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Optimisation conique : géométrie affine des barrières auto-concordantes et cônes copositifs

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Résumé

Dans cette thèse nous traitons deux thématiques différentes en optimisation, notamment la géométrie des barrières auto-concordantes pour l'optimisation conique et les cônes copositifs. La première thématique est traitée en Chapitre 1. Celui contient des résultats publiés, mais aussi quelques résultats nouveaux. L'exposition est détaillée avec preuves complètes pour la plupart des résultats présentés. Le Chapitre 2 sur la deuxième thématique constitue un survol de mes résultats publiés, obtenus en partie en collaboration avec des co-auteurs.

Géométrie des barrières auto-concordantes

Un *programme conique* est le problème de minimisation d'une fonction cible linéaire sur l'intersection d'un sous-espace affine de $\mathbb{R}^n$ avec un cône convexe $K \subset \mathbb{R}^n$. A chaque programme conique sur un cône K on peut associer un programme *dual* sur le cône dual $K^* \subset \mathbb{R}_n$, $\mathbb{R}_n$ étant l'espace dual à $\mathbb{R}^n$. Tout problème d'optimisation convexe peut être formulé sous forme d'un programme conique par homogénisation de l'ensemble faisable et minimisation sur l'épigraphe de la fonction cible. La complexité d'un programme conique ne dépend que du cône K. Des classes bien connues de programmes coniques sont les programmes linéaires (LP), coniques quadratiques (SOCP) et semi-définis (SDP).

Ces programmes sont omniprésent dans la recherche opérationnelle, l'ingénierie [15], l'analyse de systèmes [32], le contrôle [183], le routage de réseaux [223], l'apprentissage automatique [71, 129], l'analyse en composantes principales [47], l'acquisition comprimée [46], la reconstruction de signaux creux [118], la récupération de phase [216], la gamme d'applications s'étandant toujours. Beaucoup de problèmes non-convexes peuvent être approximés par des problèmes convexes ayant une description naturelle sous forme d'un programme conique, notamment des problèmes combinatoires comme MAX-CUT, SAT [75], le probléme de la clique maximum ou d'un stable de taille maximum [5, 89], kissing number [7], quadratic assignment [49], mais aussi des programmes linéaires mixtes avec contraintes entières [5], des problèmes quadratiques avec contraintes quadratiques [164], des problèmes d'optimisation avec contraintes polynomielles [155, 175, 176, 130]. Il existe des solveurs publics ou commerciaux pour les LP, SOCP, et SDP.

Les programmes coniques ont été développés dans les années 90 comme généralisation des programmes linéaires, pour lesquels le cône K est donné par l'orthant positif $\mathbb{R}^n_+$. Cela n'est devenu possible qu'après l'invention d'une nouvelle classe d'algorithmes pour la résolution des LP, les *algorithmes de point intérieur* (API). Les méthodes connues auparavant, notamment l'algorithme du simplexe, utilisent explicitement la structure polyhèdrale de l'ensemble faisable et ne s'adaptent pas à des ensembles faisables plus généraux.

En 1967 Dikin a construit le premier API pour LP [58]. En 1984 Karmarkar a publié le premier API avec une complexité polynomielle [115]. Cette méthode utilise des transformations projectives de l'ensemble faisable pour "centrer" le point courant à chaque itération. Or, la classe des fonctions cibles linéaires n'étant pas invariante par rapport à des transformations projectives, la fonction à minimiser doit être remplacée par une fonction linéaire fractionnelle. Cet inconvénient a motivé le développement des modifications de l'algorithme de Karmarkar qui utilisent des transformations affines, ce qui ménait à la redécouverte de la méthode de Dikin [213, 8]. Les algorithmes peuvent alors être classifiés en deux types, affines ou projectifs.

La méthode de Karmarkar peut être interprétée comme réduisant la somme de la fonction cible originale et une fonction de pénalité, la *barrière*, qui croit vers l'infinie si on s'approche du bord de l'ensemble faisable [115, 205]. La barrière la plus courante sur $\mathbb{R}^n_+$ est la fonction logarithmique $F(x) = -\sum_{j=1}^n \log x_i$.

En 1988 Yu. Nesterov et A. Nemirovski ont généralisé les API pour pouvoir résoudre des problèmes d'optimisation sur des cônes arbitraires et ont introduit la notion de programme conique [166, 167]. Cet achèvement réposait sur l'invention des *barrières auto-concordantes* [168]. Nesterov et Nemirovski ont aussi construit une théorie de la dualité conique, en généralisant la dualité bien connue des LP [170]. Deux propriétés des barrières logarithmiques utilisées pour la programmation linéiare ont été reconnues d'expliquer la performance des API, la homogénéité logarithmique et l'auto-concordance, qui est une inégalité entre les deuxièmes et troisièmes dérivées de la barrière. La théorie des barrières auto-concordantes est présentée dans l'ouvrage [171]. La plupart des méthodes proposées est de type affine. Une barrière possède un paramètre scalaire qui détermine son degré d'homogénéité logarithmique, le *paramètre d'auto-concordance*. Plus petit ce paramètre, plus rapide est la convergence des algorithmes.

La classe de cônes la plus importante pour l'optimisation est celle des *cônes symétriques*, qui inclut l'orthant positif $\mathbb{R}^n_+$, le cône de Lorentz et le cône de matrices semi-définies positives qui sont utilisés en LP, SOCP et SDP. Pour ces cônes des barrières numériquement accessibles avec un petit paramètre sont connues. En 1994 Nesterov et Todd ont observé que ces barrières possèdent une propriété qui n'est pas partagée par les barrières sur des cônes arbitraires, notamment d'être *auto-ajustées* (self-scaled) [160].

Faybusovich a remarqué que les cônes symétriques sont liés à des algèbres de Jordan formellement réelles [68], ce qui lui a permis d'étendre les API sur ces cônes [69, 70]. La propriété d'auto-ajustement a également été liée aux algèbres de Jordan et les barrières possédant cette propriété ont été classifiés [84, 83, 85, 189, 87].

Dans [116] la métrique riemannienne définie par le Hessien de la barrière a été considérée pour LP, bien que sans lien direct avec celle-ci. La variété riemannienne est l'intérieur de l'orthant positif dans le cas affine et l'ensemble des rayons dans cet intérieur dans le cas projectif. Nesterov and Nemirovski ont considéré cette métrique dans le cas général et ont montre que la dualité de Legendre est une isométrie [171, p.45]. Dans [173, 174, 113] il a été reconnu que la métrique hessienne avec les connexions affines sur l'espace $\mathbb{R}^n$ et son dual forment une *variété hessienne*, structure connue depuis longtemps en géométrie de l'information.

Dans cette thèse nous étudions la géométrie des barrières auto-concordantes $F : K^o \to \mathbb{R}$ sur des cônes convexes $K \subset \mathbb{R}^n$, notamment la relation entre la géométrie affine et la géométrie projective sur lesquelles sont basées les méthodes de ces deux types correspondants. Le point de départ était la révélation que la *géométrie différentielle affine*, une discipline qui a ses origines en début de XXème siècle, fournit un formalisme adapté à l'étude des barrières auto-concordantes. Pour employer ce formalisme, il faut considérer les surfaces de niveau de la barrière F comme plongements *centro-affines* dans $\mathbb{R}^n$. Les objets définis sur les surfaces de niveau sont alors les pendants projectifs des objets affines définies par la barrière. Or, la géométrie différentielle centro-affine s'applique dans un contexte beaucoup plus général, notamment sur des ensembles coniques arbitraires, pas nécessairement convexes. Nous appliquons cette théorie au cas des barrières auto-concordantes et trouvons des interprétations géométriques pour des objets apparaissants. En utilisant la machinerie puissante de la géométrie différentielle affine, nous montrons des résultats nouveaux sur les barrières auto-concordantes. Ci-dessous nous donnons un résumé du Chapitre 1.

En section 1.2 nous introduisons des notions géométriques nécessaires. Notamment, nous donnons en sous-section 1.2.3 une briève introduction en géométrie différentielle affine.

En section 1.3 nous considérons les barrières auto-concordantes d'un point de vue de cette théorie. L'objet principal dans ce contexte n'est pas la barrière F, mais une variété différentiable de dimension $n-1$. Une immersion de M dans $\mathbb{R}^n$ comme une surface de niveau de la fonction F définit sur M une métrique riemanienne, la *métrique centro-affine*. En sous-section 1.3.1 nous montrons que cette métrique est proportionelle à la métrique de sous-variété définie par la hessienne F'', le paramètre de la barrière étant la constante de proportionalité. En plus de la métrique, l'immersion génère sur M une *connexion affine*. La variété M peut être plongé de la même façon dans l'espace dual $\mathbb{R}_n$ comme une surface de niveau de la barrière duale F_*. Cette immersion duale génère la même métrique centro-affine sur M, mais une connexion affine différente, la *connexion duale*. La relation de cette dualité avec la dualité de Legendre sera considérée en sous-section 1.3.2. La différence entre les deux connexions est appelée la *forme cubique* de l'immersion. Le cas extrême quand la forme cubique est égale à zéro sera considéré en sous-section 1.3.3. Les conditions centrales d'auto-concordance et d'auto-ajustement seront mis en relation avec la forme cubique. L'auto-concordance peut être interprétée comme une borne uniforme sur la forme cubique, et le paramètre de la barrière comme une fonction de sa norme $||\cdot||_\infty$. Ce résultat est présenté en sous-section 1.3.1.

En section 1.4 nous appliquons le théorème de Calabi sur les *sphères affines*, un des résultats centraux en géométrie différentielle affine, pour construire la *barrière canonique*.

Un des plus importants problèmes ouverts dans la théorie de l'optimisation conique était l'existence d'une barrière avec une valeur petite du paramètre pour un cône convexe arbitraire $K \subset \mathbb{R}^n$. Il était connu qu'il existe une barrière F avec paramètre $\nu = C \cdot n$, $C \geq 1$ indépendent de K, la *barrière universelle*. Un désavantage de la barrière universelle est que sa barrière duale F_* n'est pas en général la barrière universelle pour K^*, c.-à-d. sa construction ne respecte pas la dualité de Legendre.

Le *théorème de Calabi* associe à chaque cône convexe $K \subset \mathbb{R}^n$ une famille de surfaces plongées dans l'intérieur de K, les *sphères affines*. Nous montrons que les sphères affines peuvent être considérées comme surfaces de niveau d'une barrière auto-concordante avec paramètre $\nu \leq n$. Cette barrière, désormais nommée *canonique*, est alors une construction universelle qui réalise la valeur $C = 1$ de la constante C introduite ci-dessus et montre en même temps que cette valeur est optimale. De plus, la barrière canonique respecte la dualité. Ce travail est publié dans les articles [91],[93] et constitue un résultat d'existence central dans la théorie de barrières auto-concordantes.

Nous calculons la barrière canonique explicitement pour quelques cônes non-homogènes en sous-section 1.4.4. Ces résultats ont été publiés dans [92].

La section 1.5 est dédiée aux barrières auto-ajustées, qui n'existent que sur les cônes symétriques. Cette condition est démontrée d'être équivalente à une propriété géométrique des plongements centro-affines correspondants, notamment à la disparition de la dérivée covariante de la forme cubique. La dernière est alors parallèle pour les barrières auto-ajustées. Cette condition peut être développée sous forme d'une équation quasi-linéaire de 4ème ordre aux dérivées partielles sur la barrière F. On obtient une caractérisation locale et une interprétation simple géométrique des barrières auto-ajustées.

Le lien entre le parallélisme de la forme cubique et la propriété d'auto-ajustement est fait par les algèbres de Jordan. Une description des barrières auto-ajustées par les algebres de Jordan formellement réelles est bien connue [189]. Nous donnons une interprétation de l'identité de Jordan comme condition d'intégrabilité de ladite équation aux dérivées partielles en sous-section 1.5.3. En sous-section 1.5.4 nous faisons un lien entre l'homogénéité logarithmique de la barrière et la présence d'un élément neutre dans l'algèbre de Jordan correspondante. En sous-section 1.5.5 nous montrons que la convexité de la barrière entraîne que l'algèbre de Jordan est formellement réelle. Une partie de ces résultats a été publiée dans [94].

Le lien découvert entre les algèbres de Jordan et le parallélisme de la forme cubique nous a aussi permis de résoudre des problèmes ouverts dans la géométrie différentielle affine. En sous-section 1.5.6 nous atteignons la classification des sphères affines avec une forme cubique parallèle, qui était un sujet de recherche intense depuis la fin des années 80. Cette classification se réduit à la classification bien connue des algèbres de Jordan semi-simples. Ce travail a été publié dans [96].

Cônes copositifs

Le *cône copositif* $\mathcal{C}^n$ est l'ensemble des matrices réelles symétriques A de taille $n \times n$ telles que pour tout vecteur $x \in \mathbb{R}_+^n$, le produit $x^T A x$ soit non-négatif. Une telle matrice est appelée *copositive*. Le cône copositif joue un rôle important dans l'optimisation non-convexe, parce qu'un grand nombre de tels problèmes peuvent être écrits comme programmes coniques sur ce cône, des *programmes copositifs*. Cela concerne un nombre de problèmes combinatoires [179, 180, 48, 215, 80, 181], mais des formulations copositives ont été dérivées également pour des problèmes de la programmation quadratique [182, 25, 22] et des programmes linéaires en nombres entières et mixtes [36]. La connexion entre le cône copositif et des conditions suffisantes d'optimalité pour la programmation quadratique, c.-à-d. le problème de minimisation d'une fonction quadratique sous de contraintes linéaires, a été observée déjà dans les années 70 [109, Theorem 3.2.3]. Les matrices copositives sont aussi utiles pour le calcul de fonctions de Lyapunov pour des systèmes hybrides avec le vecteur d'état contraint dans un cône polyhèdral [142, 120, 35, 19]. Plus d'applications de la programmation copositive peuvent être trouvées dans [63, 23]. Un état de l'art récent peut être trouvé dans [99, 28], une liste de problèmes ouverts dans [17]. Le cône dual du cône copositif, le *cône complètement positif* $\mathcal{C}_n^*$, se trouve en dehors de la portée de cette thèse. Pour plus d'information sur le cône complètement positif voir, e.g., [18, 28, 53].

Par conséquent, on ne peut pas espérer qu'un programme copositif général est facile à résoudre. En fait, de vérifier la copositivité d'une matrice donnée est un problème co-NP-complète [153]. Seul les programmes copositifs avec contraintes coniques jusqu'à l'ordre 4 pouvaient être résolus par des algorithmes courants de l'optimisation convexe, parce que des descriptions semi-définies des cônes copositifs correspondants sont connues. La plus courante approximation semi-définie du cône copositif $\mathcal{C}^n$ est celle par la somme du cône $\mathcal{S}_+^n$ des matrices réelles symétriques positives semi-définies et du cône $\mathcal{N}^n$ des matrices réelles symétriques non-négatives élément par élément. Un résultat classique de Diananda [51, Theorem 2] affirme que pour $n \leq 4$ cette approximation est exacte, c.-à-d. $\mathcal{C}^n = \mathcal{S}_+^n + \mathcal{N}^n$. En général, on a seulement l'inclusion $\mathcal{S}_+^n + \mathcal{N}^n \subset \mathcal{C}^n$. A. Horn a montré que cette inclusion est stricte pour $n \geq 5$ [51, p.25]. Les matrices dans la différence $\mathcal{C}^n \setminus (\mathcal{S}_+^n + \mathcal{N}^n)$ sont appelées *exceptionnelles* [111].

En 2011 j'ai abordé le thème des cônes copositifs, motivé par l'intérêt de trouver des descriptions semi-définies exactes de cônes copositifs d'ordre supérieur à 4. Mes études se concentrent sur un sujet particulier, les rayons extrêmes du cône $\mathcal{C}^n$. Un élément $x \in K$ est appelé un élément *extrémal* d'un cône convexe K si une décomposition $x = x_1 + x_2$ de x en éléments $x_1, x_2 \in K$ entraîne que $x_1 = \lambda x$, $x_2 = (1 - \lambda)x$ pour un certain $\lambda \in [0, 1]$. L'ensemble des multiples positifs d'un élément extrémal est appelé *rayon extrême* de K. L'ensemble des rayons extrêmes est une caractéristique importante d'un cône convexe, notamment si on veut déterminer si une approximation par l'intérieur du cône K par un autre cône convexe K' est exacte. Cela est le cas si et seulement si le cône K' contient tous les rayons extrêmes de K. Du fait que les rayons extrêmes d'un cône K sont en rapport avec les facettes du cône dual K^* de K, les rayons extrêmes de $\mathcal{C}^n$ sont recherchés aussi pour l'étude du cône complètement positif [52, 194, 29, 30, 193, 192].

Les rayons extrêmes de $\mathcal{C}^n$ qui sont contenus dans la somme $\mathcal{S}_+^n + \mathcal{N}^n$ ont été classifiés dans [82]. Le premier élément exceptionnel extrémal de $\mathcal{C}^n$ a été construit par A. Horn [51, p.25]. Cette *forme de Horn* est une matrice circulante de taille 5×5 dont les éléments sont contenus dans l'ensemble $\{-1, +1\}$. Diananda a observé qu'on ne peut pas soustraire d'un élément extrême exceptionnel copositif une matrice non-zéro du cône $\mathcal{N}^n$, sans perdre la propriété de copositivité [51]. Cela mène à une propriété d'irreductibilité qui est plus faible que l'extrémalité. On appelle une matrice copositive $A \in \mathcal{C}^n$ *irreductible* par rapport à $\mathcal{N}^n$ s'il n'existe pas une décomposition non-triviale $A = C + N$ avec $C \in \mathcal{C}^n$ et $N \in \mathcal{N}^n$ [11]. Cette propriété est plus facile à traiter que l'extrémalité. On la peut définir d'une façon similaire aussi par rapport à d'autres cônes que $\mathcal{N}^n$.

Les conditions d'irreductibilité peuvent être décrites en termes de présence ou d'absence de zéros avec certaines propriétés. L'importance des zéros a été reconnue déjà par Diananda qui les a introduit dans [51]. Un *zéro* d'une matrice copositive A est un vecteur non-nul $x \in \mathbb{R}_+^n$ tel que $x^T A x = 0$. L'ensemble d'index $i \in \{1, \dots, n\}$ tel que l'élément x_i d'un zéro x est strictement positif est appelé le *support* du zéro. Les ensembles des zéros et de leurs supports constituent des caractéristiques importantes d'une matrice copositive et sont un outil performant dans leur étude. Dans [51, 82, 10, 11, 12] un nombre de conditions nécessaires sur l'ensemble des supports d'une matrice extrême ou irreductible ont été élaborées, et des propriétés des matrices ont été formulées qui dépendent de leur ensemble de supports.

Ci-dessous nous fournissons un résumé de nos travaux sur les matrices copositives extrêmes décrits dans le chapitre 2 de cette thèse.

La section 2.2 est dédiée à l'étude du cône copositif d'ordre 5 et comporte des résultats publiés dans [90, 54, 55]. Nous fournissons une classification complète des rayons extrêmes du cône $\mathcal{C}^5$, un problème qui est resté ouvert depuis les années 60. Notre stratégie suit celle proposée par Baumert [10], en remplaçant la condition d'extrémalité par la condition plus faible d'irreductibilité par rapport à $\mathcal{N}^n$. Néanmoins, quelques nouvelles idées ont été nécessaires. Notamment, nous développons une approche trigonométrique, qui s'est avérée aussi très utile pour l'étude des cônes copositifs en général.

Celle-ci permet de décrire les rayons extrêmes exceptionnels de $\mathcal{C}^5$ sous forme analytique. L'approche trigonométrique fournira des résultats similaires pour toute famille de rayons extrêmes de $\mathcal{C}^n$ qui n'a que des zéros avec des supports de cardinalité au plus 3. En section 2.4 nous appliquons cette méthode aux rayons extrêmes du cône $\mathcal{C}^6$.

La seconde nouveauté était, en collaboration avec M. DÜR, P. DICKINSON et L. GIJBEN, d'élaborer une condition nécessaire et suffisante sur une matrice copositive d'être irreductible par rapport à $\mathcal{N}^n$. Celle-ci nous a permis de compléter la classification de Baumert [12] des matrices irreductibles dans $\mathcal{C}^5$. La connaissance des ces matrices a permis de trouver une description semi-définie exacte d'une certaine section affine de $\mathcal{C}^5$. Ce résultat étend l'ordre maximal des cônes dans des programmes copositifs qui peuvent être résolus par la programmation semi-définie jusqu'à 5.

La section 2.3 est dédiée à l'approche des *zéros minimaux*, publié dans l'article [95]. Un zéro minimal u d'une matrice copositive A est un zéro tel qu'il n'existe pas d'autres zéros de A avec un support strictement inclus dans le support de u. L'ensemble des supports de ses zéros minimaux est une caractéristique combinatoire d'une matrice copositive. Son utilité est issu du fait qu'elle est accessible à un traitement algorithmique. Les conditions d'irreductibilité par rapport aux cônes $\mathcal{N}^n$ et $\mathcal{S}_+^n$ peuvent être décrites en termes des zéros minimaux, ce qui mène à des conditions nécessaires supplémentaires sur l'ensemble des supports des zéros minimaux d'une matrice copositive exceptionnelle extrémale. Ces conditions sont assez fortes pour réduire le nombre des supports potentiels dans le cas du cône $\mathcal{C}^6$ à 44, un nombre raisonable pour pouvoir atteindre la classification des rayons extrêmes de $\mathcal{C}^6$. Des résultats sur $\mathcal{C}^6$ sont décrits dans la section 2.4.

La section 2.5 porte sur une étude locale du cône copositif. En collaboration avec P. DICKINSON j'ai entrepris une étude de la structure du bord du cône copositif. Notamment nous avons déterminé quand une matrice copositive est irreductible par rapport à une autre matrice copositive, en fonction des zéros minimaux. Entre autre nous avons devéloppé un algorithme pour déterminer si une matrice copositive donnée est située sur un rayon extrême, une question qui auparavant été très difficile à décider. Ces résultats ont été publiés dans [57].

En section 2.6 nous considérons des matrices copositives dont l'ensemble de supports a une certaine structure circulante. Il s'est avéré que de telles matrices peuvent être décrites à l'aide de systèmes dynamiques linéaires avec coefficients périodiques, un lien à priori assez surprenant. Nous avons construit de larges classes de matrices extrémales exceptionnelles pour d'ordres arbitraires $n \geq 5$. Ces matrices peuvent être vues comme généralisations de la forme de Horn et des autres matrices extrémales exceptionnelles de $\mathcal{C}^5$. Ce résultat a été publié dans [97].

Chapter 1

Geometry of self-concordant barriers

1.1 Introduction

1.1.1 Conic programs and interior-point methods

A *regular* convex cone is a closed convex cone in a real vector space, with non-empty interior, and containing no lines. A *conic program* over a regular convex cone $K \subset \mathbb{R}^n$ is an optimization problem of the form

$$\min_{x \in K} \langle c, x \rangle \quad : \qquad Ax = b. \tag{1.1}$$

Here the objective function is linear homogeneous, and the feasible set of the problem is the intersection of the cone with an affine subspace. It is easily seen that every convex optimization problem can be cast as a conic program by homogenization of the feasible set and minimization of the objective function value over the epigraph of the objective function. The computational complexity of a conic program depends on the cone K. To any conic program over a cone $K \in \mathbb{R}^n$ one can associate a *dual program*, which is a conic program over the dual cone $K^* = \{s \in \mathbb{R}_n \,|\, \langle x, s \rangle \geq 0 \ \forall\ x \in K\}$. Here $\mathbb{R}_n$ is the dual space to $\mathbb{R}^n$. Well-known classes of conic programs are linear programs (LP), second-order cone programs (SOCP), and semi-definite programs (SDP).

These programs are ubiquitous in operations research, engineering [15], systems analysis [32], control [183], network routing [223], machine learning [71, 129], principal component analysis [47], compressed sensing [46], sparse signal reconstruction [118], phase recovery [216], with a constantly widening scope of applications. Many non-convex problems can be approximated by convex problems having a natural description as a conic program, in particular combinatorial problems such as MAX-CUT, SAT [75], clique number, stable set [5, 89], kissing number [7], quadratic assignment [49], but also general mixed-integer linear programs [5], quadratically constrained quadratic problems [164], and polynomially constrained optimization problems [155, 175, 176, 130]. A number of public and commercial LP, SOCP, and SDP solvers is available.

Conic programs have been initially developed as a generalization of LPs. In a LP the cone K is given by the nonnegative orthant $\mathbb{R}^n_+$, and efficient solution methods for this class of optimization problems are known for decades. The first such method was the *simplex method* [45], which makes explicit use of the polyhedral structure of the feasible set. It is an iterative method which jumps along the edges of the feasible set between its vertices, until it reaches the optimal solution or detects infeasibility or unboundedness of the LP. Despite its excellent performance in practice the simplex method has an exponential worst-case behaviour [119].

Parallel to the evolution of the simplex method there appeared methods for the solution of general non-smooth convex optimization problems which were based on the construction of a succession of increasingly smaller sets containing the optimal solution. In 1965 Levin proposed the method of centered cuts [134], followed in 1972 by an algorithm of Shor which used ellipsoids [197]. The ellipsoid algorithm as it is known today has been designed by Yudin and Nemirovski in 1976 [228]. Its behaviour for LPs with rational data has been analysed by Khachiyan, who proved LP to be polynomial-time

[117]. The ellipsoid algorithm could not compete with the simplex algorithm and its variants in practice, however.

In 1967 Dikin designed the first interior-point algorithm for LP [58]. This method constructed a succession of ellipsoids inside the feasible set which converged to the optimal solution. In 1984 Karmarkar designed the first polynomial-time interior-point algorithm [115]. This method applied projective transformations to the feasible set before constructing the inscribed ellipsoid at each step. Since the class of linear objective functions is not invariant with respect to projective transformations, it had to be replaced by the wider class of linear fractional functions. This drawback motivated work on variants of Karmarkars algorithm which came along with affine transformations, which led to the rediscovery of Dikins method [213, 8]. These methods could compete with the simplex method in practice, however, only Karmarkars variant had also good theoretical properties.

Karmarkars paper was the starting point for systematic research on interior-point methods for LP. It is a primal method, as its iterates are points in the primal feasible set. The method can be interpreted as a barrier method, i.e., decreasing the sum of the original objective function and a penalty function, the *barrier*, which grows to infinity as the argument approaches the boundary of the feasible set [115, 205]. Barrier methods have been known for decades from non-linear programming. As a barrier on $\mathbb{R}^n_+$ the function $F(x) = -\sum_{j=1}^n \log x_i$ is used, it is called the *logarithmic barrier*. In the series of papers [13, 14, 127] the connections between barrier methods and Karmarkars method and its affine variants are elaborated in detail, see also [144]. In these papers the vector field of descent directions has been integrated and analyzed for different setups. The vector field for Karmarkars original method is called the *projective scaling vector field* [127], that of the variants using affine transformations the *affine scaling vector field* [14]. Both fields coincide on a 1-dimensional submanifold, the *central path*, which consists of the minimizers of the above-mentioned sums for different weights at the penalty function. In [184] a method was proposed whose iterates lie close to the central path and follow it towards the solution. This method needs fewer iterates than Karmarkars method to reach the same precision, but the iterations themselves are more costly computationally. In [125, 149, 207] primal-dual methods were proposed, which generated pairs of primal and dual iterates. Mehrotras algorithm [145] is a primal-dual method using second-order information at the current iterate to compute the next iterate. In [147] primal-dual methods with an adaptive step size were proposed. In [124, 146] infeasible primal-dual methods have been proposed, whose pairs of iterates do not necessarily lie on the affine subspaces defined by the constraints of the LP. In the course of the iterations the initial discrepancy then decreases exponentially. For surveys of these developments see, e.g., [128, 195, 76, 50, 220].

All the methods considered above used either the standard logarithmic barrier or a weighted sum of the logarithms of the individual entries and were designed for solving LPs. In 1988 Yu. Nesterov and A. Nemirovski extended the realm of interior-point methods to optimization problems over general cones, introducing the notion of conic program and showing that general convex optimization problems can be recast as conic programs [166, 167]. The main innovation which permitted this generalization was the invention of the *self-concordant barrier* [168]. In particular, polynomial-time algorithms could now be applied to solve SDPs, i.e., conic programs over the cone of positive semi-definite matrices [169]. Nesterov and Nemirovski also built a theory of conic duality, generalizing the well-known duality in LP [170].

Primal methods for the solutions of LPs have independently been extended to SDPs by Alizadeh [3, 4]. Later Alizadeh recognised that the majority of interior-point algorithms, including primal-dual methods, that have been devised for LP can be generalized in a straightforward manner also to SDP [5]. However, these methods relied on scaling transformations preserving the cone and could not be generalized to non-homogeneous cones in principle.

Two properties of the logarithmic barriers used for LP have been recognized by Nesterov and Nemirovski as being sufficient to explain the performance of interior-point methods, namely logarithmic homogeneity and self-concordance. This enabled them to employ an axiomatic approach to barriers in conic programming. In the book [171] a self-contained theory of interior-point methods for conic programs over arbitrary regular convex cones has been elaborated, which is based on self-concordant barriers.

Definition 1.1.1. [171, Definition 2.1.1] Let $C \subset \mathbb{R}^n$ be an open convex set. A convex C^3 function

$F : C \to \mathbb{R}$ is called *self-concordant* if for all $x \in C$ and all $h \in \mathbb{R}^n$ the relation

$$|F'''(x)[h,h,h]| \leq 2(F''(x)[h,h])^{3/2} \tag{1.2}$$

holds.

Here the derivatives of F are considered as multilinear maps, such that h can be interpreted as a tangent vector at x. Thus self-concordance of a function means that its third derivative is uniformly bounded in the local norm defined by its second derivative. Equivalently, the local norm defined at a given point can be used in a finite neighbourhood of this point while controlling the committed error.

Definition 1.1.2. [171, Definition 2.3.2] Let $K \subset \mathbb{R}^n$ be a regular convex cone and let $\nu > 0$. A convex C^2 function $F : \operatorname{int} K \to \mathbb{R}$ is called a *ν-logarithmically homogeneous barrier* for K if $F(x_k) \to +\infty$ for every sequence $\{x_k\}$ of points in $\operatorname{int} K$ converging to a point in ∂K, and for every $x \in \operatorname{int} K$ and every $t > 0$ the relation

$$F(tx) = F(x) - \nu \log t \tag{1.3}$$

holds. The function F is called *ν-self-concordant barrier* or *self-concordant barrier with parameter ν* if it is a self-concordant function and a ν-logarithmically homogeneous barrier.

The original notion of *normal barrier* as given in [171] has not become prevalent, instead the notion of self-concordant barrier is widely used nowadays. The condition of self-concordance arose from a thorough analysis of the Newton method. In fact, self-concordance allows the Newton method to make steps of a guaranteed step size safely.

Suppose a conic program of the form (1.1) is given. Let F be a self-concordant barrier on the cone K. Then the *central path* is defined as the curve $\{\sigma(\tau)\}_{\tau \geq 0}$ given by

$$\sigma(\tau) = \arg \min_{x \in K, Ax=b} (F(x) + \tau \langle c, x \rangle).$$

By convexity and self-concordance of F the minimum is unique. For every $\tau \in \mathbb{R}_+$ the minimum $\sigma(\tau)$ is a feasible point, and for $\tau \to +\infty$ the point $\sigma(\tau)$ tends to a solution of the original conic program.

The interior-point methods proposed in [171] are divided in two classes, the *path-following* methods and the *potential reduction* methods. Most of these methods are generalizations of the affine scaling methods.

In path-following methods the iterates stay in a neighbourhood of the central path while advancing along it towards the solution. Here the size of the neighbourhood is governed by the barrier parameter ν. The larger this parameter, the smaller is the neighbourhood and the smaller are the steps that the method can make while staying safely inside the neighbourhood. In fact, the steps taken by the so-called *short-step* algorithms are of order 1 in the local norm defined by the second derivative F'' of the barrier. In contrast, *long-step* methods may take larger steps if the state of the current iterate allows to do this safely, but their theoretical worst-case behaviour is not better than that of the short-step variants. A modification of these methods are the *predictor-corrector* methods, which separate explicitly the (predictor) step of advancing along the central path and the (corrector) step of decreasing the accumulated distance to the central path. While in primal methods the distance is measured by the local norm given by the Hessian F'' at the current iterate, primal-dual methods differ in the way they measure proximity to the central path. Prototypes of primal-dual path-following methods have been presented in [144, 125, 149] for LP, in [209] generalizations to arbitrary cones have been presented.

Potential reduction algorithms are mostly primal-dual. They decrease at each step a potential function defined on primal-dual pairs of iterates, augmented by an auxiliary variable which serves to homogenize the product of the primal and dual feasible sets. These methods may feature iterates which are far from the central path. The potential is unbounded below, and as its value tends to $-\infty$, the primal-dual pair of iterates tends to the optimal solutions of the respective conic programs. The method ensures that the potential and along with it the duality gap decreases by a certain amount at each step, thus yielding a guaranteed speed of convergence. However, the larger the parameter of the barrier, the smaller the amount by which the duality gap will decrease. Prototypes of potential reduction algorithms are presented in [203, 207] for LP, and the potentials used in algorithms developed later, e.g., in [154], are generalizations of the *Tanabe-Todd-Ye potential* introduced in these papers.

Karmarkars original method can also be interpreted as a primal potential reduction algorithm, as has been recognized already by Karmarkar himself [115].

In [154] Nesterov established, however, that the sequence of iterates generated by many potential reduction algorithms resembles that of long-step path following algorithms.

In order for an interior-point method to be efficient in solving a conic program over a cone $K \subset \mathbb{R}^n$, an efficiently computable self-concordant barrier for the cone K with a low barrier parameter has to be available. In [171, Section 5.5] a self-concordant barrier, the *universal barrier*, has been constructed for an arbitrary cone K, with barrier parameter bounded by above by a function of order n, but its computation requires the calculation of a multidimensional integral. In [77, 79] this barrier has been computed for homogeneous cones and it has been shown that its barrier parameter equals the *rank* of the homogeneous cone, and is hence bounded from above by its dimension n.

The most important class of cones for which easily computable barriers with small parameters are available are the *symmetric cones*, i.e., regular convex cones which are both homogeneous and self-dual. This class includes the nonnegative orthant $\mathbb{R}^n_+$, the Lorentz or second order cone L_n, and the cone $\mathcal{S}^n_+$ of positive semi-definite matrices.

In 1994 Nesterov and Todd observed that the logarithmic barriers on these cones have a property in common which barriers on general cones do not have, namely that of being *self-scaled* [160]. In order to introduce this notion we first have to define the dual barrier.

Definition 1.1.3. Let F be a self-concordant barrier on a cone K with parameter ν. The *dual barrier* of F is given by $F_*(s) = \max_{x \in K}(-\langle x, s\rangle - F(x))$, $s \in \operatorname{int} K^*$.

By [171, Theorem 2.4.4] F_* is indeed a self-concordant barrier on the dual cone K^* with the same parameter ν as F. In fact, $F_*(-p)$, $p \in -\operatorname{int} K^*$, is the Legendre transformation of F.

Definition 1.1.4. Let $K \subset \mathbb{R}^n$ be a regular convex cone, let K^* be its dual cone, let F be a self-concordant barrier on K, and let F_* be the dual barrier on K^*. Then F is called *self-scaled* if for every $x, w \in \operatorname{int} K$ we have

$$F''(w)x \in \operatorname{int} K^*, \qquad F_*(F''(w)x) = F(x) - 2F(w) - \nu.$$

A cone K admitting a self-scaled barrier is called *self-scaled cone*.

For every $x \in \operatorname{int} K$ and $s \in \operatorname{int} K^*$ there actually exists a unique point $w \in \operatorname{int} K$ such that $F''(w)x = s$ [161, Theorem 3.1]. The point w is called the *scaling point* of the pair (x, s). In contrast to the central path this scaling point is independent of the data of the conic program and is solely a feature of the barrier. Nesterov and Todd developed a theory of interior-point methods especially for self-scaled barriers [161, 162]. In this theory the directions of the steps, the so-called *Nesterov-Todd directions*, are computed using the local metric at the scaling point. It has a perfect primal-dual symmetry and compares favorably with other methods in practice [206, 204]. The Nesterov-Todd directions for LP have been found already in [144, 125, 149].

At about the same time Faybusovich observed that the above-mentioned cones underlying LP, SOCP, and SDP have another property in common, namely being symmetric, and hence the cone of squares of a Euclidean Jordan algebra [68]. He extended the interior-point methods for these special classes of conic programs to conic programs over arbitrary symmetric cones, using explicitly the structure of the Jordan algebra [69, 70], see also [190].

While the property of being self-scaled is primarily a property of the barrier, the property of being symmetric is a property of the cone. Nevertheless, these notions turned out to have a close connection. Several authors proved independently that the symmetric cones and the self-scaled cones form the same class, and provided a full classification of self-scaled barriers [84, 83, 85, 189, 87], for a history of these developments see [86].

Interior-point methods for self-scaled barriers became a subject of intense research at this time, see [148, 151, 201, 202, 208]. For surveys and books on this stage of development of semi-definite and conic programming see [171, 212, 221, 178, 222, 219, 185].

In [78] methods using self-scaled barriers have been extended to *hyperbolic barriers*, i.e., logarithms of polynomials defining hyperbolicity cones. In [43] methods for homogeneous cones have been developed based on the algebraic representation of these cones by T-algebras. In [156, 165] the notion of scaling point has been considered for general barriers.

At the turn of the millennium the evolution of the theory of interior-point algorithms considerably slowed, and the focus of research shifted to applications. Optimization problems arising in practice are rarely formulated as standard conic programs over a symmetric cone, and often even cannot be cast as such in principle, e.g., because they are non-convex. Therefore it is important to be able to convert optimization problems arising in different areas into symmetric cone programs, or at least to find symmetric cone relaxations. Accordingly, while in the 90s the focus of research was on the development and improvement of solution algorithms for these conic programs, later attention shifted to the problem of formulating various optimization problems as semi-definite programs or finding semi-definite relaxations, see the literature at the beginning of this paragraph.

In the last years, however, a renewed interest in interior-point methods and self-concordant barriers can be observed. In particular, new barriers have been constructed, for arbitrary convex sets or cones [93, 72, 33, 1] as well as for LP [132, Section 6.3],[133]. In [159] a generalization of self-scaled barriers called barriers of *negative curvature* has been considered, and the barrier parameter as a measure of the convergence speed has been complemented by the *recession coefficient*.

1.1.2 Geometry of self-concordant barriers

In this subsection we review past developments specific to the geometry of self-concordant barriers and associated objects. Geometry has played a prominent role in the early papers following the publication of Karmarkars method [115]. As has been mentioned in the previous subsection, this method is projectively invariant, but subsequently affinely invariant versions appeared [8, 213]. In the early geometric studies of these methods the affine and projective cases have been pursued in parallel. Bayer and Lagarias analyzed the vector fields of descent directions in the affine scaling methods [14] and the projective scaling methods [127]. It was observed that these vector fields can be stratified into straight lines by non-linear coordinate transformations which can be interpreted as Legendre transforms.

A comprehensive geometric analysis of LP has been provided in [116]. An important object in this work is the Riemannian metric defined by the Hessian of the barrier, although at first it has been introduced on its own without a connection to the barrier. The metric allows to convert gradients (cotangent vector fields) into directions (tangent vector fields), and hence yields an interpretation of the interior-point methods as steepest descent algorithms minimizing some potential function. The Riemannian manifold in the affine case is the interior of the nonnegative orthant, while in the projective case it is the set of rays in the interior of the nonnegative orthant. In the affine case the metric is flat, while in the projective case it is not. The vector fields of descent directions have been shown to be gradients of the objective function in the affine case and of some potential function in the projective case, although in the original formulation [116, Theorem 1] this is not explicit. One conclusion of the paper was that the complexity, more precisely the number of steps, grows with the curvature of the trajectories, because the curvature determines how well the continuous trajectory can be approximated by discrete steps. Estimates of the iteration complexity by the curvature of the central path have later been obtained also in [199, 229, 150, 114].

Nesterov and Nemirovski showed that the Legendre transformation which maps the interior of the primal cone K to the interior of the dual cone K^* is an *isometry* when these interiors are equipped with Hessian Riemannian metrics generated by a mutually dual pair of self-concordant barriers F, F_* on K and K^*, respectively [171, p.45], see also [163] for an explicit statement. Moreover, the third derivative F''' is mapped to $-F_*'''$ and the first derivative F' to $-F_*'$.

In the sequel the Riemannian metric played an auxiliary role, providing the local Euclidean norms which were used in the neighbourhoods of the iterates or the scaling points. In the 2000s, however, the interest in this metric as an independent geometric object renewed when the geodesics and the Riemannian distance defined by it came under investigation. In [163] the geodesics of the Riemannian metric have been computed for several sets. The product of the interiors of the primal and dual cones has also been considered as a Riemannnian manifold, equipped with the corresponding product metric. It was shown that the primal-dual central path in this product came within a factor of $\sqrt{2}$ of being a geodesic, implying that it was nearly optimal to let the primal-dual iterates follow this path. In [157, 158] the length of the primal central path was compared to the geodesic distance.

In [173, 174, 113] parallels have been drawn between the geometry of barriers and information geometry, and an iteration complexity estimate has been given in terms of the curvature of the central path. The two theories have the presence of a *dually flat structure* in common, which is a manifold carrying a Riemannian metric together with a pair of flat affine connections which are dual to each other with respect to this metric. Here the primal affine connection is the canonical affine connection of the primal space $\mathbb{R}^n$, while the dual affine connection is the canonical connection of its dual $\mathbb{R}_n$. Such a structure is also known under the name of *Hessian manifold* [196]. It has been shown that the affine scaling vector field is parallel under the dual flat connection, which is an equivalent reformulation of the result in [14] on the stratification of this vector field by the Legendre transformation.

Let us remark that the viewpoint presented in the previous paragraph bears a conceptual difference with respect to previous approaches. It considers the interiors of the primal and dual cone K, K^* as a single object, with the primal and dual structure being defined by different flat affine connections, or loosely speaking, different systems of coordinates on it.

1.1.3 Overview

In this subsection we give an overview over the contents of this chapter in the context presented in the previous subsections. We consider a self-concordant barrier F on the interior of a regular convex cone $K \subset \mathbb{R}^n$ and its Legendre transform, the dual barrier F_* on the interior of the dual cone K^*.

In Section 1.2 we briefly introduce some geometric concepts which will be needed for our exposition.

In Section 1.3 we investigate the relation between the projective and the affine geometry underlying the projective scaling and affine scaling methods elaborated for LP in the years after Karmarkars publication. It turns out that a similar relation is well-known and has been studied for decades in *centro-affine differential geometry* in a much more general context, i.e., not only for the cone $K = \mathbb{R}^n_+$, but for general conic sets, which are not necessarily convex. We give a short introduction into affine differential geometry in Subsection 1.2.3, for a detailed treatment see [172].

We give an affine differential geometric interpretation of many quantities and conditions which appear in the theory of interior-point methods. In the context of affine differential geometry, the primary object is not the barrier F on a cone $K \subset \mathbb{R}^n$, but a differentiable manifold M of dimension $n-1$. A Riemannian metric called *centro-affine metric* is generated on M by its immersion into $\mathbb{R}^n$ as a level surface of the barrier F. It turns out that this centro-affine metric is proportional to the submanifold metric induced on the level surface by the Hessian metric F'' on $\operatorname{int} K$, with the proportionality constant being the barrier parameter. This result is derived in Subsection 1.3.1. Beside the metric, the immersion generates also an *affine connection* on M, the *induced connection*. This connection is such that its geodesics, when considered as curves in $\mathbb{R}^n$, experience an acceleration which is proportional to the vector pointing to the origin of $\mathbb{R}^n$, with a negative proportionality constant. In the same way, M can be immersed into the dual space $\mathbb{R}_n$ as a level surface of the dual barrier F_*. This dual immersion generates the same affine metric on M, but a different affine connection, the *dual connection*. The relation of this duality with Legendre duality is considered in Subsection 1.3.2. The difference between the primal and dual connections is called *cubic form*, it measures the deviation of the level surfaces of F and F_* from quadrics. In the extreme case when the cubic form vanishes identically the affine metric turns the level surfaces of F into a hyperbolic space form. The corresponding barrier is the hyperbolic barrier on the Lorentz cone. This particular case is considered in Subsection 1.3.3. The central conditions of self-concordance and self-scaledness are both closely related to the cubic form. Self-concordance can be interpreted as a uniform bound on the cubic form, with the barrier parameter measuring its ∞-norm. This result will be presented in Subsection 1.3.1.

The benefit of considering self-concordant barriers from the viewpoint of affine differential geometry is not only to gain a transparent geometric interpretation of the former. Affine differential geometry is a century old branch of mathematics which has developed a powerful apparatus that can be used to solve problems related to optimization. In particular, the results concerning *affine spheres*, a class of hypersurfaces having an especially rich structure, allowed us to construct the *canonical barrier*, a primal-dual symmetric self-concordant barrier defined on arbitrary convex cones and having a barrier parameter bounded from above by the dimension of the cone. This result will be presented in Section 1.4 and has been published in [93], see also [91]. In Subsection 1.4.4 we compute the canonical barrier on several non-homogeneous cones. These results have been published in

In Section 1.5 we consider self-scaled barriers. The condition of self-scaledness is shown to be equivalent to the vanishing of the covariant derivative of the cubic form, or in other words, to the condition that the cubic form is *parallel*. This condition can also be rewritten as a 4-th order quasi-linear partial differential equation (PDE) on the barrier. Part of the results presented in Section 1.5 has been published in [94].

On the other hand, the well-developed theory of symmetric cones and its connection to Jordan algebras allows us to solve open problems in affine differential geometry, in particular to accomplish the classification of affine spheres with parallel cubic form. This result is described in Subsection 1.5.6 and has been published in [96].

In the table below we present some objects or conditions appearing in the theory of self-concordant barriers along with their centro-affine geometric counterparts.

self-concordant barriers	centro-affine immersions
Legendre duality	conormal map
Hessian metric	centro-affine metric
third derivative	cubic form
self-concordance condition	bound on cubic form
self-concordance parameter	∞-norm of the cubic form
canonical barrier	affine hypersphere
self-scaled barrier	parallel cubic form

1.2 Mathematical tools

In this section we briefly review some concepts from differential geometry which are necessary for our exposition later. This includes widely known subjects like Riemannian metrics, curvature, and affine connections, but also less common matter like affine hypersurface immersions and affine spheres. We are not able and we do not aim to give a self-contained introduction into these topics. We shall rather refer the reader to some introductory literature.

1.2.1 Tensor fields

In this subsection we provide basic definitions and define tensor fields on manifolds. Let M be a differentiable manifold of dimension d and $p \in M$ a point. Let $x : M \supset U \to \mathbb{R}^d$ define a coordinate chart on M such that $p \in U$, with $x^1, \dots, x^d : U \to \mathbb{R}$ being its components.

The *tangent space* to M at p consists of all tangent vectors to M at p and is denoted by T_pM. It is isomorphic to $\mathbb{R}^d$. In the coordinate chart given by x the k-th component of the vector $u \in T_pM$ is given by the derivative of the k-th coordinate function x^k in the direction of u. We shall denote this component by u^k.

The *cotangent space* to M at p is the dual space to T_pM and is denoted by T_p^*M. Its elements are called *cotangent vectors* or *covectors*. The components of a covector $v \in T_p^*M$, denoted $v_1, \dots, v_d$, are defined as the coefficients in the decomposition $v = \sum_{k=1}^d v_k dx^k$, where dx^k is the differential of the coordinate function x^k at p.

We shall adopt the *Eistein summation convention* throughout this chapter, implying summation over indices which appear in pairs as upper and lower indices. In particular, the value of a covector $v \in T_p^*M$ on a vector $u \in T_pM$ is given by the sum $u^k v_k := \sum_{k=1}^d u^k v_k$.

A *tensor* of *order* (m, n) at p is a multi-linear real-valued map on the direct product $(T_p^*M)^m \times (T_pM)^n$. The components of a (m, n)-tensor T, denoted by $T_{i_1 \dots i_n}^{j_1 \dots j_m}$, are the coefficients of the decomposition $T(v, \dots, y; u, \dots, z) = T_{j_1 \dots j_n}^{i_1 \dots i_m} v_{i_1} \dots y_{i_m} u^{j_1} \dots z^{j_n}$, where $v, \dots, y \in T_p^*M$ are m covectors and $u, \dots, z \in T_pM$ are n vectors. In particular, a $(0, 0)$-tensor is a real number, a $(1, 0)$-tensor is a vector, and a $(0, 1)$-tensor is a covector. Upper indices of a tensor are called *contravariant*, while lower indices are called *covariant*.

A (m,n)-*tensor field* T assigns a (m,n)-tensor to each point $p \in M$, such that the components $T^{i_1\dots i_m}_{j_1\dots j_n}$ are smooth functions in every chart on M. A $(1,0)$-tensor field is called a *vector field*, and a $(0,1)$-tensor field a *covector field*.

If $x: U \to \mathbb{R}^d$, $y: V \to \mathbb{R}^d$ are charts on M such that $p \in U \cap V$, then a coordinate change from x to y transforms the coordinates of a tensor T at p according to the rule

$$T^{i_1\dots i_m}_{j_1\dots j_n} \mapsto T^{k_1\dots k_m}_{l_1\dots l_n} \frac{\partial y^{i_1}}{\partial x^{k_1}} \cdots \frac{\partial y^{i_m}}{\partial x^{k_m}} \frac{\partial x^{l_1}}{\partial y^{j_1}} \cdots \frac{\partial x^{l_n}}{\partial y^{j_n}}, \tag{1.4}$$

where the partial derivatives are evaluated at p.

Introductions into tensor calculus can be found, e.g., in [200, 218].

1.2.2 Riemannian manifolds

In this section we provide some basics on Riemannian manifolds and objects on them such as connections or curvature.

Definition 1.2.1. A *Riemannian metric* on a connected differentiable manifold M is given a smooth symmetric positive definite $(0,2)$ tensor field $g_{\mu\nu}$, the *metric tensor*.

For a smooth curve $[0,T] \ni t \mapsto \sigma(t) \in M$, the metric defines a *length* by

$$l = \int_0^T \sqrt{g_{\mu\nu}\dot\sigma^\mu(t)\dot\sigma^\nu(t)}\, dt.$$

The extremals of this length functional are called *geodesics* and obey the Euler-Lagrange equation

$$\ddot\sigma^\mu + \frac{1}{2} g^{\mu\gamma} \left(g_{\alpha\gamma,\beta} + g_{\beta\gamma,\alpha} - g_{\alpha\beta,\gamma}\right) \dot\sigma^\alpha \dot\sigma^\beta = 0,$$

also called *geodesic equation*. A Riemannian manifold is called *complete* if every geodesic can be prolonged infinitely. The geodesic equation can be written in compact form as $\ddot\sigma^\mu + \Gamma^\mu_{\alpha\beta}\dot\sigma^\alpha\dot\sigma^\beta = 0$, where

$$\Gamma^\mu_{\alpha\beta} = \frac{1}{2} g^{\mu\gamma} \left(g_{\alpha\gamma,\beta} + g_{\beta\gamma,\alpha} - g_{\alpha\beta,\gamma}\right) \tag{1.5}$$

are the *Christoffel symbols*, which are symmetric in the lower indices. Here $g^{\mu\gamma}$ are the components of the inverse of the metric tensor $g_{\mu\nu}$, such that the sum $g^{\mu\gamma}g_{\mu\nu}$ equals the *Kronecker symbol* δ^γ_ν, which evaluates to 1 for $\gamma = \nu$ and to 0 otherwise.

The Christoffel symbols do not define a tensor field, their law of transformation under coordinate changes from coordinates x to coordinates y is rather given by

$$\Gamma^\gamma_{\alpha\beta} \mapsto \frac{\partial x^p}{\partial y^\alpha} \frac{\partial x^q}{\partial y^\beta} \Gamma^r_{pq} \frac{\partial y^\gamma}{\partial x^r} + \frac{\partial y^\gamma}{\partial x^m} \frac{\partial^2 x^m}{\partial y^\alpha \partial y^\beta}. \tag{1.6}$$

The Christoffel symbols determine an *affine connection*, i.e., a rule which defines the *parallel transport* of tensors along curves, or equivalently, to differentiate tensor fields. The affine connection generated by the metric is called the *Levi-Civita connection* and is denoted by $\hat\nabla$. Let $\sigma : [0,T] \to M$ be a smooth curve, and let u be a tangent vector at $\sigma(0)$. By parallel transport of u along the curve σ we obtain a vector-valued function on $[0,T]$ such that $u(t)$ is a tangent vector at $\sigma(t)$, obeying the parallel transport equation

$$\dot u^\gamma(t) + \Gamma^\gamma_{\alpha\beta} u^\alpha(t) \dot\sigma^\beta(t) = 0. \tag{1.7}$$

This equation says that the *covariant derivative* $\hat\nabla u$ of u along the direction $\dot\sigma$, which is given by the left-hand side of (1.7), vanishes. In general, the covariant derivative of a (m,n)-tensor field T along a vector field v is a $(m,n+1)$-tensor field given by

$$\hat\nabla_k T^{i_1\dots i_m}_{j_1\dots j_n} = \frac{\partial T^{i_1\dots i_m}_{j_1\dots j_n}}{\partial x^k} + \Gamma^{i_1}_{kl} T^{l i_2\dots i_m}_{j_1\dots j_n} + \cdots + \Gamma^{i_m}_{kl} T^{i_1\dots i_{m-1} l}_{j_1\dots j_n} - \Gamma^l_{k j_1} T^{i_1\dots i_m}_{l j_2\dots j_n} - \cdots - \Gamma^l_{k j_n} T^{i_1\dots i_m}_{j_1\dots j_{n-1} l}. \tag{1.8}$$

The covariant derivative of a scalar field is given by its partial derivative.

A tensor field T is called *parallel* if its covariant derivative $\hat{\nabla}T$ vanishes identically, i.e., T is reproduced by parallel transport along any curve. The metric tensor g itself is always parallel.

If a vector u is carried by parallel transport along a closed loop, then the vector at the end-point will in general be different from the vector at the starting point. The difference is linear in the original vector and linear up to higher order terms in the area element enclosed by the loop. The proportionality coefficients are given by the *Riemann curvature tensor*, the $(1,3)$-tensor

$$R^{\rho}_{\sigma\mu\nu} = \frac{\partial\Gamma^{\rho}_{\nu\sigma}}{\partial x^{\mu}} - \frac{\partial\Gamma^{\rho}_{\mu\sigma}}{\partial x^{\nu}} + \Gamma^{\rho}_{\mu\lambda}\Gamma^{\lambda}_{\nu\sigma} - \Gamma^{\rho}_{\nu\lambda}\Gamma^{\lambda}_{\mu\sigma}. \tag{1.9}$$

By contracting the first with the third index we obtain a symmetric $(0,2)$-tensor, the *Ricci curvature tensor*

$$R_{\sigma\nu} = R^{\mu}_{\sigma\mu\nu}. \tag{1.10}$$

A Riemannian metric g on a domain $\Omega \subset \mathbb{R}^n$ is called *Hessian metric* if it can be locally expressed as the Hessian of a real-valued function, $g = \frac{\partial^2 F}{\partial x^i \partial x^j} dx^i dx^j$. The function F is called the (local) *potential* of the Hessian metric.

A *space form* is a Riemannian manifold with Riemann tensor given by

$$R^{\rho}_{\sigma\mu\nu} = K(\delta^{\rho}_{\mu} g_{\sigma\nu} - \delta^{\rho}_{\nu} g_{\sigma\mu}), \tag{1.11}$$

where K is a constant. If $K = 0$, then the space form is *flat*, for $K < 0$ it is *hyperbolic*, and for $K > 0$ it is *elliptic*.

Let us now consider a Riemannian manifold $\mathcal{M}$ with metric G and a smooth submanifold $M \subset \mathcal{M}$. The restriction g of G to M defines a metric on M and turns M into a Riemannian manifold too. At any point $y \in M$, the tangent space $T_y\mathcal{M}$ can be decomposed into a G-orthogonal sum $T_yM \oplus N_yM$. Here N_yM is defined as the G-orthogonal complement of T_yM in $T_y\mathcal{M}$ and is called the *normal subspace* to M at y. The submanifold M is called *totally geodesic* if if every M-geodesic is also an $\mathcal{M}$-geodesic.

An introduction into Riemannian geometry can be found in [65, 200].

1.2.3 Affine hypersurface immersions

Affine hypersurface immersions have first been studied in the pioneering works of Tzitzeica [210] and Blaschke [20]. This branch of differential geometry deals with properties of submanifolds, in particular, submanifolds of codimension 1, of affine real space which are invariant with respect to the special linear group of affine transformations.

In the previous subsection we considered the Levi-Civita connection $\hat{\nabla}$ generated by a Riemannian metric. One may also consider affine connections and define notions like parallel transport, geodesics, or curvature independently of any metric. For a general affine connection ∇ on a manifold M, the Christoffel symbols Γ^k_{ij} in the transformation rule (1.6), the parallel transport equation (1.7), the formula for the covariant derivative (1.8), and the curvature tensors (1.9),(1.10) have to replaced by the corresponding coefficients of the connection ∇^k_{ij}. We deal only with torsion-free connections, whose coefficients are symmetric in the lower indices. The Ricci tensor (1.10) defined by such a connection is in general no more symmetric, however. From (1.6) it follows that the components of the difference of any two affine connections transform like a $(1,2)$-tensor under coordinate changes. By adding such a tensor to one connection, we hence obtain another connection.

A classical example of an affine connection is the canonical connection D on $\mathbb{R}^n$. In the usual coordinate system on $\mathbb{R}^n$ the coefficients of the connection vanish identically, and the covariant derivative with respect to D just equals the usual partial derivative ∂. The subject of affine differential geometry are the structures generated by the connection D on smooth hypersurfaces of $\mathbb{R}^n$.

Let M be an $(n-1)$-dimensional differentiable manifold and $f : M \to \mathbb{R}^n$ a smooth hypersurface immersion. Let $\xi : M \to \mathbb{R}^n$ be a smooth transversal vector field on M, i.e., such that at any point $y \in M$, every tangent vector $u \in T_{f(y)}\mathbb{R}^n$ can be decomposed into a sum of a tangential component in $f_*[T_yM]$ and a component parallel to $\xi(y)$. Then there exists a unique affine connection ∇ and a unique symmetric $(0,2)$-tensor field h on M such that for every ∇-geodesic $\sigma(t)$ on M we have

$$\frac{d^2 f(\sigma(t))}{dt^2} + h(\dot\sigma(t),\dot\sigma(t))\cdot\xi(\sigma(t)) = 0. \tag{1.12}$$

This can be written equivalently as $D - \nabla = -h\otimes\xi$, and ∇ can be interpreted as projection of D onto the tangent space to M along ξ. The tensor h is called the *affine fundamental form*, and ∇ is called the *induced connection*. If h is non-degenerate everywhere on M, then f is called *non-degenerate* and h is called the *affine metric*.

Given a hypersurface immersion $f: M\to\mathbb{R}^n$ and a transversal vector field $\xi: M\to\mathbb{R}^n$, we may define another hypersurface immersion $\nu: M\to\mathbb{R}_n$ into the dual space of $\mathbb{R}^n$, as follows. For $y\in M$ we define the image $\nu(y)$ as the vector $v\in\mathbb{R}_n$ which is zero on the tangent space $f_*[T_yM]$ and 1 on the transversal vector $\xi(y)$. It turns out that this *conormal map* defines the same quadratic form h on M, but a different affine connection $\bar\nabla$, which is called the *dual affine connection*. The conormal map of the immersion ν is the original immersion f, so the correspondence $f\leftrightarrow\nu$ is a duality.

The induced connection ∇ on M does in general not coincide with the Levi-Civita connection $\hat\nabla$ of the affine metric h. Their difference $K^\gamma_{\alpha\beta} = \nabla^\gamma_{\alpha\beta} - \hat\nabla^\gamma_{\alpha\beta}$ is called the *difference tensor*. Although the covariant derivative of h with respect to $\hat\nabla$ vanishes, its covariant derivative with respect to ∇ is in general not zero. The covariant derivative $C_{\alpha\beta\gamma} = \nabla_\alpha h_{\beta\gamma}$ is called the *cubic form*.

In this thesis we shall deal exclusively with *hyperbolic centro-affine hypersurface immersions* $f: M\to\mathbb{R}^n$, whose transversal vector field is defined by the relation $\xi = -f$ and whose affine metric is positive definite. This implies that the image of the immersion is convex such that its convex hull and the origin lie on opposite sides of the surface. Centro-affine immersions have further particular properties. Their cubic form C is symmetric and can be expressed by the difference tensor as $C_{\alpha\beta\gamma} = -2h_{\alpha\sigma}K^\sigma_{\beta\gamma}$, with inverse relation $K^\sigma_{\beta\gamma} = -\frac{1}{2}h^{\alpha\sigma}C_{\alpha\beta\gamma}$. The curvature tensors (1.9),(1.10) of the induced connection ∇ are given by

$$R^\rho_{\sigma\mu\nu} = h_{\sigma\nu}\delta^\rho_\mu - h_{\sigma\mu}\delta^\rho_\nu, \qquad R_{\sigma\nu} = (n-2)h_{\sigma\nu}.$$

The images under f of the ∇-geodesics are always contained in 2-dimensional linear subspaces of $\mathbb{R}^n$, which are spanned by ξ and the image of the velocity vector.

If the cubic form is symmetric, then there exists a simple relation between the Levi-Civita connection $\hat\nabla$ of the affine metric, the dual connection $\bar\nabla$, and the induced connection ∇. Namely, we have $\hat\nabla = \frac{1}{2}(\nabla+\bar\nabla)$, or equivalently $\bar\nabla - \nabla = -2K$ [172, Section I, Corollary 4.4]. The cubic form hence measures the difference between the primal and dual connections.

There exist, however, also other choices of the transversal vector field. In the absence of a distinguished point in $\mathbb{R}^n$ which can serve as the origin, i.e., when the target space of the immersion is merely an affine space, the most natural choice of the transversal vector field is the *affine normal*. If the immersion is locally convex, as will be the case with the level surface of barriers, the affine normal can be interpreted as follows. Choose a point $y\in M$ and a neighbourhood $U\subset M$ of y such that $f[U]$ is a convex surface. Consider the image $f_*[T_yM]$ of the tangent space at some point y as an affine hyperplane H which is tangent to the immersion $f[M]$ at the point $f(y)$. Consider a family of hyperplanes H_α which is parallel to H. Then the hyperplane H_α intersects the convex hull of $f[U]$ in some compact convex set C_α with center of gravity γ_α. The centers of gravity form a curve γ with end-point $f(y)$. The tangent to γ at $f(y)$ is the direction of the affine normal ξ at y, see Fig. 1.1. The definition of the affine normal assumes the existence of an affinely invariant volume form on $\mathbb{R}^n$, and therefore it is defined only up to a multiplicative constant in the absence of such a volume form. Affine hypersurface immersions equipped with the affine normal as transversal vector field are called *Blaschke immersions*.

A *proper affine hypersphere* is a hypersurface immersion with all affine normals meeting in a point. It is convenient to consider this point to be the origin of $\mathbb{R}^n$. This definition involves only the direction of the affine normals and is hence independent of the volume form chosen on $\mathbb{R}^n$. Moreover, it turns out that the affine normal of a proper affine hypersphere is always equal to a constant times the centro-affine transversal vector field, $\xi = \mathit{const}\cdot f$. Only the value of this constant depends on the volume form.

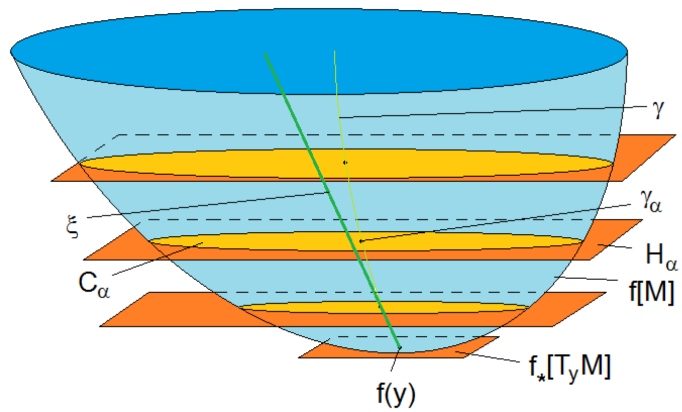

Figure 1.1: Direction of the affine normal for convex hypersurfaces immersions

An excellent general reference on affine differential geometry is the book [172]. Centro-affine hypersurface immersions are treated in detail in the first chapter.

1.2.4 Lie derivative

There exist also derivations which are not defined by affine connections. Let M be a differentiable manifold and v a vector field on M. Then v defines a flow $\Phi_t : M \to M$ on M by the differential equation $\frac{dx}{dt} = v(x)$. The *Lie derivative* $\mathcal{L}_v T$ of a tensor field T on M is defined by the rate of change of T along the flow Φ_t. It is a tensor field of the same type as T. The Lie derivative of T vanishes if and only if the flow Φ_t leaves T invariant.

The coordinate expression of the Lie derivative of a tensor field $T^{i_1\dots i_m}_{j_1\dots j_n}$ along a vector field v^k is given by [226, eq.(I.3.26)]

$$(\mathcal{L}_v T)^{i_1\dots i_m}_{j_1\dots j_n} = v^k \frac{\partial T^{i_1\dots i_m}_{j_1\dots j_n}}{\partial x^k} - \frac{\partial v^{i_1}}{\partial x^k} T^{k i_2\dots i_m}_{j_1\dots j_n} - \dots - \frac{\partial v^{i_m}}{\partial x^k} T^{i_1\dots i_{m-1}k}_{j_1\dots j_n} + \frac{\partial v^k}{\partial x^{j_1}} T^{i_1\dots i_m}_{k j_2\dots j_n} + \dots + \frac{\partial v^k}{\partial x^{j_n}} T^{i_1\dots i_m}_{j_1\dots j_{n-1}k}.$$

If M possesses in addition an affine connection ∇, then the partial derivatives can be replaced by the covariant derivatives with respect to ∇ [226, eq.(I.3.27)],

$$\begin{aligned}(\mathcal{L}_v T)^{i_1\dots i_m}_{j_1\dots j_n} = {} & v^k \nabla_k T^{i_1\dots i_m}_{j_1\dots j_n} - \nabla_k v^{i_1} T^{k i_2\dots i_m}_{j_1\dots j_n} - \dots - \nabla_k v^{i_m} T^{i_1\dots i_{m-1}k}_{j_1\dots j_n} + \\ & + \nabla_{j_1} v^k T^{i_1\dots i_m}_{k j_2\dots j_n} + \dots + \nabla_{j_n} v^k T^{i_1\dots i_m}_{j_1\dots j_{n-1}k}.\end{aligned}$$

In particular, we have $\mathcal{L}_v \delta^i_j = 0$ for the Lie derivative of the Kronecker symbol. Let now $T_{\alpha\beta}$ be a non-degenerate $(0,2)$ tensor field and $S^{\alpha\beta}$ the inverse $(2,0)$ tensor field, such that $T_{\alpha\beta}S^{\beta\gamma} = \delta^\gamma_\alpha$. Then we have by the Leibniz rule

$$S^{\beta\gamma}\mathcal{L}_v T_{\alpha\beta} + T_{\alpha\beta}\mathcal{L}_v S^{\beta\gamma} = 0$$

and hence $\mathcal{L}_v S^{\mu\gamma} = -S^{\mu\alpha}S^{\beta\gamma}\mathcal{L}_v T_{\alpha\beta}$. Therefore $\mathcal{L}_v S = 0$ if and only if $\mathcal{L}_v T = 0$.

The Lie derivative $\mathcal{L}_v$ commutes with the covariant derivative with respect to ∇ if and only if the affine flow Φ_t defined by v leaves the affine connection ∇ invariant [226, Theorem I.4.2]. In particular, we have the following result.

Lemma 1.2.2. *Let $U \subset \mathbb{R}^n$ be a domain and let v be a vector field on U. Let D be the canonical flat affine connection of $\mathbb{R}^n$. Then the Lie derivative $\mathcal{L}_v$ commutes with D if and only if the vector field v is linear-affine in affine coordinates on U.* □

A treatment of the Lie derivative can be found in many books on differential geometry or general relativity, e.g., [218]. For a specialized monograph see [226].

1.3 Barriers from the viewpoint of affine differential geometry

In this section we establish how logarithmically homogeneous barriers, which are functions F defined on domains in $\mathbb{R}^n$, relate to centro-affine geometry, which deals with hypersurfaces in $\mathbb{R}^n$. The key result which relates these two objects is the splitting of the metric defined by the Hessian F'' into a trivial 1-dimensional radial part and a non-trivial $(n-1)$-dimensional part modelled on the level surfaces of F, which turns out to be proportional to the centro-affine metric. Then we consider how the cubic form on the level surface relates to the third derivative F'''. The main result will be the characterization of self-concordant barriers by the centro-affine geometry of their level surfaces, in particular, the equivalence between the condition of self-concordance and the uniform boundedness of the cubic form. This will yield also an interpretation of the barrier parameter as a measure of the difference between the primal and dual affine connections on the level surface. We shall present this result in Subsection 1.3.1. In Subsection 1.3.2 we consider the relation between Legendre duality and the conormal map. In Subsection 1.3.3 we then consider the simplest possible case, namely centro-affine immersions with vanishing cubic form, for which the primal and dual affine connections coincide with the Levi-Civita connection of the centro-affine metric. We show that this case corresponds the hyperbolic barrier on the Lorentz cone.

The viewpoint on barriers as functions on the interior of the cone can be associated to the class of affine-scaling methods. The viewpoint of centro-affine geometry puts in the focus the level surface of the barrier, which is canonically isomorphic to the manifold of rays in the interior of the cone, and can thus be associated to projective-scaling methods. One of the reasons for developing the theory presented in this chapter is to lay a theoretical foundation onto which one can build projective-scaling methods for general cones.

Another advantage of the presented connection between affine differential geometry and self-concordant barriers is that results from geometry can be applied to yield new insights in the theory of barriers. We shall present several applications in the subsequent sections.

1.3.1 Self-concordance and cubic form

The splitting result presented below is not limited to self-concordant barriers, but is valid for arbitrary logarithmically homogeneous functions. Let $F : K^o \to \mathbb{R}$ be a smooth locally strongly convex function on the interior of a regular convex cone K satisfying the logarithmic homogeneity condition (1.3) with some $\nu > 0$. Let $F_\alpha = \{x \in K^o \,|\, F(x) = \alpha\}$ be the level surfaces of F. For every $\alpha \in \mathbb{R}$, there exists a diffeomorphism $I_\alpha : F_\alpha \times \mathbb{R}_+ \to K^o$ given by $I_\alpha : (x, \beta) \mapsto \beta x$. The following result states that the Hessian metric defined by F on K^o splits into a direct product under the inverse of I_α.

Proposition 1.3.1. *[139, Theorem 1, p.428] Assume the notations and conditions of the previous paragraph. Then the Riemannian manifold (K^o, F''), consisting of the interior of K equipped with the Hessian metric generated by F, is isometric under I_α^{-1} to the product $(F_\alpha, \nu h) \times (\mathbb{R}_+, \nu\beta^{-2}d\beta^2)$, where h is the centro-affine metric of the inclusion $F_\alpha \hookrightarrow \mathbb{R}^n$, considered as centro-affine immersion.*

Thus the affine metric on the level surface F_α is given by ν^{-1} times the restriction of the Hessian metric F'' on this level surface, while the metric on a ray has metric tensor $\nu\beta^{-2}$, where β is the natural coordinate on the ray. Since all 1-dimensional Riemannian manifolds are locally isometric to the Euclidean space $\mathbb{R}^1$, all the information contained in the metric F'' is concentrated in the non-trivial $(n-1)$-dimensional factor and is encoded by the centro-affine metric h of the level surfaces of F. Note also that all level surfaces F_α are mutually isometric.

All the necessary ingredients to prove this result have already been provided in [171, Section 2.3.3]. For the case of homogeneous cones equipped with the universal barrier it has been proven in [187]. However, even convexity and non-degeneracy are not necessary. A proof in this general case can be found in [96, Theorem 2.2].

The barrier parameter ν appears as a proportionality coefficient between the centro-affine metric on the level surfaces of F and the Hessian metric F''. From the viewpoint of centro-affine geometry it is therefore convenient to consider logarithmically homogeneous functions of homogeneity degree $\nu = 1$, because in this case the centro-affine metric is directly reproduced as the submanifold metric generated by the Hessian. This yields also a simple means to compute the centro-affine fundamental form on an arbitrary smooth hypersurface. To this end one has to construct a 1-logarithmically homogeneous function F in a neighbourhood of the hypersurface, such that F is constant on the surface itself, and then take the restriction of the Hessian F'' to the hypersurface.

In the same way the second derivative F'' is related to the centro-affine metric on the level surfaces of F, the third derivative is related to their cubic forms.

Lemma 1.3.2. *Assume above notations and conditions. Then for every $\alpha \in \mathbb{R}$, the cubic form of the inclusion $F_\alpha \hookrightarrow \mathbb{R}^n$, considered as centro-affine immersion, equals the restriction of the symmetric $(0,3)$ tensor field $\nu^{-1}F'''$ on F_α.*

Proof. Let $y \in F_\alpha$ be an arbitrary point and let $u \in T_yF_\alpha$ be a tangent vector at y. We shall now compute the value $C[u,u,u]$ of the cubic form on this vector. Let ∇ be the induced centro-affine connection on F_α and D the canonical affine connection on D. We then have $C = \nabla h = \nu^{-1}\nabla F''$ by the definition of the cubic form and by Proposition 1.3.1.

Let $\sigma(t)$ be the ∇-geodesic through $y = \sigma(0)$ with velocity u. Then by definition $u(t) = \dot\sigma(t)$ is the vector obtained by ∇-parallel transport of u from y to $\sigma(t)$ along σ. Applying (1.12) we get

$$\dot u(t) - h(u(t),u(t)) \cdot \sigma(t) = 0. \tag{1.13}$$

Let further $\gamma(t) = F''(\sigma(t))[u(t),u(t)]$ be the value of F'' on the vector $u(t)$. On the one hand, we get by differentiation

$$\begin{aligned}\dot\gamma(t) &= F'''(\sigma(t))[\dot\sigma(t),u(t),u(t)] + 2F''(\sigma(t))[\dot u(t),u(t)]\\ &= F'''(\sigma(t))[u(t),u(t),u(t)] + 2h(u(t),u(t))F''(\sigma(t))[\sigma(t),u(t)]\\ &= F'''(\sigma(t))[u(t),u(t),u(t)].\end{aligned}$$

Here the second equality comes from (1.13), and the third equality holds because the position vector $\sigma(t)$ and the tangent vector $u(t)$ are orthogonal by virtue of Proposition 1.3.1. On the other hand, we have

$$\dot\gamma(t) = \nabla_{u(t)}\gamma(t) = (\nabla F'')(\sigma(t))[u(t),u(t),u(t)] = \nu C(\sigma(t))[u(t),u(t),u(t)].$$

Here the first equality holds because the covariant derivative of a scalar equals its partial derivative. The second equality holds by the Leibniz rule, taking into account that the ∇-derivative of u vanishes because $u(t)$ is ∇-parallel. The third equality comes from the definition of the cubic form C.

Equalling the two expressions for $\dot\gamma(t)$ completes the proof. □

By Lemma 1.3.2 self-concordance of F implies that the cubic form on the level surfaces of F is uniformly bounded. However, the converse implication is not immediately evident, because the affine metric and the cubic form on the level surface F_α determine the derivatives F'', F''' only on those vectors which are tangent to F_α. We can, however, restore the values of these derivatives on arbitrary vectors from the values on the vectors tangent to F_α only, which allows to obtain the following result.

Lemma 1.3.3. *Let $F : K^o \to \mathbb{R}$ be a logarithmically homogeneous convex C^3 function with homogeneity degree ν on a convex cone $K \subset \mathbb{R}^n$, $n \geq 2$, let $x \in K^o$ be a point, and set $\alpha = F(x)$. Assume that F'' is positive definite everywhere on K^o. Then $|F'''(x)[u,u,u]| \leq 2(F''(x)[u,u])^{3/2}$ holds for all vectors $u \in \mathbb{R}^n$ if and only if the cubic form C on the level surface F_α at x has ∞-norm not exceeding 2ϑ with $\vartheta = \frac{\nu-2}{\sqrt{\nu-1}}$ as measured in the affine metric h at x.*

Proof. Differentiating (1.3) with respect to t at $t = 1$ and with respect to x we obtain $F'(x)[x] = -\nu$, $F''(x)[x] = -F'(x)$, see also [171, eqs. (2.3.12–13)]. Differentiating further with respect to x, we get $F'''(x)[x] = -2F''(x)$, see also [163].

Let $v \in T_xF_\alpha$ be a vector tangent to F_α, and set $u = v + \beta x$ with $\beta \in \mathbb{R}$. By Proposition 1.3.1 and Lemma 1.3.2 we have $F''(x) = \nu h(x)$, $F'''(x) = \nu C(x)$ on v. Using the above formulas recursively and the condition that v is tangent to the level surface of F we obtain

$$\begin{aligned} F'''(x)[u,u,u] &= F'''(x)[v,v,v] + 3\beta F'''(x)[v,v,x] + 3\beta^2 F'''(x)[v,x,x] + \beta^3 F'''(x)[x,x,x] \\ &= F'''(x)[v,v,v] - 6\beta F''(x)[v,v] + 6\beta^2 F'(x)[v] - 2\beta^3 \nu \\ &= \nu(C(x)[v,v,v] - 6\beta h(x)[v,v] - 2\beta^3), \end{aligned} \tag{1.14}$$

$$\begin{aligned} F''(x)[u,u] &= F''(x)[v,v] + 2\beta F''(x)[v,x] + \beta^2 F''(x)[x,x] \\ &= F''(x)[v,v] - 2\beta F'(x)[v] - \beta^2 F'(x)[x] = \nu(h(x)[v,v] + \beta^2). \end{aligned} \tag{1.15}$$

Therefore we have $|F'''(x)[u,u,u]| \leq 2(F''(x)[u,u])^{3/2}$ for all $u \in \mathbb{R}^n$ if and only if we have

$$|C(x)[v,v,v] - 6\beta h(x)[v,v] - 2\beta^3| \leq 2\nu^{1/2}(h(x)[v,v] + \beta^2)^{3/2}$$

for all $v \in T_x F_\alpha$ and $\beta \in \mathbb{R}$. By squaring the inequality we get the equivalent condition

$$4\nu(h(x)[v,v] + \beta^2)^3 - (C(x)[v,v,v] - 6\beta h(x)[v,v] - 2\beta^3)^2 \geq 0. \tag{1.16}$$

The left-hand side is a polynomial p in β. We shall now determine the triples $(\nu, h(x)[v,v], C(x)[v,v,v])$ for which $p(\beta)$ is nonnegative on the real axis. If $v = 0$, then $p(\beta) = 4(\nu-1)\beta^6$, and p is nonnegative if and only if $\nu \geq 1$. If $v \neq 0$, and such v exist by our assumption $n \geq 2$, then $h(x)[v,v] > 0$, and we may make the substitution $\beta = \tilde\beta\sqrt{h(x)[v,v]}$. With $\vartheta = \frac{C(x)[v,v,v]}{2(h(x)[v,v])^{3/2}}$ we get

$$p(\beta) = (h(x)[v,v])^3 \left[4\nu(1+\tilde\beta^2)^3 - (2\vartheta - 6\tilde\beta - 2\tilde\beta^3)^2\right].$$

The polynomial in brackets is nonnegative if and only if it is a sum of squares of cubic polynomials in $\tilde\beta$, which by a standard procedure [175] can equivalently be expressed by the matrix inequality

$$\exists\ \mu,\rho,\tau: \quad \begin{pmatrix} 4(\nu-1) & 0 & \mu & 4\vartheta+\rho \\ 0 & 12(\nu-2)-2\mu & -\rho & \tau \\ \mu & -\rho & 12(\nu-3)-2\tau & 12\vartheta \\ 4\vartheta+\rho & \tau & 12\vartheta & 4\nu-4\vartheta^2 \end{pmatrix} \succeq 0.$$

By Schur complements this is in turn equivalent to the linear matrix inequality (LMI)

$$\exists\ \mu,\rho,\tau: \quad A = \begin{pmatrix} 4(\nu-1) & 0 & \mu & 4\vartheta+\rho & 0 \\ 0 & 12(\nu-2)-2\mu & -\rho & \tau & 0 \\ \mu & -\rho & 12(\nu-3)-2\tau & 12\vartheta & 0 \\ 4\vartheta+\rho & \tau & 12\vartheta & 4\nu & 2\vartheta \\ 0 & 0 & 0 & 2\vartheta & 1 \end{pmatrix} \succeq 0,$$

which is linear in (ν,ϑ). Hence the feasible set of this LMI is convex. We shall show that this set equals the set $S = \{(\nu,\vartheta) \mid \nu \geq 2,\ |\vartheta| \leq \frac{\nu-2}{\sqrt{\nu-1}}\}$.

Indeed, inserting the values $\nu = 2$, $\vartheta = \rho = 0$, $\mu = -4$, $\tau = -8$ into A above yields a block-diagonal positive semi-definite rank 3 matrix and shows that the point $(2,0)$ is feasible. Let now $\tilde\beta \in (-1,1)\setminus\{0\}$ and set $\hat\nu = \frac{1+\tilde\beta^2}{\tilde\beta^2}$, $\hat\vartheta = -\frac{1-\tilde\beta^2}{\tilde\beta}$, $\hat\mu = -\frac{8\tilde\beta^2-4}{\tilde\beta^2}$, $\hat\tau = -4(\tilde\beta^2+1)$, $\hat\rho = 0$. Inserting these values into the matrix A defined above, we obtain the matrix

$$\hat A = \begin{pmatrix} \frac{4}{\tilde\beta^2} & 0 & \frac{4(1-2\tilde\beta^2)}{\tilde\beta^2} & -\frac{4(1-\tilde\beta^2)}{\tilde\beta} & 0 \\ 0 & \frac{4(1+\tilde\beta^2)}{\tilde\beta^2} & 0 & -4(1+\tilde\beta^2) & 0 \\ \frac{4(1-2\tilde\beta^2)}{\tilde\beta^2} & 0 & \frac{4(2\tilde\beta^4-4\tilde\beta^2+3)}{\tilde\beta^2} & -\frac{12(1-\tilde\beta^2)}{\tilde\beta} & 0 \\ -\frac{4(1-\tilde\beta^2)}{\tilde\beta} & -4(1+\tilde\beta^2) & -\frac{12(1-\tilde\beta^2)}{\tilde\beta} & \frac{4(1+\tilde\beta^2)}{\tilde\beta^2} & -\frac{2(1-\tilde\beta^2)}{\tilde\beta} \\ 0 & 0 & 0 & -\frac{2(1-\tilde\beta^2)}{\tilde\beta} & 1 \end{pmatrix}.$$

By computing the determinants of the principal minors in the upper left corner one can check that this matrix is positive semi-definite of rank 4. It can be checked directly that the kernel of $\hat A$ is generated by the vector $w = (\tilde\beta^4, \tilde\beta^3, \tilde\beta^2, \tilde\beta, 2(1-\tilde\beta^2))^T$. Therefore the pair $(\nu, \vartheta) = (\frac{1+\tilde\beta^2}{\tilde\beta^2}, -\frac{1-\tilde\beta^2}{\tilde\beta})$ is feasible for all $\tilde\beta \in (-1,1) \setminus \{0\}$. Thus all extremal points of the set S defined above are feasible, and S is contained in the feasible set of the LMI.

On the other hand, for every positive semi-definite matrix A as above we have

$$w^T A w = 4(\tilde\beta^2+1)^2(2\vartheta\tilde\beta + \tilde\beta^2\nu + \tilde\beta^4\nu - 4\tilde\beta^2 - \tilde\beta^4 + 1) \geq 0,$$

leading to the linear inequality $2\tilde\beta(\vartheta - \hat\vartheta) + \tilde\beta^2(1+\tilde\beta^2)(\nu - \hat\nu) \geq 0$. It is not hard to check that the set S equals the intersection of the closed half-planes defined by these inequalities, with the parameter $\tilde\beta$ running through the set $(-1,1) \setminus \{0\}$. Therefore the feasible set of the LMI is contained in S.

We have shown that (1.16) holds for all $v \in T_x F_\alpha$ and all $\beta \in \mathbb{R}$ if and only if $\nu \geq 2$ and $|C(x)[v,v,v]| \leq 2\frac{\nu-2}{\sqrt{\nu-1}}(h(x)[v,v])^{3/2}$ for all $v \in T_x F_\alpha$. Clearly the condition $\nu \geq 2$ is redundant, which completes the proof. □

Corollary 1.3.4. *Let $F : K^o \to \mathbb{R}$ be a logarithmically homogeneous convex C^3 function with homogeneity degree ν on a convex cone $K \subset \mathbb{R}^n$, $n \geq 2$. Then F is self-concordant if and only if the cubic form on the level surfaces of F has ∞-norm not exceeding 2ϑ with $\vartheta = \frac{\nu-2}{\sqrt{\nu-1}}$ as measured in the affine metric.* □

If we want to perform computations with geometric objects on the level surfaces of a barrier F, we need to introduce a coordinate system on these level surfaces. While the interior of the cone K can be conveniently parameterized by any linear coordinate system on $\mathbb{R}^n$, the level surfaces are curved and such a coordinate system cannot be used directly. We shall map the level surface by a radial bijection to the interior of a compact proper affine section S of the cone and then use an affine coordinate system on this section, as shown in Fig. 1.2. The next result shows how to express the affine metric and the

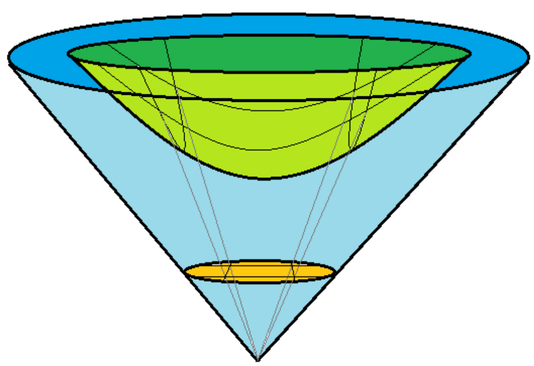

Figure 1.2: Coordinate system on level surface of F defined by radial projection onto affine section

cubic form in such a coordinate system.

Lemma 1.3.5. *Let $F : K^o \to \mathbb{R}$ be a self-concordant barrier with parameter ν on some regular convex cone $K \subset \mathbb{R}^n$. Let S be a compact proper affine section of K. Let F_α be a level surface of F, equipped with the centro-affine metric h and the cubic form C. Define a bijection $\iota : F_\alpha \to S^o$ such that for every point $p \in F_\alpha$, the image point $\iota(p) \in S^o$ is a multiple of p. Let $y : S^o \to \mathbb{R}^{n-1}$ be an affine coordinate chart on S^o and let $x = y \circ \iota : F_\alpha \to \mathbb{R}^{n-1}$ be the corresponding coordinate chart on F_α. Let $f = F \circ \iota : F_\alpha \to \mathbb{R}$ be the scalar function defined by the restriction of F to the interior of the section*

S. Then we have

$$h_{\alpha\beta} = \nu^{-1}\frac{\partial^2 f}{\partial x^\alpha \partial x^\beta} - \nu^{-2}\frac{\partial f}{\partial x^\alpha}\frac{\partial f}{\partial x^\beta}, \tag{1.17}$$

$$C_{\alpha\beta\gamma} = \nu^{-1}\frac{\partial^3 f}{\partial x^\alpha \partial x^\beta \partial x^\gamma} - 2\nu^{-2}\left(\frac{\partial^2 f}{\partial x^\alpha \partial x^\beta}\frac{\partial f}{\partial x^\gamma} + \frac{\partial^2 f}{\partial x^\alpha \partial x^\gamma}\frac{\partial f}{\partial x^\beta} + \frac{\partial^2 f}{\partial x^\beta \partial x^\gamma}\frac{\partial f}{\partial x^\alpha}\right) + 4\nu^{-3}\frac{\partial f}{\partial x^\alpha}\frac{\partial f}{\partial x^\beta}\frac{\partial f}{\partial x^\gamma}. \tag{1.18}$$

Proof. Let $x \in F_\alpha$ be a point on the level surface and $y = \iota(x)$ the projection of x to the affine section S. Note that homotheties map level surfaces of F to level surfaces and leave the transversal vector field invariant. Hence the affine metric and the cubic form on the level surfaces are also mapped to each other. Moreover, the coordinate charts x defined by the affine section S are also mapped to each other, i.e., in these coordinates a homothety is the identity map. We may hence assume without loss of generality that the level surface F_α passes through the point y, and in fact $x = y$, by applying an appropriate homothety.

Let now $v \in T_xF_\alpha$ be a vector tangent to the level surface, and $u = \iota_* v$ its image in the tangent space to S. Then $u = v + \beta x$ for some $\beta \in \mathbb{R}$, because in a neighbourhood of x the surface F_α is projected to S parallel to the vector x, up to terms of higher order. We have $F'(x)[u] = F'(x)[v] + \beta F'(x)[x] = -\beta\nu$, giving $\beta = -\nu^{-1}F'(x)[u]$. Formulas (1.15),(1.14) then yield

$$F'''(x)[u,u,u] = \nu C(x)[v,v,v] + 6F'(x)[u]h(x)[v,v] + 2\nu^{-2}(F'(x)[u])^3,$$
$$F''(x)[u,u] = \nu h(x)[v,v] + \nu^{-1}(F'(x)[u])^2.$$

Solving this system for h and C we obtain

$$h(x)[v,v] = \nu^{-1}F''(x)[u,u] - \nu^{-2}(F'(x)[u])^2,$$
$$C(x)[v,v,v] = \nu^{-1}F'''(x)[u,u,u] - 6\nu^{-2}F'(x)[u]F''(x)[u,u] + 4\nu^{-3}(F'(x)[u])^3.$$

Now $F'(x)[u] = f'(x)[v]$, $F''(x)[u,u] = f''(x)[v,v]$, $F'''(x)[u,u,u] = f'''(x)[v,v,v]$ by definition of f. The claim of the lemma readily follows. □

The affine metric h and the cubic form C of a level surface of a barrier F can be seen as the projective counterparts of the Hessian metric F'' and the third derivative F'''. Indeed, in the case of LP, i.e., when $K = \mathbb{R}^n_+$, the projective metric introduced by Karmarkar [116, Section 2] on the interior of the standard simplex is proportional to the centro-affine metric on the level surfaces of the logarithmic barrier $F(x) = -\sum_{j=1}^n \log x_j$ on $\mathbb{R}^n_+$, as can be seen by applying (1.17) to the restriction of F to the affine section of $\mathbb{R}^n_+$ given by $\sum_{j=1}^n x_j = 1$.

Sometimes it is convenient to consider the level surface F_α not as a submanifold of the ambient space $\mathbb{R}^n$ but as an abstract $(n-1)$-dimensional manifold equipped with a metric h and a cubic form C, modelled on the interior of a compact affine section of K, with h and C given by (1.17),(1.18). These data suffice to recover both the barrier, up to an additive constant and a multiplicative factor determining the barrier parameter, and the cone K, up to linear isomorphisms of $\mathbb{R}^n$. Indeed, by raising an index of C by means of h we may reconstruct the difference tensor $\bar\nabla - \nabla$. The Levi-Civita connection $\hat\nabla = \frac{1}{2}(\nabla + \bar\nabla)$ then allows to recover both connections $\nabla, \bar\nabla$. Uniqueness of the centro-affine immersion of M as a submanifold of $\mathbb{R}^n$ then follows from the fundamental uniqueness result [172, Theorem 8.1].

In order to be a self-concordant barrier with parameter ν for a cone $K \subset \mathbb{R}^n$, it is not sufficient for a smooth convex ν-logariathmically homogeneous function $F : K^o \to \mathbb{R}$ to be a self-concordant function. We must also have $F(x) \to +\infty$ for $x \to \partial K$. This condition can also be rewritten in terms of the level surfaces of F. We shall need the following definition.

Definition 1.3.6. Let $K \subset \mathbb{R}^n$ be a regular convex cone. A hyperbolic centro-affine hypersurface $M \subset K^o$ is called *asymptotic to* K if every ray in K^o intersects M in exactly one point and for every compact proper affine section S of K and some Euclidean metric on $\mathbb{R}^n$, the distance between the intersections $\partial K \cap S$ and $\alpha M \cap S$ is positive for all $\alpha > 0$.

Since all Euclidean metrics on $\mathbb{R}^n$ are equivalent, we may also replace "some Euclidean metric" by "every Euclidean metric". Let S be a proper compact affine section of K. For a surface M which is asymptotic to K, the intersections $S_\alpha = \alpha M \cap S^o$ are closed, because every limit point of S_α must also be in S^o and hence in S_α by continuity of M. By convexity of M the convex hull of S_α equals the union $S_{\geq\alpha} = \bigcup_{\beta\geq\alpha} S_\beta$. Hence for decreasing α we have that $S_{\geq\alpha}$ is an increasing sequence of compact convex sets whose union equals the interior of S and who have a positive distance from the boundary $\partial S = \partial K \cap S$. This situation is shown on Fig. 1.3. We have the following result.

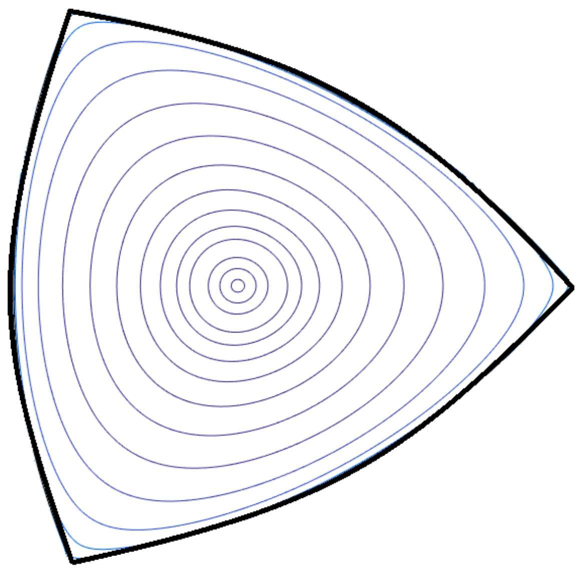

Figure 1.3: Intersections $S_\alpha = \alpha M \cap S^o$ for different α

Lemma 1.3.7. *Let $K \subset \mathbb{R}^n$ be a regular convex cone and $F : K^o \to \mathbb{R}$ a ν-logarithmically homogeneous smooth convex function for some $\nu > 0$. Then the following are equivalent:*

(a) the level surfaces of F are hyperbolic centro-affine surfaces which are asymptotic to K;

(b) for every sequence of points $x_k \in K^o$ tending to a boundary point $x \in \partial K$ we have $F(x_k) \to +\infty$.

Proof. $(a) \Rightarrow (b)$: Let $x \in \partial K$ be a non-zero point, and let S be a proper compact affine section of K containing x. Let $x_k \in K^o$ be a sequence of points tending to x. Project x_k radially on S to obtain a point $\tilde{x}_k \in S^o$. Then $\tilde{x}_k = \alpha_k x_k$ for some $\alpha_k > 0$, and $\lim_{k\to\infty} \alpha_k = 1$, because the sequence $\tilde{x}_k$ tends to the same point as the sequence x_k. By logarithmic homogeneity of F we have $F(\tilde{x}_k) = F(x_k) - \nu \log \alpha_k$, and $\lim_{k\to\infty} \nu \log \alpha_k = 0$. Therefore $F(x_k) \to +\infty$ if and only if $F(\tilde{x}_k) \to +\infty$ as $k \to +\infty$. However, $F(\tilde{x}_k) \to +\infty$, because the level set $\{x \in S^o \,|\, F(x) \leq \alpha\}$ has a positive distance from ∂S for every $\alpha > 0$.

Let now $x = 0$ and let $x_k \in K^o$ be a sequence of points tending to x. Choose a proper compact affine section S of K and an arbitrary point $y \in S^o$. Let $\alpha_k > 0$ be the unique number such that $x_k \in \alpha_k S$. The level set $\{x \in S^o \,|\, F(x) \leq F(y)\}$ is non-empty and has a positive distance from ∂S. It is hence closed by continuity of F, because every limit point has to be in S^o. It is also bounded and therefore compact, hence F attains a global minimum t^* on S^o. It follows that the minimum of F on the section αS is given by $t^* - \nu \log \alpha$ for every $\alpha > 0$. In particular, $F(x_k) \geq t^* - \nu \log \alpha_k \to +\infty$ for $k \to +\infty$, because $\lim_{k\to\infty} \alpha_k = 0$. This proves (b).

$(b) \Rightarrow (a)$: Since F is convex, its level surfaces are convex. By logarithmic homogeneity the function F is strictly decreasing along the rays of K^o, hence the level surfaces intersect every ray in exactly one point and are curved away from the origin, i.e., hyperbolic. Let S be a proper compact affine section of K. Then the restriction of F to S^o is convex and tends to $+\infty$ along every sequence of points tending to some point in ∂S. It follows that the level sets $\{x \in S^o \,|\, F(x) \leq \alpha\}$ have a positive distance from ∂S for every α. This shows (a). □

We are now ready to formulate the main result of this subsection.

Theorem 1.3.8. *Let $M \hookrightarrow \mathbb{R}^n$ be a smooth hyperbolic centro-affine hypersurface immersion which is asymptotic to some regular convex cone $K \subset \mathbb{R}^n$. Let C be the cubic form and h the centro-affine metric of the immersion, and let $||C||_\infty = \sup\{\frac{|C(x)[u,u,u]|}{(h(x)[u,u])^{3/2}} \,|\, x \in M, \; u \in T_xM, \; h(x)[u,u] \neq 0\}$ be the ∞-norm of C as measured in the metric h. Then for every $\nu > 0$ such that $||C||_\infty \leq \frac{2(\nu-2)}{\sqrt{\nu-1}}$, the function $F : K^o \to \mathbb{R}$ given by $F[\alpha M] = \{-\nu \log \alpha\}$ for every $\alpha > 0$ is a self-concordant logarithmically homogeneous barrier for K with parameter ν.*

On the other hand, let $F : K^o \to \mathbb{R}$ be a self-concordant logarithmically homogeneous barrier for some regular convex cone $K \subset \mathbb{R}^n$ with parameter ν. Then every level surface of F is a hyperbolic centro-affine hypersurface immersion, asymptotic to K, such that the ∞-norm of its cubic form, as measured in its affine metric, does not exceed the value $\frac{2(\nu-2)}{\sqrt{\nu-1}}$.

The theorem follows directly from Corollary 1.3.4 and Lemma 1.3.7.

The function $\nu \mapsto \frac{2(\nu-2)}{\sqrt{\nu-1}}$ is monotonic for $\nu \geq 2$ with inverse function $c \mapsto \frac{16+c^2+c\sqrt{16+c^2}}{8}$. The ∞-norm $||C||_\infty$ of the cubic form of the level surfaces of a self-concordant barrier F hence yields a lower bound $\frac{16+||C||_\infty^2+||C||_\infty\sqrt{16+||C||_\infty^2}}{8}$ on the barrier parameter. The relation between the ∞-norm of the cubic form and the barrier parameter is somewhat obscured by the fact that the barrier parameter is defined as the degree of logarithmic homogeneity. For given level surfaces of the barrier this degree can be chosen in an arbitrary manner, the sole condition to respect is inequality (1.2). Whether this inequality is tight or not has no influence on the barrier parameter. In order to highlight the role of the cubic form we shall introduce the following definition.

Definition 1.3.9. For a self-concordant logarithmically homogeneous barrier F, we define the *effective barrier parameter* of F as the lowest barrier parameter which can be achieved by dividing F by a positive constant $\alpha \geq 1$ while maintaining the property of self-concordance.

From Theorem 1.3.8 we then get immediately the following result.

Lemma 1.3.10. *Let F be a self-concordant logarithmically homogeneous barrier for some regular convex cone $K \subset \mathbb{R}^n$, $n \geq 2$, and let C be the centro-affine cubic form of any level surface of F. Let $||C||_\infty$ be the ∞-norm of C in the affine metric of the surface. Then the effective barrier parameter of F is given by $\frac{16+||C||_\infty^2+||C||_\infty\sqrt{16+||C||_\infty^2}}{8}$.* □

As mentioned in Subsection 1.2.3, the cubic form can be obtained by lowering an index of the difference tensor between the dual connection and the induced connection on the level surface. Hence $||C||_\infty$ is also the infinity norm of the difference between these connections. The barrier parameter can therefore be seen as estimating this difference from above.

1.3.2 Legendre duality and the conormal map

As mentioned in Subsection 1.1.1, to every self-concordant barrier F on a cone $K \subset \mathbb{R}^n$ with parameter ν one can associate a dual barrier F_* on the dual cone $K^* \subset \mathbb{R}_n$ with the same parameter ν. In this subsection we show that this notion of duality is closely linked to the duality in affine differential geometry defined by the conormal map.

By applying the first order optimality condition to the maximization problem $\max_{x \in K}(-\langle x, s\rangle - F(x))$ in Definition 1.1.3 we obtain the condition $s = -F'(x)$. Let us denote the corresponding map from K^o to $\mathbb{R}_n$ by Φ, $\Phi(x) = -F'(x)$. By [171, Theorem 2.4.4] the image of Φ is exactly the interior of the dual cone K^*. Positive definiteness of the Hessian F'' implies that Φ is actually a bijection between the interiors of K and K^*. Moreover, it is an isometry when the interiors of K, K^* are equipped with the Hessian metrics F'', F_*'', respectively [171, p.45],[163]. By the Definition 1.1.3 of the dual barrier we have

$$F(x) + F_*(\Phi(x)) = -\langle x, \Phi(x)\rangle = \langle x, F'(x)\rangle = -\nu, \tag{1.19}$$

and hence Φ maps level surfaces of F to level surfaces of F_*. As a consequence, the isometry Φ preserves the product structure in Proposition 1.3.1, but as is easily seen from (1.19), the orientation of the rays is reversed: a ray pointing away from the origin in the primal cone is mapped to a ray pointing towards the origin in the dual cone.

Let us now choose $\alpha \in \mathbb{R}$ and consider the level surface $F_\alpha = \{x \in K^o \mid F(x) = \alpha\}$. By definition the conormal map of the hypersurface immersion $F_\alpha \hookrightarrow \mathbb{R}^n$ maps the point $x \in F_\alpha$ to $p \in \mathbb{R}_n$ such that p is proportional to $F'(x)$ and $\langle p, -x \rangle = 1$. From the identity $F'(x)[x] = -\nu$ we obtain the explicit expression $p = \nu^{-1}F'(x) = -\nu^{-1}\Phi(x)$. We get the following result.

Lemma 1.3.11. *Let $F : K^o \to \mathbb{R}$ be a self-concordant barrier on a regular convex cone $K \subset \mathbb{R}^n$ with parameter ν. Let F_α be a level surface of F. Then the conormal map of the hypersurface immersion $F_\alpha \hookrightarrow \mathbb{R}^n$ is given by $-\nu^{-1}\Phi$, where Φ is the isometry between the interiors of K and K^* defined by Legendre duality.* □

1.3.3 Lorentz cones and hyperbolic barriers

As we have seen in Subsection 1.3.1, the effective barrier parameter of a self-concordant barrier with a given level surface is a monotonic function of the ∞-norm of the cubic form C of this surface. Here the lowest possible norm of the cubic form, $||C||_\infty = 0$, corresponds to the parameter value 2. In this subsection we shall consider this case in detail. We show that the only cone which admits a self-concordant barrier with parameter $\nu = 2$ is the Lorentz cone with its usual hyperbolic barrier.

By an extension of the Pick-Berwald theorem a centro-affine hypersurface with vanishing cubic form must be given by a quadratic equation [172, Section IV.6]. If it is in addition hyperbolic and asymptotic to a cone, it must be a hyperboloid and the cone must be linearly isomorphic to the Lorentz cone $L_n = \{x = (x_0, x_1, \dots, x_{n-1})^T \mid x_0 \geq \sqrt{\sum_{j=1}^{n-1} x_j^2}\}$. We immediately obtain the following result.

Lemma 1.3.12. *Let $F : K^o \to \mathbb{R}$ be a self-concordant logarithmically homogeneous barrier on a cone $K \subset \mathbb{R}^n$, $n \geq 2$. Then the value of its barrier parameter is at least 2. If its parameter equals 2, then there exists a basis of $\mathbb{R}^n$ such that in the corresponding coordinate system we have $K = L_n$ and $F(x) = -\log(x_0^2 - \sum_{j=1}^{n-1} x_j^2) + const.$* □

The cubic form measures the deviation of the level surface of a barrier F from a quadric. This is not surprising, since by Lemma 1.3.2 it is given by the third derivative F''', which measures the deviation of F from a quadratic function. We would like to stress an important difference between the affine and the projective viewpoint, however. If $F''' = 0$, then the level surfaces of F become paraboloids, while in the case of a vanishing cubic form they become hyperboloids. A paraboloid cannot be asymptotic to a convex cone, and that is why the self-concordance parameter cannot be zero. The "ideal barrier" in the affine case thus does not exist, while in the projective case it is a well-known object. There are also practical consequences. In the methods using affine scaling each iteration consists of a Newton-type step in an affine space. This step can never be exact, because the deviation of F from a quadratic function is always non-zero. In the projective case this drawback disappears.

Let us now compute the affine metric on the hyperboloid. We project the hyperboloid radially to the affine section of L_n given by $x_0 = 1$. The hyperboloid is thus mapped to the open $(n-1)$-dimensional unit ball, parameterized by the coordinates $x = (x_1, \dots, x_{n-1})^T$. The restriction of F to this section is given by $f(x) = -\log(1 - \sum_{j=1}^{n-1} x_j^2)$. Formula (1.17) then yields

$$h = \frac{1}{2} \cdot \frac{2(1 - ||x||^2)I + 4xx^T}{(1 - ||x||^2)^2} - \frac{1}{4} \cdot \frac{2x}{1 - ||x||^2} \cdot \frac{2x^T}{1 - ||x||^2} = \frac{(1 - ||x||^2)I + xx^T}{(1 - ||x||^2)^2}$$

for the affine metric. Thus we obtain the Beltrami-Klein model of hyperbolic space. The geodesics of the affine metric in this model are straight lines.

1.4 Canonical barrier

1.4.1 Introduction

In this section we present the main result of [93], the construction of the *canonical barrier*. This result is a consequence of a deep theorem in affine differential geometry, the *Calabi theorem*. The connections which have been made in the previous section between affine differential geometry and logarithmically homogeneous functions allow to rewrite the Calabi theorem as an existence and uniqueness result for the solution of a certain PDE on the interior of an arbitrary regular convex cone. That this solution is a self-concordant barrier will then be deduced from a curvature estimate.

The canonical barrier is a universal construction, in the sense that it assigns a self-concordant barrier to every regular convex cone. It is, however, not the first such construction. In [171, Section 2.5] Nesterov and Nemirovski introduce the *universal barrier*. This is a self-concordant logarithmically homogeneous barrier which exists and is unique, up to an additive constant[1], for any regular convex cone $K \subset \mathbb{R}^n$. Its barrier parameter ν is of order $O(n)$, i.e., there exists a constant $C > 0$, independent of K and n, such that ν can be chosen equal to Cn [171, Theorem 2.5.1, Remark 2.5.1, p.50]. In [77, Cor. 4.1, p.868] Güler showed that the universal barrier on a regular convex cone K is, up to an additive constant, equal to C times the logarithm of the *characteristic function* of K. The latter object was introduced by Koranyi in [126] and is given by the expression

$$\varphi(x) = \int_{K^*} e^{-\langle x,y\rangle} dy \tag{1.20}$$

for $x \in K^o$. A similar function was introduced by Koecher in [121] on so-called *domains of positivity*, which are self-dual cones[2] K such that the isomorphism between K and K^* is a self-adjoint map. Some interesting properties of a particular level surface of the characteristic function, the *constant volume envelope*, have been deduced in [73, Sections 3,4]. From definition (1.20) it follows that the universal barrier on a product cone is the sum of the universal barriers on the factor cones, thus it is compatible with the operation of taking product cones. Moreover, it is invariant with respect to any automorphism of K with determinant 1, i.e., the unimodular automorphism subgroup. Note that this property ensures that for homogeneous cones, the level surfaces of the universal barrier are the orbits of the unimodular subgroup of automorphisms. The universal barrier does not behave well with respect to duality, however: in [6] an example of a self-dual cone was given on which the duality mapping defined by the universal barrier is not involutive, and hence the universal barrier is not equal to its dual barrier.

The canonical barrier is another self-concordant logarithmically homogeneous barrier which exists and is unique, up to an additive constant, for every regular convex cone. It can be obtained as the potential of a natural Hessian metric on the interior of K, the *Cheng-Yau metric*, which was first introduced in [42]. The canonical barrier shares with the universal barrier all invariance properties, but in addition it behaves well under duality. It can be represented as the solution of the PDE $\log\det F'' = 2F$ with boundary condition $F|_{\partial K} = +\infty$. On homogeneous cones its level surfaces equal those of the universal barrier, and on this class of cones the two barriers are essentially the same object. That the universal barrier on homogeneous cones satisfies above PDE has been shown already by Güler [77, Theorem 4.4, p.868]. Güler also conjectured that the solution of this PDE defines a self-concordant barrier for general cones.

We give a precise statement of the Calabi theorem on affine spheres in Subsection 1.4.2, where we also list some properties of the Cheng-Yau metric. As with the universal barrier, which can easily be obtained as the logarithm of the long-known characteristic function of K, the difficulty with the canonical barrier is to show that it is indeed a barrier, in particular, that it satisfies the self-concordance condition (1.2). The proof of this fact is the main result of this section and will be accomplished in Subsection 1.4.3. It turns out that the barrier parameter of the canonical barrier equals the dimension n of K. Like with the universal barrier, it may be possible to lower the barrier parameter of the canonical barrier by multiplying it by a positive constant smaller than 1, i.e., the effective barrier parameter of the canonical barrier may be strictly smaller than n. In Subsection 1.4.4 we give expressions for

[1] This constant is determined by the choice of the volume form on K^* when integrating (1.20).

[2] Here we understand self-dual in the wider sense that K is linearly isomorphic to its dual cone K^*.

the canonical barrier on a class of cones including the 3-dimensional power cone in order to provide nontrivial examples.

The self-concordance of the canonical barrier has been obtained independently by Daniel Fox in [72]. In that paper he applies methods that are more sophisticated than those used here, and he obtains more general results. He also mentions that the barrier parameter of the canonical barrier can be obtained by the easier method presented here.

1.4.2 Affine hyperspheres and the Calabi theorem

A proper affine sphere is a hypersurface in $\mathbb{R}^n$ whose affine normals all meet in a point, which may be conveniently considered as the origin. The Calabi theorem, originally formulated as the *Calabi conjecture* in [39, p.22], is an existence and uniqueness result on hyperbolic affine spheres. The conjecture has been proven by the efforts of many authors, a synthesis of the proof is given in [135, Section 2].

Theorem 1.4.1 (Calabi theorem). *Let $K \subset \mathbb{R}^n$ be a regular convex cone. Then there exists a unique foliation of the interior K^o into a family of mutually homothetic proper hyperbolic affine hyperspheres which are asymptotic to K.*

Since the direction of the affine normal is invariant under affine transformations of $\mathbb{R}^n$, we have that this foliation is invariant under linear isomorphisms of the cone. Let us formalize this result as follows.

Corollary 1.4.2. *Let $A : \mathbb{R}^n \to \mathbb{R}^n$ be an invertible linear map, let $K \subset \mathbb{R}^n$ be a regular convex cone, and let $K' = A[K]$ be its image. Then A maps the foliation of K^o into proper affine spheres which are asymptotic to K to the foliation of $\operatorname{int} K'$ into proper affine spheres which are asymptotic to K'.* □

The Calabi theorem is closely linked to another existence and uniqueness result involving regular convex domains in $\mathbb{R}^n$. Here *regular* means that the domain is non-empty and does not contain any line.

Proposition 1.4.3. *Let $\Omega \subset \mathbb{R}^n$ be a regular convex domain. Then there exists a unique locally strongly convex smooth solution $F : \Omega \to \mathbb{R}$ of the PDE*

$$\log \det F'' = 2F \tag{1.21}$$

with boundary condition $\lim_{x \to \partial\Omega} F(x) = +\infty$.

Existence of the solution is proven in [42, Theorem 4.4, p.365], while uniqueness follows from [41, Proposition 5.5, p.528]. The Hessian F'' of the solution defines a complete Einstein-Hessian metric on Ω, the *Cheng-Yau metric*. Here *Einstein-Hessian* means that an appropriate complexification of the Riemannian manifold has its Ricci curvature tensor equal to a multiple of the metric tensor [196, Def. 3.3, p.41].

For domains Ω which can be represented as a product of two domains, we have the following evident result.

Lemma 1.4.4. *Let $\Omega_n \subset \mathbb{R}^n$, $\Omega_m \subset \mathbb{R}^m$ be regular convex domains, and let $F_n : \Omega_n \to \mathbb{R}$, $F_m : \Omega_m \to \mathbb{R}$ be the solutions of the boundary value problem in Proposition 1.4.3 for the domains Ω_n, Ω_m. Then the solution of this boundary value problem on the product domain $\Omega = \Omega_n \times \Omega_m$ is given by $F(x, y) = F_n(x) + F_m(y)$.* □

Equation (1.21) is invariant with respect to affine transformations of $\mathbb{R}^n$. It can be checked directly that if $x \mapsto \tilde{x} = Ax + b$ is an affine coordinate transformation of $\mathbb{R}^n$, then the solution $\tilde{F}(\tilde{x})$ of (1.21) in the new coordinates is given by

$$\tilde{F}(\tilde{x}) = F(x) - \log|\det A|. \tag{1.22}$$

In particular, F remains invariant if $\det A = \pm 1$, i.e., if the affine map preserves the volume from on $\mathbb{R}^n$. If no distinguished volume form is given, then the solution of (1.21) may change by an additive constant under coordinate transformations, due to the coordinate dependence of the definition of the determinant.

We wish to use the solution F as a barrier for conic programming, and hence our interest is in the case when the domain Ω is the interior of a regular convex cone $K \subset \mathbb{R}^n$. Then the homothety $x \mapsto \tilde{x} = \alpha x$ is an automorphism of K^o for all $\alpha > 0$. We therefore obtain from (1.22) that $F(\alpha x) = F(x) - n \log \alpha$ for all $\alpha > 0$, i.e., the solution F satisfies (1.3) with $\nu = n$. That the potential of the Cheng-Yau metric on regular convex cones is logarithmically homogeneous was already mentioned in [139, pp.426–427] without a detailed proof. By Lemma 1.3.7 and by virtue of the boundary condition in Proposition 1.4.3 it follows that the level surfaces of the solution F of (1.21) form a family of mutually homothetic centro-affine surfaces which are asymptotic to the cone K and foliate its interior. Sasaki [188, pp.73–74] has shown that these level surfaces are exactly the hyperbolic affine hyperspheres from the Calabi Theorem 1.4.1. This relation has been later rediscovered as the main result of [139]. A more comprehensive review of the literature and an independent derivation can be found in [72], where the solution of (1.21) was termed *canonical potential* of the cone K.

The solution F shares with the universal barrier of Nesterov and Nemirovski its existence and uniqueness as well as the invariance properties with respect to unimodular automorphisms and the behaviour under the operation of taking products of cones.

In contrast to the universal barrier, whose dual barrier on the dual cone is in general not the universal barrier of the dual cone, affine hyperspheres also behave well under duality. In particular, we have the following result.

Proposition 1.4.5. *[74, Prop. 1, p.391] Let $M \subset \mathbb{R}^n$ be an affine hypersphere. Then the image of M under the conormal map is also an affine hypersphere.*

By Lemma 1.3.11 the conormal map is proportional to the isometry Φ between the interiors of the cones K, K^* defined by Legendre duality. Therefore Φ maps the foliation of K^o by affine spheres to the corresponding foliation of the interior of K^*.

1.4.3 Self-concordance

In this subsection we prove the self-concordance of the solution F of equation (1.21). By Theorem 1.3.8 this property is equivalent to the uniform boundedness of the ∞-norm of the cubic form of the level surfaces of F. However, in the previous subsection we have seen that these level surfaces are exactly the affine spheres which are asymptotic to the cone K. In [135, Corollary 2.6.5, p.128] a uniform bound on the 2-norm of the cubic form of hyperbolic affine spheres has been deduced by a purely algebraic argument from estimates of the Ricci curvature of the affine metric. We shall provide a similar argument for bounding the ∞-norm. The proof provided here is somewhat different from that in [93] and has been published in the related paper [91].

The Ricci curvature tensor Ric_h of the centro-affine metric h on complete hyperbolic affine spheres of dimension $n-1$ satisfies the inequalities $-(n-2)h \preceq \mathrm{Ric}_h \preceq 0$. The first inequality comes from [39, eq. (2.7), p.24], the second one from [39, Theorem 5.1, p.31].

The utility of these bounds comes from the fact that the Ricci tensor and the cubic form are algebraically dependent. The Ricci curvature of the affine metric is explicitly given by [191, p.3]

$$R_{ij} = -(n-2)h_{ij} + \frac{1}{4}h^{kr}h^{ls}C_{ikl}C_{jrs}, \tag{1.23}$$

where h^{ij} is, as usual, the inverse of the matrix h_{ij} of the centro-affine metric.

Moreover, the cubic form of an affine sphere satisfies the *apolarity condition* [172, Section II, Theorem 4.4]

$$h^{ij}C_{ijk} = 0. \tag{1.24}$$

We shall need the following auxiliary inequality.

Lemma 1.4.6. *Let $n \geq 3$ and $\lambda_1, \dots, \lambda_{n-2} \leq 1$ be such that $\sum_{i=1}^{n-2} \lambda_i = -1$. Then*

$$\frac{3}{4}\sum_{i=1}^{n-2} \lambda_i^2 - \frac{1}{2}\sum_{i=1}^{n-2} \lambda_i^3 \geq \frac{3n-4}{4(n-2)^2}.$$

Proof. Define $c_i = (n-2)\lambda_i + 1$. Then $\sum_{i=1}^{n-2} c_i = 0$ and $c_i \leq n-1$ for all i. It follows that $c_i^3 \leq (n-1)c_i^2$ for all i. We then have

$$\begin{aligned}
\frac{3}{4}\sum_{i=1}^{n-2}\lambda_i^2 - \frac{1}{2}\sum_{i=1}^{n-2}\lambda^3 - \frac{3n-4}{4(n-2)^2} &= \frac{3}{4(n-2)^2}\sum_{i=1}^{n-2}(c_i-1)^2 - \frac{1}{2(n-2)^3}\sum_{i=1}^{n-2}(c_i-1)^3 - \frac{3n-4}{4(n-2)^2} \\
&= \left(\frac{3}{4(n-2)} + \frac{1}{2(n-2)^2} - \frac{3n-4}{4(n-2)^2}\right) - \left(\frac{3}{2(n-2)^2} + \frac{3}{2(n-2)^3}\right)\sum_{i=1}^{n-2} c_i \\
&\quad + \left(\frac{3}{4(n-2)^2} + \frac{3}{2(n-2)^3}\right)\sum_{i=1}^{n-2} c_i^2 - \frac{1}{2(n-2)^3}\sum_{i=1}^{n-2} c_i^3 \\
&\geq \left(\frac{3n}{4(n-2)^3} - \frac{n-1}{2(n-2)^3}\right)\sum_{i=1}^{n-2} c_i^2 = \frac{n+2}{4(n-2)^3}\sum_{i=1}^{n-2} c_i^2 \geq 0.
\end{aligned}$$

This completes the proof. □

For $n = 2$ every regular convex cone is isomorphic to $\mathbb{R}_+^2$, which is homogeneous. Therefore the condition $n \geq 3$ in the lemma does not restrict generality.

Corollary 1.4.7. *Let B be a real symmetric $(n-1)\times(n-1)$ matrix with vanishing trace. Then $\frac{3}{4}\lambda_{\max}(B)\operatorname{tr} B^2 - \frac{1}{2}\operatorname{tr} B^3 \geq \frac{n(n-1)}{4(n-2)^2}\lambda_{\max}^3(B)$.*

Proof. If $\lambda_{\max}(B) = 0$, then $B = 0$ and the assertion of the corollary is evident.

Suppose now that $\lambda_{\max}(B) > 0$. Let $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-2} \leq \lambda_{n-1} = 1$ be the eigenvalues of the matrix $\tilde{B} = \frac{B}{\lambda_{\max}(B)}$ in increasing order. Then $\sum_{i=1}^{n-2}\lambda_i = -1$ and $\lambda_i \leq 1$ for all i. We then have

$$\begin{aligned}
\frac{3}{4}\lambda_{\max}(B)\operatorname{tr} B^2 - \frac{1}{2}\operatorname{tr} B^3 - \frac{n(n-1)}{4(n-2)^2}\lambda_{\max}^3(B) &= \lambda_{\max}^3(B)\left(\frac{3}{4}\operatorname{tr}\tilde{B}^2 - \frac{1}{2}\operatorname{tr}\tilde{B}^3 - \frac{n(n-1)}{4(n-2)^2}\right) \\
&= \lambda_{\max}^3(B)\left[\frac{3}{4}\left(1 + \sum_{i=1}^{n-2}\lambda_i^2\right) - \frac{1}{2}\left(1 + \sum_{i=1}^{n-2}\lambda_i^3\right) - \frac{n(n-1)}{4(n-2)^2}\right] \geq 0,
\end{aligned}$$

where the inequality comes from the preceding lemma. □

We are now in a position to estimate the norm $||C(p)||_\infty = \max_{u\in T_pM:\ h(p)[u,u]=1} C(p)[u,u,u]$ of the cubic form at a point p of a complete hyperbolic affine sphere M of dimension $n-1$. Let $p \in M$ be an arbitrary point, let $\xi \in T_pM$ be a maximizer of the cubic form on the unit sphere in T_pM. We shall now drop the argument p from the tensors h, C.

Define the symmetric $(0,2)$-tensor $B_{ij} = C_{ijk}\xi^k$. Note that B is traceless by the apolarity condition (1.24), i.e., $h^{ij}B_{ij} = 0$, and that $B_{ij}\xi^i\xi^j = ||C||_\infty$. Moreover, by the optimality conditions [135, Lemma 2.2.3.19, p.106] on ξ we have that $B_{ij}\xi^i\eta^j = 0$ and $B_{ij}\eta^i\eta^j \leq \frac{1}{2}B_{ij}\xi^i\xi^j \leq ||C||_\infty$ for every unit length vector η which is orthogonal to ξ. It follows that ξ is also a maximizer of B on the unit sphere in T_pM. In particular, we have

$$B_{ij}\xi^j = ||C||_\infty h_{ij}\xi^j \tag{1.25}$$

as the first order optimality condition, and $||C||_\infty$ is the maximal eigenvalue of the matrix of B in any orthonormal basis of T_pM.

In an orthonormal basis of T_pM the matrix of the centro-affine metric h is given by the identity matrix I_{n-1}. Let $\{\xi, \eta_1, \dots, \eta_{n-2}\}$ be an orthonormal basis of T_pM, then we have

$$\begin{aligned}
||C||_\infty^2 &= (B_{ij}\xi^i\xi^j)^2 = \left(-\sum_{k=1}^{n-2} B_{ij}\eta_k^i\eta_k^j\right)^2 \leq (n-2)\sum_{k=1}^{n-2}(B_{ij}\eta_k^i\eta_k^j)^2 \leq (n-2)\sum_{k=1}^{n-2} B_{il}B_j^l\eta_k^i\eta_k^j \\
&= (n-2)\left(B_{il}B^{li} - B_{il}B_j^l\xi^i\xi^j\right) = (n-2)\left(C_{ilj}C_k^{li}\xi^j\xi^k - ||C||_\infty^2\right) \\
&= 4(n-2)(R_{jk} + (n-2)h_{jk})\xi^j\xi^k - (n-2)||C||_\infty^2 \leq 4(n-2)^2 - (n-2)||C||_\infty^2.
\end{aligned}$$

Here the second equality holds because B is traceless. The next two inequalities are due to Bunjakowski-Schwarz. The third equality holds because $\sum_{k=1}^{n-2} \eta_k \eta_k^T = I_{n-1} - \xi\xi^T$. We used (1.25) and (1.23) in the last two equalities, respectively, and the non-positivity of the Ricci curvature [39, Theorem 5.1, p.31] in the last inequality.

Since the point $p \in M$ was arbitrary, it follows that $||C||_\infty \leq \frac{2(n-2)}{\sqrt{n-1}}$. Theorem 1.3.8 then yields the following result.

Lemma 1.4.8. *Let $K \subset \mathbb{R}^n$ be a regular convex cone and let F be the solution of* (1.21) *on K^o. Then F is a self-concordant logarithmically homogeneous barrier on K with barrier parameter $\nu = n$.* □

Definition 1.4.9. We call the barrier given by the solution F of (1.21) the *canonical barrier.*

Corollary 1.4.10. *Let $K \subset \mathbb{R}^n$ be a regular convex cone. Then the barrier parameter of the optimal barrier on K does not exceed n.* □

We shall summarize the obtained results in the following theorem.

Theorem 1.4.11. *Let $K \subset \mathbb{R}^n$ be a regular convex cone. Fix a basis of $\mathbb{R}^n$ and consider in the corresponding coordinate system the boundary value problem*

$$\log\det\left(\frac{\partial^2 F(x)}{\partial x^2}\right) = 2F(x),\ x \in K^o; \qquad F|_{\partial K} = +\infty. \tag{1.26}$$

This problem has a unique locally strictly convex solution $F : K^o \to \mathbb{R}$. This solution is a smooth logarithmically homogeneous self-concordant barrier, the canonical barrier, on K with barrier parameter n, and gives rise to an Einstein-Hessian metric F'' on K^o. It is invariant under unimodular basis changes of $\mathbb{R}^n$ and is determined up to an additive constant under arbitrary basis changes. In particular, it is invariant under the group of unimodular automorphisms of the cone K. The dual barrier F_* : $\operatorname{int} K^* \to \mathbb{R}$ differs from the solution of the above boundary value problem on the dual cone K^* by an additive constant, and hence its Hessian is an Einstein-Hessian metric on $\operatorname{int} K^*$. If $K = K_1 \times K_2$ is a product of regular convex cones, then the canonical barrier F on K is the sum of the canonical barriers on the individual factor cones K_1, K_2. □

From the invariance properties it follows that the canonical barrier has the same level surfaces as the universal barrier on the class of homogeneous cones, see also [77, Theorem 4.4, p.868]. In particular, all classical barriers used in interior-point methods for solving conic programs over irreducible symmetric cones have the same level surfaces as the canonical barrier. This shows at the same time that the effective barrier parameter of the canonical barrier may be strictly smaller than the dimension n of the cone. Below in Section 1.4.4 we shall demonstrate this on the example of a non-homogeneous cone.

The canonical barrier is in general not optimal, i.e., on a given cone K there may exist self-concordant barriers with parameter strictly smaller than the effective parameter of the canonical barrier. An example is the symmetric cone $L_3 \times \mathbb{R}_+ = \left\{x \in \mathbb{R}^4 \,|\, x_1 \geq \sqrt{x_2^2 + x_3^2},\ x_4 \geq 0\right\}$. The optimal barrier $-\log(x_1^2 - x_2^2 - x_3^2) - \log x_4$ on this cone has barrier parameter $\nu = 3$, while the canonical barrier $-\frac{3}{2}\log\frac{x_1^2 - x_2^2 - x_3^2}{3} - \log x_4$ has effective barrier parameter 4.

1.4.4 Examples

In this subsection we provide analytic expressions for the canonical barrier on several non-homogeneous cones. As this barrier is a solution of a non-linear PDE, such expressions are notoriously difficult to obtain and likely do not exist is most cases. Most promising are cones K possessing a rich continuous symmetry group, which allows to reduce the dimension of the PDE by using its invariance properties. In particular, if the orbits of the automorphism group of the cone have codimension 1, then the PDE can be reduced to an ordinary differential equation (ODE). Here we consider the canonical barrier on the *power cone* in arbitrary dimension and on 3-dimensional cones with a non-trivial symmetry group, which we call *semi-homogeneous*. In general, the canonical barrier can be expressed by elliptic functions in these cases. These results have been published in [93] and [92], respectively. In recent years a promising approach based on loop groups has been developed to compute the hyperbolic affine spheres which are asymptotic to general 3-dimensional cones [62, 137, 136], by using the especially rich complex-analytic structure of these surfaces [217, 198].

Generalized power cone

Let $n \geq 3$, let $p, q \in (1, +\infty)$ such that $\frac{1}{p} + \frac{1}{q} = 1$, and consider the cone

$$K = \left\{ (x, y, z^T)^T \in \mathbb{R}^n \,|\, x \geq 0,\ y \geq 0,\ ||z||_2 \leq (\sqrt{p}x)^{1/p}(\sqrt{q}y)^{1/q} \right\}.$$

For $n = 3$, i.e., z scalar, we obtain a linear image of the *power cone*, a well-known non-homogeneous self-dual cone. For general n the cones K have been considered in [40, p.94] and are also self-dual.

The cone K is invariant under unimodular automorphisms of the form

$$x \mapsto \alpha^{-1-\frac{n-2}{q}}x, \quad y \mapsto \alpha^{1+\frac{n-2}{p}}y, \quad z \mapsto \alpha^{\frac{1}{q}-\frac{1}{p}}Uz,$$

where $\alpha > 0$ and U is an orthogonal matrix of size $n-2$. Hence the canonical barrier on K, which must be invariant under these automorphisms and satisfies (1.3) with $\nu = n$, can be written in the form

$$F(x, y, z) = -\left(1 + \frac{n-2}{p}\right)\log(\sqrt{p}x) - \left(1 + \frac{n-2}{q}\right)\log(\sqrt{q}y) + \phi\left((\sqrt{p}x)^{-1/p}(\sqrt{q}y)^{-1/q}||z||\right),$$

where $\phi : [0, 1) \to \mathbb{R}$ is a function of a scalar variable such that $\lim_{t=1}\phi(t) = +\infty$.

Setting $t = (\sqrt{p}x)^{-1/p}(\sqrt{q}y)^{-1/q}||z||$ and inserting above expression into PDE (1.21) and integrating, we obtain

$$\log t = -\frac{1}{2p}\log\left(1 + \frac{p+n-2}{\rho}\right) - \frac{1}{2q}\log\left(1 + \frac{q+n-2}{\rho}\right),$$
$$\phi = \frac{1}{2}\left(1 + \frac{n-2}{p}\right)\log(\rho + p + n - 2) + \frac{1}{2}\left(1 + \frac{n-2}{q}\right)\log(\rho + q + n - 2),$$

where $\rho = t\frac{d\phi}{dt}$. These relations give a parametric representation of the solution curve $(t, \phi(t))$, with the parameter ρ ranging from 0 to $+\infty$. It is also seen that for $p \neq 2$ there exists no closed-form expression for $\phi(t)$.

Numerical calculations indicate the following conjecture.

Conjecture 1.4.12. *The effective barrier parameter of the canonical barrier F on the cone K equals* $\nu = \frac{n \max(p,q)}{\max(p,q)+n-2}$.

The conjecture can be formulated equivalently as the nonnegativity of a certain multivariate polynomial. For $n = 3$, i.e., when K is isomorphic to the power cone, this polynomial can be shown to be a sum of squares. The corresponding value $\nu = \frac{3\max(p,q)}{\max(p,q)+1}$ of the barrier parameter is smaller than the best-known values $\nu = 3$ (analytically) and $\nu = 3 - \frac{2}{\max(p,q)}$ (numerically) reported in [40, Section 3.1]. In Fig. 1.4 the self-concordance parameters of the barriers proposed in [40] and of the canonical barrier are depicted as a function of p.

Homogenized epigraph of the exponential function

Consider the closure of the homogenization of the epigraph of the exponential function given by

$$K = \{(x, y, 0)^T \,|\, x \leq 0,\ y \geq 0\} \cup \left\{ (x, y, z)^T \,\middle|\, \frac{y}{z} \geq \exp\frac{x}{z},\ z > 0 \right\}.$$

This cone is invariant with respect to the unimodular subgroup of automorphisms $(x, y, z) \mapsto (e^t(x - 3tz), e^{-2t}y, e^t z)$, $t \in \mathbb{R}$. Invariance of the canonical barrier with respect to this group leads to the Ansatz

$$F(x, y, z) = -\log y - 2\log z + \phi\left(\log\frac{y}{z} - \frac{x}{z}\right).$$

Here $\phi : \mathbb{R}_{++} \to \mathbb{R}$ is a scalar function. Inserting F into (1.21) and integrating, we obtain the parametric representation

$$\begin{pmatrix} t \\ \phi \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \log(1+\kappa) + 2\kappa \\ \log(1+\kappa) - 3\log\kappa \end{pmatrix}$$

of the function $\phi(t)$, where $\kappa = -\frac{1}{\dot\phi}$ runs through all positive reals.

It is not hard to check that the effective barrier parameter of the canonical barrier for this cone equals 3.

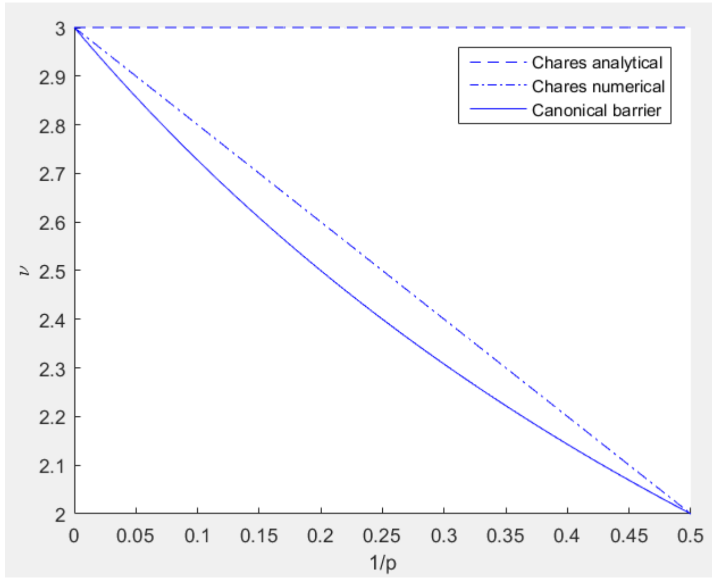

Figure 1.4: Effective self-concordance parameters of barriers for the power cone

Asymmetric power cone

Consider the cone

$$K = \{(x,y,z)^T \mid -\alpha x^{1/p}y^{1/q} \leq z \leq x^{1/p}y^{1/q}\}$$

with $\alpha \in (0,1]$, $p \in [2,+\infty)$, and $q \in (1,2]$ such that $\frac{1}{p}+\frac{1}{q}=1$. This cone is invariant with respect to the unimodular group of automorphisms $(x,y,z) \mapsto (e^{(2p-1)t}x, e^{-(p+1)t}y, e^{-(p-2)t}z)$. The canonical barrier on K must be invariant with respect to this symmetry group and therefore has the form

$$F = -\frac{p+1}{p}\log x - \frac{q+1}{q}\log y + \phi\left(x^{-1/p}y^{-1/q}z\right), \tag{1.27}$$

where $\phi : (-\alpha, 1) \to \mathbb{R}$ is a scalar function.

In order to represent this function, we shall need the cubic polynomial $P(\xi) = 4(p+q)(\xi-1)(\xi+p)(\xi+q)+c^2$ depending on a parameter $c \in [0, 2(p+q))$ which we shall choose further below. This polynomial has 3 real roots ξ_1, ξ_2, ξ_3 satisfying $1 \geq \xi_1 > 0 > \xi_2 \geq -q \geq -p \geq \xi_3$. Define the function

$$G(\zeta) = \left(\frac{1}{\zeta^2+\xi_1-1} - \frac{1}{p(\zeta^2+\xi_1+p)} - \frac{1}{q(\zeta^2+\xi_1+q)}\right)\left(\zeta - \frac{\sqrt{(1-\xi_1)(1-\xi_2)(1-\xi_3)}}{\sqrt{(\zeta^2+\xi_1-\xi_2)(\zeta^2+\xi_1-\xi_3)}}\right).$$

This function has a simple pole at $\zeta = -\sqrt{1-\xi_1}$ with residue 1 and is analytic elsewhere on $\mathbb{R}$. Left of the pole it is negative, right of the pole positive, decreasing in absolute value as $|\zeta|^{-3}$. We now choose the parameter c such that

$$\log \alpha = -\int_0^{+\infty} G(\zeta - \sqrt{1-\xi_1}) + G(-\zeta - \sqrt{1-\xi_1})\, d\zeta.$$

The pole of the function G cancels out in the integrand and the integral is finite and positive. It can be checked that $c \in [0, 2(p+q))$ is mapped bijectively to $\alpha \in (0,1]$ by this equation.

A parametric description of the function $\phi(t)$ is then given by

$$t = \begin{cases} \exp\left(-\int_\zeta^{+\infty} G(\zeta)\, d\zeta\right), & \zeta \in (-\sqrt{1-\xi_1}, +\infty), \\ -\alpha \cdot \exp\left(\int_{-\infty}^\zeta G(\zeta)\, d\zeta\right), & \zeta \in (-\infty, -\sqrt{1-\xi_1}), \\ 0, & \zeta = -\sqrt{1-\xi_1}, \end{cases}$$

$$\phi = \log \frac{\sqrt{(1-\xi_1)(1-\xi_2)(1-\xi_3)} + \zeta\sqrt{(\zeta^2+\xi_1-\xi_2)(\zeta^2+\xi_1-\xi_3)}}{t\sqrt{p+q}}.$$

The integrals over $G(\zeta)$ can be expressed by elliptic functions [38], see also [2].

Symmetric power cone

Specializing the value of α from the previous subsection to 1 leads to the power cone

$$K = \{(x,y,z)^T \,|\, |z| \leq x^{1/p}y^{1/q}\}.$$

The value $\alpha = 1$ corresponds to the value $c = 0$, which yields the roots $\xi_1 = 1$, $\xi_2 = -q$, $\xi_3 = -p$ of the polynomial P. The canonical barrier of K is still given by (1.27), but the integrals have analytic expressions and the parametric representation of the scalar function $\phi : (-1,1) \to \mathbb{R}$ can be simplified. Namely, we have

$$\begin{pmatrix} t \\ \phi \end{pmatrix} = \begin{pmatrix} (\zeta^2+p+1)^{-\frac{1}{2p}}(\zeta^2+q+1)^{-\frac{1}{2q}}\zeta \\ -\frac{1}{2}\log(p+q) + \frac{p+1}{2p}\log(\zeta^2+p+1) + \frac{q+1}{2q}\log(\zeta^2+q+1) \end{pmatrix}$$

with parameter $\zeta \in \mathbb{R}$.

Intersection of the power cone with a half-space

For the value $\alpha = 0$ we obtain the cone

$$K = \{(x,y,z)^T \,|\, 0 \leq z \leq x^{1/p}y^{1/q}\},$$

which is an intersection of the power cone with the closed half-space given by the inequality $z \geq 0$. The canonical barrier for this cone is given by (1.27) with the function $\phi : (0,1) \to \mathbb{R}$ given parametrically by

$$\begin{aligned} t &= (\sqrt{\xi+p+q-1}+\sqrt{p+q})\left(\frac{\xi}{(\sqrt{\xi+p+q-1}+\sqrt{p+q-1})^2}\right)^{\frac{\sqrt{p+q-1}}{\sqrt{p+q}}} \cdot \\ &\cdot \left(\frac{\sqrt{\xi+p+q-1}+\sqrt{q-1}}{\xi+p}\right)^{\frac{1}{p}}\left(\frac{\sqrt{\xi+p+q-1}+\sqrt{p-1}}{\xi+q}\right)^{\frac{1}{q}}, \\ \phi &= \log\left(1+\frac{\xi\sqrt{\xi+p+q-1}}{\sqrt{p+q}}\right) - \log t, \end{aligned}$$

where the parameter runs through $\xi \in (0,+\infty)$. The effective barrier parameter of the canonical barrier for this cone equals 3.

Intersection of L_3 with a half-space

For the special case $p = q = 2$ in the previous subsection we get the cone

$$K = \{(x,y,z)^T \,|\, 0 \leq z \leq \sqrt{xy}\},$$

which is isomorphic to the cone built over a half-disc. The canonical barrier for K is given by (1.27) with the parametrization of ϕ simplifying to

$$\begin{aligned} t &= \left(\frac{\sqrt{\xi}}{\sqrt{\xi+3}+\sqrt{3}}\right)^{\sqrt{3}} \cdot \frac{(\sqrt{\xi+3}+2)(\sqrt{\xi+3}+1)}{\xi+2}, \\ \phi &= \log\left(1+\frac{\xi\sqrt{\xi+3}}{2}\right) + \sqrt{3}\log\frac{\sqrt{\xi+3}+\sqrt{3}}{\sqrt{\xi}} - \log\frac{(\sqrt{\xi+3}+2)(\sqrt{\xi+3}+1)}{\xi+2}, \end{aligned}$$

with parameter $\xi \in (0,+\infty)$. The effective barrier parameter of the canonical barrier for this cone equals 3.

Power cone plus orthant

The cone dual to the intersection of the power cone with a half-space is isomorphic to

$$K = \{(x, y, z)^T \mid z \geq -x^{1/p} y^{1/q}\},$$

which equals the sum of the power cone and the nonnegative orthant of $\mathbb{R}^3$. The canonical barrier for this cone is given by (1.27) with the function $\phi : (-1, +\infty) \to \mathbb{R}$ given parametrically by

$$\begin{aligned} t = &\frac{1-\xi}{\sqrt{\xi+p+q-1}+\sqrt{p+q}} \left(\frac{\sqrt{\xi+p+q-1}+\sqrt{p+q-1}}{\sqrt{\xi+p+q-1}-\sqrt{p+q-1}} \right)^{\frac{\sqrt{p+q-1}}{\sqrt{p+q}}} \cdot \\ &\cdot (\sqrt{\xi+p+q-1}+\sqrt{q-1})^{-\frac{1}{p}} (\sqrt{\xi+p+q-1}+\sqrt{p-1})^{-\frac{1}{q}}, \\ \phi = \log &\frac{\sqrt{p+q}-\xi\sqrt{\xi+p+q-1}}{\sqrt{p+q}\,t} = \log \frac{1+\xi+\frac{\xi^2}{p+q}}{1+\xi\sqrt{1+\frac{\xi-1}{p+q}}} + \log \frac{1-\xi}{t}, \end{aligned}$$

where the parameter runs through $\xi \in (0, +\infty)$. The effective barrier parameter of the canonical barrier for this cone equals 3.

Sum of L_3 and an orthant

Specializing to $p = q = 2$ in the previous subsection we get

$$K = \{(x, y, z)^T \mid z \geq -\sqrt{xy}\},$$

which equals the sum of an inclined Lorentz cone and the nonnegative orthant of $\mathbb{R}^3$. The canonical barrier for this cone is given by (1.27) with the function $\phi : (-1, +\infty) \to \mathbb{R}$ given parametrically by

$$\begin{aligned} t &= \frac{1-\xi}{(\sqrt{\xi+3}+2)(\sqrt{\xi+3}+1)} \left(\frac{\sqrt{\xi+3}+\sqrt{3}}{\sqrt{\xi+3}-\sqrt{3}} \right)^{\frac{\sqrt{3}}{2}} \\ \phi &= \log \frac{1+\xi+\frac{\xi^2}{4}}{1+\xi\sqrt{1+\frac{\xi-1}{4}}} + \log(\sqrt{\xi+3}+2) + \log(\sqrt{\xi+3}+1) + \frac{\sqrt{3}}{2} \log \frac{\sqrt{\xi+3}-\sqrt{3}}{\sqrt{\xi+3}+\sqrt{3}}, \end{aligned}$$

where the parameter runs through $\xi \in (0, +\infty)$. The effective barrier parameter of the canonical barrier for this cone equals 3.

Semi-homogeneous 3-dimensional cones

The computation of the canonical potential in the cases listed above was possible due to a reduction of PDE (1.21) to an ODE by virtue of a non-trivial automorphism group of the cone. We shall call regular convex cones $K \subset \mathbb{R}^n$ whose automorphism group has orbits of codimension 1 *semi-homogeneous*. The following result, whose proof can be found in [92], shows that every 3-dimensional semi-homogeneous cone is isomorphic to one of the cases computed above.

Theorem 1.4.13. *Let $K \subset \mathbb{R}^3$ be a regular convex cone such that* $\dim \mathrm{Aut}\, K \geq 2$. *Then K is isomorphic to exactly one of the following cones.*

1. *the cone obtained by the homogenization of the epigraph of the exponential function,*
2. *the positive orthant $\mathbb{R}^3_+$,*
3. *the cone given by $\{x \mid z \geq -x^{1/p}y^{1/q},\ x \geq 0,\ y \geq 0\}$ for some $p \in [2, \infty)$, $\frac{1}{p} + \frac{1}{q} = 1$,*
4. *the cone given by $\{x \mid -\alpha x^{1/p}y^{1/q} \leq z \leq x^{1/p}y^{1/q},\ x \geq 0,\ y \geq 0\}$ for some $p \in [2, \infty)$, $\frac{1}{p} + \frac{1}{q} = 1$, $\alpha \in (0, 1]$,*
5. *the cone given by $\{x \mid 0 \leq z \leq x^{1/p}y^{1/q},\ x \geq 0,\ y \geq 0\}$ for some $p \in [2, \infty)$, $\frac{1}{p} + \frac{1}{q} = 1$.*

1.5 Self-scaled barriers and parallel cubic forms

1.5.1 Introduction

In this section we study the centro-affine geometry of the level surfaces of self-scaled barriers. We show that self-scaledness of a barrier is characterized by the vanishing of the covariant derivative of the cubic form on its level surfaces. Therefore from the viewpoint of affine differential geometry the self-scaled barriers are the simplest class of self-concordant logarithmically homogeneous barriers after the hyperbolic barrier on the Lorentz cone, which is characterized by the vanishing of the cubic form itself.

Self-scaled barriers have been classified completely, with the first steps done by Hauser [84, 83, 85] and the classification being completed independently by Schmieta [189], Güler [86], and Lim [87]. Hauser showed that a self-scaled barrier $F_{K\times K'}(x,y)$ on a product of cones K, K' decomposes into a sum $F_K(x) + F_{K'}(y)$ of self-scaled barriers on the factor cones, with the decomposition being unique up to an additive constant. The other authors showed that an irreducible self-scaled cone must be symmetric and every self-scaled barrier on it must be an affine scaling of the universal barrier. These results rely on the connection between symmetric cones and Jordan algebras.

Definition 1.5.1. A *Jordan algebra* J over a field $\mathbb{K}$ is a vector space over $\mathbb{K}$ endowed with a bilinear operation $\bullet : J \times J \to J$ satisfying the following conditions:

i) commutativity: $x \bullet y = y \bullet x$ for all $x, y \in J$,

ii) Jordan identity: $x \bullet (x^2 \bullet y) = x^2 \bullet (x \bullet y)$ for all $x, y \in J$, where $x^2 = x \bullet x$.

The Jordan algebra is called *Euclidean* or *formally real* if $\mathbb{K} = \mathbb{R}$ and the identity $\sum_{k=1}^m x_k^2 = 0$ entails $x_k = 0$, $k = 1, \dots, m$, for all elements $k_1, \dots, k_m \in J$.

The symmetric cones can then be characterized as sets of the form $\{x^2 \,|\, x \in J\}$ or as closures of sets of the form $\{\exp(x) \,|\, x \in J\}$, where J is a Euclidean Jordan algebra [214, Theorem 3],[122]. Most of the material on Jordan algebras used in this section can be looked up in [123]. Other references on Jordan algebras are [110] or [143].

The Euclidean Jordan algebras have been completely classified in [112]. Every Euclidean Jordan algebra can in a unique manner be represented as a direct sum of simple or irreducible Euclidean Jordan algebras [112, p.38]. The simple Euclidean Jordan algebras have been listed in [112, Fundamental Theorem 2].

In this section we shall work a lot with the partial derivatives of a barrier F. We will denote the partial derivatives of F short-hand by indices after a comma. Thus $\frac{\partial F}{\partial x^\alpha} = F_{,\alpha}$, $\frac{\partial^2 F}{\partial x^\alpha \partial x^\beta} = F_{,\alpha\beta}$ etc. The elements of the inverse of the Hessian F'' will be denoted by upper indices after a comma, $(F'')^{-1} = (F^{,\alpha\beta})_{\alpha,\beta=1,\dots,n}$, such that $F_{,\alpha\beta}F^{,\beta\gamma} = \delta_\alpha^\gamma$.

Güler and Schmieta associate to every self-scaled barrier F on a cone $K \subset \mathbb{R}^n$ a Euclidean Jordan algebra J by the formula

$$(u \bullet v)^\gamma = -\frac{1}{2} F^{,\gamma\delta} F_{,\alpha\beta\delta} u^\alpha v^\beta. \tag{1.28}$$

The cone of squares of the algebra J then coincides with the original symmetric cone K. This approach can be traced back to Koecher [123] for the more general case of ω-domains, see also [211].

Given the Jordan algebra J, it is, however, not possible to recover the derivatives F'', F''' in a unique manner from its structure tensor. It is easily seen, e.g., that the right-hand side of (1.28) remains invariant under multiplication of F by a constant. In order to be obtain a one-to-one correspondence between the algebra and the derivatives of the barrier, we have to augment the definition of Jordan algebra as follows.

Definition 1.5.2. A *metrised algebra* is a pair (A, σ) such that A is an algebra and σ is a non-degenerate symmetric invariant bilinear form on A, i.e.,

$$\sigma(a, b \bullet c) = \sigma(a \bullet b, c) \tag{1.29}$$

for all $a, b, c \in A$.

If A is commutative, then condition (1.29) is equivalent to the condition that the operator L_a of left multiplication by a is self-adjoint with respect to σ for all $a \in A$.

The Hessian F'' is invariant with respect to the algebra defined by (1.28), because the third derivative F''' is symmetric. Given the metrised Jordan algebra (J, F''), it is then possible to recover the third derivative. The concept of metrised algebra has been introduced in [31] by Bordemann, but in the context of Jordan algebras it has been essentially used and studied already by Koecher [123, Theorem III.10, p.64].

Here we shall establish a different link between Jordan algebras and barriers. Let F be a logarithmically homogeneous function F with non-degenerate Hessian, and let C be the cubic form of a level surface of F. We show that the integrability condition of the quasi-linear fourth order PDE $\hat{\nabla} C = 0$ is exactly the Jordan identity for the algebra (1.28). This implies that a non-degenerate centro-affine hypersurface immersion satisfying the condition $\hat{\nabla} C = 0$ defines a metrised Jordan algebra (1.28) with invariant form F''. Thus self-scaledness, the metrised Jordan algebra structure, and the parallelism of the cubic form are all equivalent expressions of the same condition. This provides also a radically different view on self-scaled barriers, because these are initially defined by a global algebraic property, while the parallelism condition is local and geometric. We consider these connections in Subsection 1.5.3.

A similar parallelism condition turns out to be equivalent to condition (1.3) of logarithmic homogeneity. Namely, a scalar function F on a domain in $\mathbb{R}^n$ is logarithmically homogeneous with respect to some central point if and only if the first derivative F' is parallel with respect to the Levi-Civita connection defined by the Hessian F''. This yields a differential-geometric description of logarithmic homogeneity. This relation is considered in Subsection 1.5.2.

We show (Theorem 1.5.14) that given a Hessian manifold satisfying $\hat{D}Dg = 0$, the existence of a Hessian potential F satisfying $\hat{D}F' = 0$ is equivalent to unitality of the metrised Jordan algebra associated to the manifold, where D is the canonical affine connection of the manifold and $\hat{D}$ the Levi-Civita connection of g.

The correspondence between Euclidean Jordan algebras and symmetric cones can be generalized to the non-convex case [214, Theorem 4], see also [123],[140],[122]. In a similar manner, the relation between the condition that the cubic form of the level surface of a logarithmically homogeneous function F is parallel and the condition that the algebra defined by virtue of (1.28) is Jordan still holds for non-convex functions F and non-Euclidean Jordan algebras. This equivalence can be used to reduce problems about centro-affine hypersurface immersions with parallel cubic form to problems about metrised Jordan algebras. We used this approach in [96] to solve the problem of classifying affine spheres with parallel cubic form. We shall briefly present this result in Subsection 1.5.6.

1.5.2 Parallel first derivative

In this subsection we consider the condition on a general Hessian metric F'' that the first derivative F' of the Hessian potential is parallel with respect to the Levi-Civita connection $\hat{D}$ defined by F''. We show that this condition is equivalent to the logarithmic homogeneity of F. Since the condition $\hat{D}F' = 0$ is invariant with respect to affine transformations of the underlying space, the central point of the homogeneity might not coincide with the origin of $\mathbb{R}^n$. Therefore we consider potentials F which are defined on an affine real space $\mathbb{A}^n$ rather than the vector space $\mathbb{R}^n$.

Let $U \subset \mathbb{A}^n$ be a simply connected domain in n-dimensional real affine space. Consider a C^3 function $F : U \to \mathbb{R}$ with non-degenerate Hessian. The function F turns U into a Hessian pseudo-Riemannian manifold with metric F''. Let D be the canonical flat affine connection on U, $\hat{D}$ the Levi-Civita connection of the Hessian metric F'', and $K = D - \hat{D}$ the difference tensor. The difference tensor is a tensor of type $(1, 2)$ which is symmetric in the two lower indices.

In an affine coordinate system, the Christoffel symbols of the Levi-Civita connection $\hat{D}$ have the form $\Gamma^\gamma_{\alpha\beta} = \frac{1}{2} F_{,\alpha\beta\delta} F^{,\gamma\delta}$, while the Christoffel symbols of D vanish. Hence the difference tensor can be expressed by the derivatives of F as

$$K^\gamma_{\alpha\beta} = -\Gamma^\gamma_{\alpha\beta} = -\frac{1}{2} F_{,\alpha\beta\delta} F^{,\gamma\delta}. \tag{1.30}$$

The covariant derivative of $F' = DF$ with respect to $\hat{D}$ is given by

$\hat{D}_\beta F_{,\alpha} = F_{,\alpha\beta} - \frac{1}{2}F_{,\delta}F^{,\gamma\delta}F_{,\alpha\beta\gamma}$. Hence F' is $\hat{D}$-parallel if and only if

$$F_{,\delta}F^{,\gamma\delta}F_{,\alpha\beta\gamma} = 2F_{,\alpha\beta}. \tag{1.31}$$

Let $F : U \to \mathbb{R}$ be a solution of (1.31). Define the vector field $e^\gamma = -F_{,\delta}F^{,\gamma\delta}$ on U. We then have

$$D_\alpha e^\gamma = -F_{,\alpha\delta}F^{,\gamma\delta} + F_{,\delta}F^{,\gamma\rho}F_{,\rho\sigma\alpha}F^{,\sigma\delta} = -\delta^\gamma_\alpha + 2F^{,\gamma\rho}F_{,\rho\alpha} = \delta^\gamma_\alpha. \tag{1.32}$$

Let x^α be an affine coordinate system on $\mathbb{A}^n$. By (1.32) the vector field e differs on U from the position vector field x by a constant $c = x - e$. This difference distinguishes a point $c \in \mathbb{A}^n$, which we call the *center*. Let us shift the coordinate system in $\mathbb{A}^n$ such that $c = 0$, and the position vector field x coincides with e. By definition of e we then have

$$F_{,\delta} + F_{,\gamma\delta}x^\gamma = 0. \tag{1.33}$$

Integrating, we obtain

$$F_{,\gamma}x^\gamma = -\nu, \tag{1.34}$$

where $\nu \in \mathbb{R}$ is an integration constant. Integrating (1.34) along the rays emanating from c, we obtain

$$F(\alpha x) = -\nu \log \alpha + F(x) \tag{1.35}$$

for all $x \in U$ and $\alpha > 0$ such that the ray segment between x and αx lies in U. This means that F is locally logarithmically homogeneous with homogeneity parameter ν.

On the other hand, we have the following result.

Lemma 1.5.3. *Let $F : U \to \mathbb{R}$ be a locally logarithmically homogeneous function on some domain $U \subset \mathbb{R}^n$ with homogeneity parameter ν and with non-degenerate Hessian. Then $\hat{D}F' = 0$, where $\hat{D}$ is the Levi-Civita connection of F''. Moreover, the vector field $e^\beta = -F_{,\alpha}F^{,\alpha\beta}$ equals the position vector field x^β on U.*

Proof. Differentiating (1.35) with respect to α at $\alpha = 1$ yields (1.34). Differentiating (1.34) yields (1.33). Differentiating (1.33) and eliminating x by virtue of (1.33) then gives back (1.31). The equality $x = e$ also follows from (1.33). □

Combining with the preceding consideration, we obtain the following result.

Theorem 1.5.4. *Let $F : U \to \mathbb{R}$ be a C^3 function defined on some simply connected domain $U \subset \mathbb{A}^n$. Suppose that F has a non-degenerate Hessian and denote by $\hat{D}$ the Levi-Civita connection of the Hessian metric F''. Then the first derivative F' is $\hat{D}$-parallel if and only if F is locally logarithmically homogeneous with some homogeneity parameter ν with respect to some central point $c \in \mathbb{A}^n$.* □

In particular, for every logarithmically homogeneous function $F : K^o \to \mathbb{R}^n$ on the interior of a regular convex cone $K \subset \mathbb{R}^n$ with non-degenerate Hessian we have that the first derivative F' is parallel with respect to the Levi-Civita connection defined by F''.

1.5.3 Parallel third derivative

In this subsection we analyze the condition $\hat{D}F''' = 0$, where $\hat{D}$ is the Levi-Civita connection of the Hessian metric F''. Actually, we do not need to require that F'' is positive definite, it is sufficient for the considerations in this subsection that F'' is non-degenerate.

Let $U \subset \mathbb{R}^n$ be a simply connected domain and consider a C^5 function $F : U \to \mathbb{R}$ with non-degenerate Hessian. The covariant derivative of F''' with respect to $\hat{D}$ is given by

$$\hat{D}_\delta F_{,\alpha\beta\gamma} = F_{,\alpha\beta\gamma\delta} - \frac{1}{2}F^{,\rho\sigma}(F_{,\alpha\beta\rho}F_{,\gamma\sigma\delta} + F_{,\alpha\gamma\rho}F_{,\beta\sigma\delta} + F_{,\beta\gamma\rho}F_{,\alpha\sigma\delta}). \tag{1.36}$$

Hence F''' is parallel with respect to $\hat{D}$ if and only if F is a solution of the quasi-linear fourth order PDE

$$F_{,\alpha\beta\gamma\delta} = \frac{1}{2}F^{,\rho\sigma}(F_{,\alpha\beta\rho}F_{,\gamma\delta\sigma} + F_{,\alpha\gamma\rho}F_{,\beta\delta\sigma} + F_{,\alpha\delta\rho}F_{,\beta\gamma\sigma}). \tag{1.37}$$

Note that F is a solution of (1.37) if and only if $F+l$ is a solution, where l is an arbitrary affine-linear function, i.e., a function satisfying $l''=0$. The functions F and $F+l$ define also the same pseudo-metric F'' and the same difference tensor K. We may also obtain other solutions of (1.37) by multiplying a solution F by non-zero constants or performing an affine change of coordinates in U.

Let us deduce the integrability condition of PDE (1.37). Introduce affine coordinates x^α on U. Differentiating (1.37) with respect to the coordinate x^η and substituting the appearing fourth order derivatives of F by the right-hand side of (1.37), we obtain after simplification

$$\begin{aligned} F_{,\alpha\beta\gamma\delta\eta} \;=\; & \frac{1}{4}F^{,\rho\sigma}F^{,\mu\nu}\left(F_{,\beta\eta\nu}F_{,\alpha\rho\mu}F_{,\gamma\delta\sigma}+F_{,\alpha\eta\mu}F_{,\rho\beta\nu}F_{,\gamma\delta\sigma}+F_{,\gamma\eta\nu}F_{,\alpha\rho\mu}F_{,\beta\delta\sigma}+F_{,\alpha\eta\mu}F_{,\rho\gamma\nu}F_{,\beta\delta\sigma}\right. \\ & +F_{,\beta\eta\nu}F_{,\gamma\rho\mu}F_{,\alpha\delta\sigma}+F_{,\gamma\eta\mu}F_{,\rho\beta\nu}F_{,\alpha\delta\sigma}+F_{,\beta\eta\nu}F_{,\delta\rho\mu}F_{,\alpha\gamma\sigma}+F_{,\delta\eta\mu}F_{,\rho\beta\nu}F_{,\alpha\gamma\sigma} \\ & \left.+F_{,\delta\eta\nu}F_{,\alpha\rho\mu}F_{,\beta\gamma\sigma}+F_{,\alpha\eta\mu}F_{,\rho\delta\nu}F_{,\beta\gamma\sigma}+F_{,\delta\eta\nu}F_{,\gamma\rho\mu}F_{,\alpha\beta\sigma}+F_{,\gamma\eta\mu}F_{,\rho\delta\nu}F_{,\alpha\beta\sigma}\right). \end{aligned}$$

The right-hand side must be symmetric in all 5 indices. Commuting the indices δ,η and equating the resulting expression with the original one we obtain

$$\begin{aligned} F^{,\rho\sigma}F^{,\mu\nu}&\left(F_{,\beta\eta\nu}F_{,\delta\rho\mu}F_{,\alpha\gamma\sigma}+F_{,\alpha\eta\mu}F_{,\rho\delta\nu}F_{,\beta\gamma\sigma}+F_{,\gamma\eta\mu}F_{,\rho\delta\nu}F_{,\alpha\beta\sigma}\right. \\ &\left.-F_{,\beta\delta\nu}F_{,\eta\rho\mu}F_{,\alpha\gamma\sigma}-F_{,\alpha\delta\mu}F_{,\rho\eta\nu}F_{,\beta\gamma\sigma}-F_{,\gamma\delta\mu}F_{,\rho\eta\nu}F_{,\alpha\beta\sigma}\right)=0. \end{aligned}$$

Raising the index η by the inverse metric $F^{,\mu\nu}$, we get by virtue of (1.30) the integrability condition

$$K^\eta_{\alpha\mu}K^\mu_{\delta\rho}K^\rho_{\beta\gamma}+K^\eta_{\beta\mu}K^\mu_{\delta\rho}K^\rho_{\alpha\gamma}+K^\eta_{\gamma\mu}K^\mu_{\delta\rho}K^\rho_{\alpha\beta}=K^\mu_{\alpha\delta}K^\eta_{\rho\mu}K^\rho_{\beta\gamma}+K^\mu_{\beta\delta}K^\eta_{\rho\mu}K^\rho_{\alpha\gamma}+K^\mu_{\gamma\delta}K^\eta_{\rho\mu}K^\rho_{\alpha\beta}.$$

This condition is satisfied if and only if $K^\eta_{\alpha\mu}K^\mu_{\delta\rho}K^\rho_{\beta\gamma}u^\alpha u^\beta u^\gamma v^\delta=K^\mu_{\alpha\delta}K^\eta_{\rho\mu}K^\rho_{\beta\gamma}u^\alpha u^\beta u^\gamma v^\delta$ for all tangent vectors fields u,v on U, which can be written as

$$K(K(K(u,u),v),u)=K(K(u,v),K(u,u)). \tag{1.38}$$

Consider an arbitrary point $y\in U$. The difference tensor K defines a bilinear map $T_yU\times T_yU\to T_yU$ by $(u,v)\mapsto K(u,v)$. Equipped with this bilinear map, the tangent space T_yU becomes an algebra A_y. We shall denote the multiplication in this algebra by $\bullet$, such that $u\bullet v=K(u,v)$. The left multiplication operator with the element u will be denoted by L_u, such that $L_uv=u\bullet v$ for all u,v. Further, we define the positive powers of an element u recursively by $u^1=u$, $u^{k+1}=u\bullet u^k=L_u^ku$. If the algebra has a unit element e, then we put also $u^0=e$.

Lemma 1.5.5. *Let $F:U\to\mathbb{R}$ be a C^5 solution of PDE (1.37) with non-degenerate Hessian and let $y\in U\subset\mathbb{R}^n$ be a point. Let A_y be the algebra defined by the difference tensor $K=D-\hat{D}$ on T_yU, where D is the canonical affine connection on $\mathbb{R}^n$ and $\hat{D}$ the Levi-Civita connection of F''. Let σ_y be the bilinear form defined on T_yU by the Hessian pseudo-metric $F''=D^2F$. Then the pair (A_y,σ_y) is a metrised Jordan algebra.*

Proof. The tensor K is symmetric in the lower indices, and hence the multiplication $\bullet$ of the algebra A_y is commutative. Condition (1.38) is equivalent to the Jordan identity $u\bullet(u^2\bullet v)=u^2\bullet(u\bullet v)$, and thus A_y is a Jordan algebra.

For arbitrary vectors $u,v,w\in A_y$ we have

$$\begin{aligned} \sigma_y(u\bullet v,w) &= F_{,\beta\gamma}K^\beta_{\delta\rho}u^\delta v^\rho w^\gamma=-\frac{1}{2}F_{,\beta\gamma}F_{,\delta\rho\sigma}F^{,\sigma\beta}u^\delta v^\rho w^\gamma=-\frac{1}{2}F_{,\delta\rho\gamma}u^\delta v^\rho w^\gamma \\ &= -\frac{1}{2}F_{,\beta\delta}u^\delta F_{,\rho\gamma\sigma}F^{,\sigma\beta}v^\rho w^\gamma=F_{,\delta\beta}u^\delta K^\beta_{\rho\gamma}v^\rho w^\gamma=\sigma_y(u,v\bullet w). \end{aligned} \tag{1.39}$$

Here the second and fifth equation come from (1.30). Hence the form σ_y satisfies (1.29) and is an invariant form. Finally, σ_y is non-degenerate and symmetric because F'' is. □

Lemma 1.5.6. *Let $F:U\to\mathbb{R}$ be a C^5 solution of (1.37) with non-degenerate Hessian, defined on a connected domain $U\subset\mathbb{R}^n$, and let $y,y'\in U$ be different points. Let (A_y,σ_y),$(A_{y'},\sigma_{y'})$ be the metrised Jordan algebras defined on the tangent spaces $T_yU,T_{y'}U$ as in Lemma 1.5.5. Then (A_y,σ_y),$(A_{y'},\sigma_{y'})$ are isomorphic.*

Proof. Assume the conditions of the lemma. Let γ be a smooth path connecting the points y, y'. The parallel transport with respect to the Levi-Civita connection $\hat{D}$ along γ defines a non-degenerate linear map $J : T_yU \to T_{y'}U$. Now both F'' and F''' are parallel with respect to $\hat{D}$. Hence the difference tensor K is also $\hat{D}$-parallel. It then follows that J is an isomorphism mapping (A_y, σ_y) to $(A_{y'}, \sigma_{y'})$. □

In particular, a closed path leading back to y defines an automorphism of the metrised Jordan algebra (A_y, σ_y).

We have seen how a solution of (1.37) defines a metrised Jordan algebra. We shall now consider the reverse direction.

Lemma 1.5.7. *Let (A, σ) be a metrised Jordan algebra. Then there exists a neighbourhood $U \subset A$ of zero such that the analytic function $F : U \to \mathbb{R}$ defined by*

$$F(x) = \sum_{k=2}^{\infty} \frac{(-1)^k}{k} \sigma(x, x^{k-1}) \tag{1.40}$$

is a solution of (1.37).

Proof. First note that the expression $\sigma(x, x^{k-1})$ is a homogeneous polynomial of degree k in the entries of x, and the right-hand side of (1.40) is an ordinary Taylor series. It is also easily seen that the convergence radius of the series is nonzero, and hence F is defined on some neighbourhood $U \subset A$ of zero. On this neighbourhood F is analytic. By possibly shrinking U, we shall also assume that the matrix L_x has spectral radius strictly smaller than 1 for all $x \in U$.

The partial derivative of x^k in the direction u is given by

$$\begin{aligned} D_u x^k &= D_u(L_x^{k-1}x) = \sum_{l=1}^{k-1} L_x^{l-1} L_u L_x^{k-1-l} x + L_x^{k-1} u = \sum_{l=1}^{k-1} L_x^{l-1} L_u x^{k-l} + L_x^{k-1} u \\ &= \sum_{l=1}^{k} L_x^{l-1} L_{x^{k-l}} u, \end{aligned}$$

where L_{x^0} is by convention the identity matrix. The derivative of F is then given by

$$\begin{aligned} D_u F &= \sum_{k=2}^{\infty} \frac{(-1)^k}{k} \left(\sigma(D_u x, x^{k-1}) + \sigma(x, D_u x^{k-1}) \right) \\ &= \sum_{k=2}^{\infty} \frac{(-1)^k}{k} \left(\sigma(u, x^{k-1}) + \sum_{l=1}^{k-1} \sigma(x, L_x^{l-1} L_{x^{k-1-l}} u) \right) \\ &= \sum_{k=2}^{\infty} \frac{(-1)^k}{k} \left(\sigma(x^{k-1}, u) + \sum_{l=1}^{k-1} \sigma(L_{x^{k-1-l}} L_x^{l-1} x, u) \right) = \sum_{k=2}^{\infty} (-1)^k \sigma(x^{k-1}, u) \\ &= \sum_{k=1}^{\infty} (-1)^{k+1} \sigma(x^k, u) = \sigma((I + L_x)^{-1} x, u), \end{aligned} \tag{1.41}$$

where the fourth equality comes from power-associativity of the Jordan algebra A and all sums define analytic functions on U. Note that $I + L_x$ and its inverse are self-adjoint with respect to σ.

The next derivatives are given by

$$\begin{aligned} D_v D_u F &= \sigma((I + L_x)^{-1} v, u) - \sigma((I + L_x)^{-1} L_v (I + L_x)^{-1} x, u), \\ D_v^2 D_u F &= -2\sigma((I + L_x)^{-1} L_v (I + L_x)^{-1} v, u) + 2\sigma((I + L_x)^{-1} L_v (I + L_x)^{-1} L_v (I + L_x)^{-1} x, u), \\ D_v^3 D_u F &= 6\sigma(((I + L_x)^{-1} L_v)^2 (I + L_x)^{-1} v, u) - 6\sigma(((I + L_x)^{-1} L_v)^3 (I + L_x)^{-1} x, u). \end{aligned}$$

At $x = 0$ we hence get

$$\begin{aligned} D_v D_u F &= \sigma(v, u), \\ D_v^2 D_u F &= -2\sigma(v^2, u), \\ D_v^4 F &= 6\sigma(v^3, v) = 6\sigma(v^2, v^2). \end{aligned}$$

Using these expressions we obtain

$$\begin{aligned}&\left[F_{,\alpha\beta\gamma\delta} - \frac{1}{2}F^{,\rho\sigma}(F_{,\alpha\beta\rho}F_{,\gamma\delta\sigma} + F_{,\alpha\gamma\rho}F_{,\beta\delta\sigma} + F_{,\alpha\delta\rho}F_{,\beta\gamma\sigma})\right] u^\alpha u^\beta u^\gamma u^\delta \\ &= 6\sigma(u^2, u^2) + (F_{,\alpha\beta\rho}K^\rho_{\gamma\delta} + F_{,\alpha\gamma\rho}K^\rho_{\beta\delta} + F_{,\alpha\delta\rho}K^\rho_{\beta\gamma})u^\alpha u^\beta u^\gamma u^\delta \\ &= 6\sigma(u^2, u^2) + 3D^2_{\mathbb{R}u} D_{u^2} F = 0.\end{aligned}$$

It follows that (1.37) is satisfied at $x = 0$.

For $x \in U$ an arbitrary point, we shall identify the tangent space T_xU with A. Fix a vector $w \in A$, and define the vector field $v(x) = (I + L_x)w = w + x \bullet w$ on U. Since the vector field v is affine-linear in x, the Lie derivative $\mathcal{L}_v$ commutes with the directional derivative D on U by Lemma 1.2.2.

We shall now compute the Lie derivative of (1.36) with respect to the vector field v. By (1.41) we have

$$\mathcal{L}_v F = \sigma((I + L_x)^{-1}x, (I + L_x)w) = \sigma(x, w),$$

and the Lie derivative of F is a linear function in x. It follows that $\mathcal{L}_v DF = D\mathcal{L}_v F$ is a constant 1-form, and $\mathcal{L}_v D^k F = D^{k-1}\mathcal{L}_v DF = 0$ for every $k \geq 2$. Hence the Lie derivative $\mathcal{L}_v$ of (1.36) vanishes on U.

We thus have $\hat{D}F''' = 0$ at $x = 0$ and $\mathcal{L}_v(\hat{D}F''') = 0$ for all $w \in A$ and all $x \in U$. Since $I + L_x$ is regular, we have $\{v = (I + L_x)w \,|\, w \in A\} = T_xU$ for all $x \in U$. If U is connected, which we may assume without restriction of generality, then it follows that $\hat{D}F''' = 0$ identically on U and (1.37) is satisfied by the function F. This completes the proof. □

Lemmas 1.5.5 and 1.5.7 show how to construct a metrised Jordan algebra from a solution of (1.37) and vice versa. We now show that the corresponding maps are the inverse of one another in the sense of the following lemmas.

Lemma 1.5.8. *Let $F : U \to \mathbb{R}$ be a C^5 solution of (1.37) on a domain $U \subset \mathbb{R}^n$ and $y \in U$ a point. Let (A_y, σ_y) be the metrised Jordan algebra defined by F as in Lemma 1.5.5. Let $\tilde{U} \subset A_y = T_yU \simeq \mathbb{R}^n$ be the neighbourhood of zero and $\tilde{F} : \tilde{U} \to \mathbb{R}$ the solution of (1.37) defined by (A_y, σ_y) as in Lemma 1.5.7.*

Then there exists a neighbourhood $V \subset U \cap (y + \tilde{U})$ of y such that the difference $d(x) = F(x) - \tilde{F}(x - y)$ is affine-linear on V.

Proof. The functions $F(x)$ and $\tilde{F}(x - y)$ are both defined on $U \cap (y + \tilde{U})$ and are C^5 solutions of (1.37). We shall now compare the second and third derivatives of these functions at $x = y$. For tangent vectors $u, v, w \in A_y$ we have by definition of σ_y and by (1.39) that

$$F''(u, v) = \sigma_y(u, v), \qquad F'''(u, v, w) = -2\sigma_y(u \bullet v, w).$$

On the other hand, the quadratic and cubic terms in the Taylor series (1.40) yield

$$\tilde{F}''(u, u) = \sigma_y(u, u), \qquad \tilde{F}'''(u, u, u) = -2\sigma_y(u, u \bullet u).$$

Thus the second and third derivatives of $F(x)$ and $\tilde{F}(x - y)$ coincide at $x = y$.

Consider a ray $\gamma(t) = y + tz$ emanating from y. On this ray equation (1.37) defines an ODE on the vector of second and third partial derivatives of F and $\tilde{F}$, respectively. By the preceding paragraph, both ODEs have the same initial condition at $t = 0$. Since the second derivative is non-degenerate, the ODEs satisfy the conditions of the Picard-Lindelöf theorem [138] on the existence and uniqueness of the solution. Therefore the restriction of the second derivative $D^2 d$ to the ray γ is identically zero on some interval $[0, T]$ with $T > 0$. The Lipschitz constant of the right-hand side of the ODE, which is involved in the proof of the Picard-Lindelöf theorem and defines a strictly positive lower bound on T, is a continuous function of the direction z of the ray. This bound then also depends continuously on z. By letting z run through the unit sphere, it follows that there exists a neighbourhood V of y where $D^2 d$ identically vanishes. On this neighbourhood d is an affine-linear function. This completes the proof. □

Lemma 1.5.9. *Let (A, σ) be a metrised Jordan algebra, let $U \subset A$ be the neighbourhood of zero and $F : U \to \mathbb{R}$ the solution of* (1.37) *defined by (A, σ) as in Lemma 1.5.7. Let (A_0, σ_0) be the metrised Jordan algebra defined by F at the point $y = 0$ as in Lemma 1.5.5. Then, under identification of A with T_0U, we have $(A_0, \sigma_0) = (A, \sigma)$.*

Proof. By (1.40) we have for arbitrary $u \in T_0U$ that

$$F''(u, u) = \sigma(u, u), \qquad F'''(u, u, u) = -2\sigma(u, u \bullet u),$$

where $\bullet$ denotes the multiplication in A. From the first relation it follows that $\sigma_0 = \sigma$. Since A is commutative and σ is a symmetric invariant form, it follows from the second relation that for all $u, v, w \in T_0U$ we have $F'''(u, v, w) = -2\sigma(u \bullet v, w)$. By (1.30) we then get $K(u, v) = u \bullet v$. But $K(u, v)$ defines the multiplication in A_0, which proves also $A_0 = A$. □

From Lemma 1.5.8 we have also the following corollary.

Corollary 1.5.10. *Let F be a C^4 solution of* (1.37)*. Then F is analytic.*

Proof. If F is C^4, then the right-hand side of (1.37) is continuously differentiable. But then the left-hand side is continuously differentiable, and F is actually C^5. By Lemma 1.5.8 F then locally coincides with an analytic function. Hence F is analytic. □

In this subsection we have shown that the local isomorphism classes of Hessian metrics g on domains $U \subset \mathbb{R}^n$ with $\hat{D}$-parallel derivative Dg are in one-to-one correspondence with the isomorphism classes of metrised Jordan algebras, where D is the canonical affine connection on $\mathbb{R}^n$ and $\hat{D}$ the Levi-Civita connection of g. In the next subsection we shall specialize this correspondence to Hessian metrics with logarithmically homogeneous potentials.

1.5.4 Parallel first and third derivatives

In this subsection we consider the situation when both conditions $\hat{D}F' = 0$ and $\hat{D}F''' = 0$ are satisfied, where $\hat{D}$ is the Levi-Civita connection of the Hessian metric F''. We show that for a logarithmically homogeneous solution of (1.37) the corresponding Jordan algebra is *unital*, i.e., possesses a unit element e, and that the converse implication also holds up to an additive affine-linear term. On the other hand, we show that a logarithmically homogeneous function F is a solution of (1.37) if and only if the cubic form C of the level surfaces of F is parallel with respect to the Levi-Civita connection $\hat{\nabla}$ of the affine metric h.

Lemma 1.5.11. *Let $F : U \to \mathbb{R}$ be a solution of* (1.37) *on some domain $U \subset \mathbb{R}^n$, and let $y \in U$ be a point. Let (A_y, σ_y) be the metrised Jordan algebra defined by F as in Lemma 1.5.5. If F in addition satisfies* (1.31)*, then the Jordan algebra A_y possesses a unit element, which is given by $e^\gamma = -F_{,\delta}F^{,\gamma\delta}$.*

Proof. Raising the index β in (1.31), we obtain by (1.30) that $-F_{,\delta}F^{,\gamma\delta}K^\beta_{\alpha\gamma} = \delta^\beta_\alpha$. The left-hand side of this equation defines the multiplication operator L_e of the algebra A_y corresponding to the vector $e^\gamma = -F_{,\delta}F^{,\gamma\delta}$. The right-hand side is the identity operator on T_yU, and hence e is a unit element of A_y. □

Corollary 1.5.12. *Let $F : U \to \mathbb{R}$ be a logarithmically homogeneous solution of* (1.37) *on some domain $U \subset \mathbb{R}^n$, and let $y \in U$ be a point. Let (A_y, σ_y) be the metrised Jordan algebra defined by F as in Lemma 1.5.5. Then y is the unit element of A_y.*

The corollary is a direct consequence of Lemmas 1.5.3 and 1.5.11.

Lemma 1.5.13. *Let $F : U \to \mathbb{R}$ be a solution of* (1.37) *on some domain $U \subset \mathbb{A}^n$ in affine space, let $y \in U$ be a point, and (A_y, σ_y) the metrised Jordan algebra defined by F as in Lemma 1.5.5. Suppose A_y possesses a unit element. Then there exists a potential $\tilde{F}$ of the Hessian metric F'' on U which satisfies* (1.31)*.*

Proof. Assume the conditions of the lemma. Since A_y has a unit element, for every $x \in U$ the similarly defined Jordan algebra A_x has also a unit element, because by Lemma 1.5.6 the algebras A_y and A_x are isomorphic. Let e be the vector field on U defined by these unit elements. We then have

$$K^{\beta}_{\alpha\gamma} e^{\gamma} = \delta^{\beta}_{\alpha}, \tag{1.42}$$

where $K = D - \hat{D}$ is the $(1,2)$-tensor field of the structure tensors of the algebras A_x, $x \in U$. Note that the difference tensor K as well as the Kronecker symbol are $\hat{D}$-parallel, because F is a solution of (1.37). Let v be an arbitrary smooth vector field on U. Applying the covariant derivative $\hat{D}_v$ to both sides of (1.42), we obtain $K^{\beta}_{\alpha\gamma}\hat{D}_v e^{\gamma} = 0$, or equivalently $u \bullet \hat{D}_v e = 0$ for all vector fields u, v.

This implies $L_{\hat{D}_v e} u = 0$ for all u, v. Note that in a unital algebra with unit element e the condition $L_w = 0$ implies $L_w e = w = 0$. Therefore the covariant derivative $\hat{D}e$ vanishes identically on U. Writing this out, we get $\frac{\partial}{\partial x^{\delta}} e^{\gamma} + \Gamma^{\gamma}_{\beta\delta} e^{\beta} = \frac{\partial}{\partial x^{\delta}} e^{\gamma} - K^{\gamma}_{\beta\delta} e^{\beta} = 0$. By (1.42) we then get

$$D_{\beta} e^{\gamma} = \frac{\partial e^{\gamma}}{\partial x^{\beta}} = \delta^{\gamma}_{\beta}. \tag{1.43}$$

Lowering the index β in (1.42), we get by virtue of (1.30) that

$$-\frac{1}{2} F_{,\alpha\beta\gamma} e^{\gamma} = F_{,\alpha\beta}. \tag{1.44}$$

Hence the second derivative

$$\frac{\partial^2 (F_{,\gamma} e^{\gamma})}{\partial x^{\alpha} \partial x^{\beta}} = F_{,\gamma\alpha\beta} e^{\gamma} + F_{,\gamma\alpha}\delta^{\gamma}_{\beta} + F_{,\gamma\beta}\delta^{\gamma}_{\alpha} = F_{,\gamma\alpha\beta} e^{\gamma} + 2F_{,\alpha\beta}$$

vanishes on U. Here we have used (1.43) to express the derivatives of the vector field e. It follows that the function $\tilde{F} = F - F_{,\gamma} e^{\gamma}$ satisfies $\tilde{F}'' = F''$, $\tilde{F}''' = F'''$, and is a potential of the Hessian metric F''. Moreover, we have

$$\tilde{F}_{,\alpha} = F_{,\alpha} - F_{,\gamma\alpha} e^{\gamma} - F_{,\gamma} \frac{\partial e^{\gamma}}{\partial x^{\alpha}} = F_{,\alpha} - F_{,\gamma\alpha} e^{\gamma} - F_{,\gamma}\delta^{\gamma}_{\alpha} = -\tilde{F}_{,\gamma\alpha} e^{\gamma},$$

whence $e^{\gamma} = -\tilde{F}_{,\alpha}\tilde{F}^{,\alpha\gamma}$. Inserting this into (1.44) finally yields (1.31). □

Combining the two lemmas, we obtain the following theorem.

Theorem 1.5.14. *Let $F : U \to \mathbb{R}$ be a solution of (1.37) on a domain $U \subset \mathbb{A}^n$ in affine space, let $y \in U$ be a point, and (A_y, σ_y) the metrised Jordan algebra defined by F as in Lemma 1.5.5. Then the following are equivalent.*

1. A_y possesses a unit element.

2. There exists another solution $\tilde{F}$ of (1.37) on U, generating the same Hessian metric $F'' = \tilde{F}''$ on U and the same metrised Jordan algebra (A_y, σ_y) on T_yU, such that $\hat{D}\tilde{F}' = 0$, where $\hat{D}$ is the Levi-Civita connection of F''. □

Recall that by Theorem 1.5.4 the condition $\hat{D}\tilde{F}' = 0$ is equivalent to logarithmic homogeneity of F with respect to some central point.

We shall now assume logarithmic homogeneity of F and find an equivalent condition of (1.37) in terms of the centro-affine cubic form of the level surfaces of F.

Lemma 1.5.15. *Let $U \subset \mathbb{R}^n$ be a conic domain, $\alpha \in \mathbb{R}$ an arbitrary number, and $F : U \to \mathbb{R}$ a logarithmically homogeneous function with homogeneity parameter $\nu > 0$ and positive definite Hessian. Let $\hat{D}$ be the Levi-Civita connection of the metric F'', $F_{\alpha} = \{x \in U \,|\, F(x) = \alpha\}$ a level surface of F, h the centro-affine metric and C the cubic form on F_{α}, and $\hat{\nabla}$ the Levi-Civita connection of h. Then $\hat{D}F''' = 0$ if and only if $\hat{\nabla}C = 0$.*

Proof. Since F is logarithmically homogeneous with homogeneity parameter $\nu > 0$, the level surfaces of F are homothetic images of each other and $F_\alpha \hookrightarrow U$ is indeed a centro-affine hypersurface immersion.

Let $x \in F_\alpha$ be an arbitrary point. By Proposition 1.3.1 the tangent space T_xU splits into an F''-orthogonal sum $T_xF_\alpha \oplus \{tx \,|\, t \in \mathbb{R}\}$. Let Π be the orthogonal projection of T_xU onto the first summand. This projection is a $(1,1)$-tensor with components

$$\Pi^\gamma_\beta = \delta^\gamma_\beta + \nu^{-1}x^\gamma F_{,\beta} = \delta^\gamma_\beta - \nu^{-1}F^{,\gamma\delta}F_{,\delta}F_{,\beta}.$$

Define a symmetric $(0,3)$-tensor T on T_xU by $T[u,u,u] = F'''[\Pi u, \Pi u, \Pi u]$, or in coordinate notation

$$\begin{aligned} T_{\beta\gamma\delta} &= \Pi^\rho_\beta \Pi^\sigma_\gamma \Pi^\tau_\delta F_{,\rho\sigma\tau} = (\delta^\rho_\beta + \nu^{-1}x^\rho F_{,\beta})(\delta^\sigma_\gamma + \nu^{-1}x^\sigma F_{,\gamma})(F_{,\rho\sigma\delta} - 2\nu^{-1}F_{,\delta}F_{,\rho\sigma}) \\ &= (\delta^\rho_\beta + \nu^{-1}x^\rho F_{,\beta})(F_{,\rho\gamma\delta} - 2\nu^{-1}F_{,\gamma}F_{,\rho\delta} - 2\nu^{-1}F_{,\delta}F_{,\rho\gamma} + 2\nu^{-2}F_{,\gamma}F_{,\delta}F_{,\rho}) \\ &= F_{,\beta\gamma\delta} - 2\nu^{-1}(F_{,\beta}F_{,\gamma\delta} + F_{,\gamma}F_{,\beta\delta} + F_{,\delta}F_{,\beta\gamma}) + 4\nu^{-2}F_{,\beta}F_{,\gamma}F_{,\delta}. \end{aligned}$$

Here we used that $F'''(x)[x] = -2F''(x)$, $F''(x)[x] = -F'(x)$, $F'(x)[x] = -\nu$. Thus the difference $F''' - T$ depends on F', F'' only.

Extend T to a tensor field on U by varying $x \in F_\alpha$ and the parameter α of the level surface. We have that F'' is $\hat{D}$-parallel, and F' is also $\hat{D}$-parallel by Lemma 1.5.3. Hence the difference $F''' - T$ is $\hat{D}$-parallel and $\hat{D}F''' = 0$ if and only if $\hat{D}T = 0$.

By Lemma 1.3.2 we have that T can be represented as a direct sum $T = \nu C \oplus 0$, where the first summand is a tensor on the tangent subspace T_xF_α and the second is the null tensor on the radial subspace $\{tx \,|\, t \in \mathbb{R}\}$ of T_xU. But the Riemannian manifold (U, F'') is a direct product with first factor $(F_\alpha, \nu h)$ by Proposition 1.3.1. Hence $\hat{D}T = 0$ if and only if $\hat{\nabla}C = 0$. This completes the proof. □

Remark 1.5.16. The condition that F'' is positive definite can be replaced by the weaker condition that F'' is non-degenerate. The proof of this stronger result is similar, with Proposition 1.3.1 replaced by [96, Theorem 2.2].

1.5.5 Self-scaled barriers and parallel cubic form

We are now in a position to apply the theory developed in the previous subsections to self-concordant logarithmically homogeneous barriers. First we add the convexity of the Hessian potential F as a condition.

Lemma 1.5.17. *Let $F : U \to \mathbb{R}$ be a solution of both* (1.37) *and* (1.31) *with positive definite Hessian on a domain $U \subset \mathbb{R}^n$, let $y \in U$ be a point, and (A_y, σ_y) the metrised Jordan algebra defined by F as in Lemma 1.5.5. Then A_y is a Euclidean Jordan algebra.*

The lemma follows immediately from [123, Theorem VI.12], which states that if the invariant bilinear form σ of a metrised Jordan algebra (A, σ) is positive definite, then the algebra A is Euclidean.

Now the metrised Jordan algebras (A, σ), where A is Euclidean and σ is non-degenerate, can be completely classified. By [123, Corollary VI.5] a Euclidean Jordan algebra is semi-simple, i.e., $\tau(u,v) = tr\, L_{u \bullet v}$ is a non-degenerate bilinear form, the *trace form*. The trace form is actually itself invariant [123, Lemma III.4] and positive definite [123, Theorem VI.12]. By [123, Theorem III.10] there exists a central element $z \in A$ (i.e., an element satisfying $z \bullet (u \bullet v) = u \bullet (z \bullet v)$ for all u, v) such that $\sigma(u,v) = \tau(z \bullet u, v) = tr\, L_{(z \bullet u) \bullet v}$ for all $u, v \in A$. This central element z is invertible, and every invertible central element gives rise to an invariant non-degenerate bilinear form in this way [123, Theorem III.10; item (v), pp.71–72]. The semi-simple algebra A can be decomposed in a unique manner as a direct sum $A = A^1 \oplus \cdots \oplus A^m$ of simple ideals [123, Theorem III.11], which have been completely classified in [112, Fundamental Theorem 2] and are in one-to-one correspondence with the irreducible symmetric cones. Let $e_1, \dots, e_m$ be the unit elements of these simple ideals. Then every central element $z \in A$ has a unique representation as a sum $z = \sum_{j=1}^m \alpha_j e_j$, where α_j are real numbers [112, p.46].

Lemma 1.5.18. *Let A be a Euclidean Jordan algebra with simple summands $A_1, \dots, A_m$. Then every positive definite invariant bilinear form σ on A can be represented as*

$$\sigma(u,v) = \sum_{j=1}^m \alpha_j tr\, L_{u_j \bullet v_j} \tag{1.45}$$

for some positive real numbers $\alpha_1, \dots, \alpha_m$, where $u_j, v_j \in A_j$ are the components of the elements u, v in the simple summands, respectively.

On the other hand, for every $\alpha_1, \dots, \alpha_m > 0$ the form σ defined in (1.45) *is a positive definite invariant bilinear form on A.*

Proof. By the above every invariant bilinear form σ on A has the form (1.45) for some $\alpha_j \in \mathbb{R}$, and all m-tuples $(\alpha_1, \dots, \alpha_m)$ give rise to invariant bilinear forms. Since the trace forms on the summand algebras are positive definite, the form (1.45) is positive definite if and only if all coefficients α_j are positive. □

This characterization of metrised Euclidean Jordan algebras allows to classify also all logarithmically homogeneous solutions of (1.37) with positive definite Hessian. We need the following uniqueness result.

Lemma 1.5.19. *Let $F : U \to \mathbb{R}$ be a logarithmically homogeneous solution of* (1.37) *on a conic domain $U \subset \mathbb{R}$ and with homogeneity parameter ν. Let $y \in U$ be a point and let (A_y, σ_y) be the metrised Jordan algebra defined on T_yU as in Lemma 1.5.5. Let $\tilde{F} : U \to \mathbb{R}$ be another logarithmically homogeneous solution of* (1.37) *which generates the same metrised Jordan algebra (A_y, σ_y) on T_yU. Then $\tilde{F} = F + const$ and the homogeneity parameter of $\tilde{F}$ also equals ν.*

Proof. By Lemma 1.5.8 the functions $F, \tilde{F}$ differ by an affine-linear function on U, and $\tilde{F}'' = F''$. By Lemma 1.5.3 the first derivative of a logarithmically homogeneous function can be written as $F_{,\alpha} = -F_{,\alpha\beta}x^\beta$, with x the position vector field. Therefore the first derivatives of $F, \tilde{F}$ also coincide on U. Therefore F and $\tilde{F}$ differ by an additive constant, and by (1.34) have also the same homogeneity parameter. □

We shall now construct an explicit logarithmically homogeneous solution of (1.37) which produces a given metrised Euclidean Jordan algebra (A, σ). To this end we need to introduce the determinant of an element $x \in A$.

In a Euclidean Jordan algebra A, there exists for every element $x \in A$ a complete system of mutually orthogonal idempotents $\epsilon^1, \dots, \epsilon^m$ and distinct reals $\lambda_1, \dots, \lambda_m$ such that $x = \sum_{j=1}^m \lambda_j \epsilon^j$ [112, Theorem 6]. The numbers λ_j are called the *eigenvalues* of x, and $d_j = tr\, L_{\epsilon^j}$ is their multiplicity. The sum $\sum_{j=1}^m d_j$ depends on the algebra A only and is called its *rank*. Clearly we have $x^k = \sum_{j=1}^m \lambda_j^k \epsilon^j$ for the powers of x, and hence $tr\, L_{x^k} = \sum_{j=1}^m \lambda_j^k d_j$. The *determinant* of x is defined as the product $\prod_{j=1}^m \lambda_j^{d_j}$. It is a homogeneous polynomial of degree rk A in x. The point x is in the interior of the symmetric cone K corresponding to A if and only if all its eigenvalues are positive. The unit element e of A can be expressed as sum $e = \sum_{j=1}^m \epsilon^j$ and is an element of K^o.

Let τ be the trace form on A, and let $x = \sum_{j=1}^m \lambda_j e^j \in A$ be such that all eigenvalues λ_j lie in the open interval $(-1, 1)$. Let d_j be the multiplicities of λ_j. Then we have $e + x = \sum_{j=1}^m (1 + \lambda_j) e^j$, and hence

$$\begin{aligned} -\log\det(e+x) &= -\sum_{j=1}^m d_j \log(1+\lambda_j) = \sum_{j=1}^m d_j \sum_{l=1}^\infty \frac{(-1)^l}{l}\lambda_j^l = \sum_{l=1}^\infty \frac{(-1)^l}{l} tr\, L_{x^l} \\ &= -tr\, L_x + \sum_{k=2}^\infty \frac{(-1)^k}{k}\tau(x, x^{k-1}). \end{aligned} \tag{1.46}$$

By Lemma 1.5.7 the function $F(x) = -\log\det(e+x)$, and after a coordinate change $F(x) = -\log\det x$, is hence a solution of (1.37).

Lemma 1.5.20. *Let (A, σ) be a metrised Euclidean Jordan algebra, $A_1, \dots, A_m$ its simple summands, with σ given by* (1.45) *for some $\alpha_j > 0$. Let $e \in A$ and $e_j \in A_j$ be the unit elements of the corresponding algebras. Then the function*

$$F(x) = -\sum_{j=1}^m \alpha_j \log\det x_j$$

is a logarithmically homogeneous solution of (1.37), *defined on the interior of the symmetric cone K corresponding to A. The metrised Euclidean Jordan algebra (A_e, σ_e) defined by F on T_eK^o as in Lemma 1.5.5 coincides with (A, σ).*

Proof. The cone K can be represented as direct product $K_1 \times \cdots \times K_m$, where K_j is the irreducible symmetric cone corresponding to the algebra A_j. The function $F_j(x_j) = -\log\det x_j$ is a logarithmically homogeneous solution of (1.37) on the interior of K_j, with homogeneity parameter rk A_j. But then $F(x) = \sum_{j=1}^m \alpha_j F_j(x)$ is also a solution of (1.37), defined on K^o and with homogeneity parameter $\sum_{j=1}^m \alpha_j \operatorname{rk} A_j$.

Let τ_j be the trace form on A_j. Then by Lemma 1.5.9 and (1.46) the metrised Jordan algebra defined by F_j at e_j equals (A_j, τ_j). It follows that the solution $\alpha_j F_j$ generates the metrised algebra $(A_j, \alpha_j \tau_j)$ at e_j, and hence F generates the metrised algebra (A, σ) at e. □

This result allows to explicitly characterize the logarithmically homogeneous convex solutions of (1.37).

Theorem 1.5.21. *Let $U \subset \mathbb{R}^n$ be a conic domain, and let $F : U \to \mathbb{R}$ be a logarithmically homogeneous C^4 function with positive definite Hessian. Then F is a solution of* (1.37) *if and only if there exists a Euclidean Jordan algebra $A = A_1 \oplus \cdots \oplus A_m$, where A_j are the simple summands of A, with corresponding symmetric cone $K \subset \mathbb{R}^n$, positive numbers $\alpha_1, \dots, \alpha_m$, and a constant $c \in \mathbb{R}$ such that $U \subset K^o$ and*

$$F(x) = -\sum_{j=1}^m \alpha_j \log\det x_j + c, \tag{1.47}$$

where $x_j \in A_j$ are the components of x.

Proof. Let F be a solution of (1.37) and $y \in U$ an arbitrary point. Let (A_y, σ_y) be the metrised Euclidean Jordan algebra defined by F on T_yU as in Lemma 1.5.5. Denote by $A_1, \dots, A_m$ the simple summands of A_y. By Lemma 1.5.18 there exist numbers $\alpha_1, \dots, \alpha_m$ such that the form σ_y is given by (1.45).

Let K be the symmetric cone corresponding to A_y. By Corollary 1.5.12 the element y is the unit of A_y and hence $y \in K^o$. Define the function $\tilde{F} : K^o \to \mathbb{R}$ by

$$\tilde{F}(x) = -\sum_{j=1}^m \alpha_j \log\det x_j,$$

where $x_j \in A_j$ are the components of x. By Lemma 1.5.20 the function $\tilde{F}$ is a logarithmically homogeneous solution of (1.37) and generates the same metrised algebra (A_y, σ_y) on T_yU as F. By Lemma 1.5.19 the functions $F, \tilde{F}$ differ by a constant in a neighbourhood of y. Since both functions are analytic by Corollary 1.5.10, we obtain $F = \tilde{F} + c$ for some $c \in \mathbb{R}$ on the intersection $K^o \cap U$.

Now $\tilde{F}$ cannot be continued analytically beyond ∂K, because $\tilde{F}(x) \to +\infty$ for $x \to \partial K$. Therefore we must have $U \subset K^o$. This proves one side of the equivalence.

The opposite implication is evident: a function $\tilde{F}(x)$ of the form defined above is a solution of (1.37) by Lemma 1.5.20, and it remains a solution if one adds a constant to it. □

This allows us to formulate our main result, the characterization of self-scaled barriers.

Theorem 1.5.22. *Let $K \subset \mathbb{R}^n$ be a regular convex cone and $F : K^o \to \mathbb{R}$ a logarithmically homogeneous self-concordant barrier on K. Then the following conditions are equivalent:*

(a) F is self-scaled;

(b) F is a solution of (1.37)*;*

(c) the dual barrier F_* is a solution of (1.37)*;*

(d) the cubic form C on the level surfaces of F is parallel with respect to the Levi-Civita connection $\hat{\nabla}$ of the centro-affine metric h on these level surfaces.

Proof. (a) $\Rightarrow$ (b). Let F be self-scaled. Then K is a symmetric cone [86]. Let $K = K_1 \times \cdots \times K_m$ be its decomposition into irreducible symmetric cones, and let A_j be simple Euclidean Jordan algebras such that their cones of squares equal K_j. By [189, Theorem 4] the function F has the form (1.47) for some $c \in \mathbb{R}$, $\alpha_j \geq 1$, where $x_j \in A_j$ are the components of x corresponding to the product decomposition of K. By Theorem 1.5.21 the function F satisfies (1.37).

(b) $\Rightarrow$ (a). Suppose F satisfies (1.37). By Theorem 1.5.21 there exists a Euclidean Jordan algebra $A = A_1 \oplus \cdots \oplus A_m$, where A_j are its simple summands, such that F has the form (1.47) for some $c \in \mathbb{R}$ and $\alpha_j > 0$, and $K \subset K_A$, where K_A is the cone of squares for A. By [189, Theorem 2] we actually have $\alpha_j \geq 1$ as a consequence of the self-concordance condition (1.2). By (1.47) we have $F(x) \to +\infty$ for $x \to \partial K_A$ and by assumption for $x \to \partial K$. Hence $K = K_A$. Finally, [189, Theorem 4] shows that F is a self-scaled barrier.

(b) $\Leftrightarrow$ (d). This is the assertion of Lemma 1.5.15.

(c) $\Leftrightarrow$ (d). Condition (d) is invariant under the conormal map. Hence this equivalence is again the assertion of Lemma 1.5.15, but applied to the dual barrier F_*. □

If the interiors of K and K^* are identified under the isometry $\Phi : x \mapsto -F'(x)$ defined by Legendre duality, then the canonical flat affine connection $\bar{D}$ of the dual space $\mathbb{R}_n$ can be carried over to the interior of K. By (1.6) the Christoffel symbols of $\bar{D}$ are given by $\Gamma^\gamma_{\alpha\beta} = F^{,\gamma m} F_{,m\alpha\beta}$. Hence by virtue of (1.30) we have $\hat{D} = \frac{1}{2}(D + \bar{D})$, as is always the case in a Hessian structure.

Now Legendre duality maps the third derivative F''' to $-F_*'''$ in dual space [171, p.45]. Therefore the condition $\bar{D}F''' = 0$ is equivalent to the condition $\frac{d^4 F_*}{ds^4} = 0$, i.e., the dual barrier is a cubic polynomial. Likewise, the condition $DF''' = 0$ means that F is a cubic polynomial. Thus the self-scaledness condition $\hat{D}F''' = 0$ can be interpreted as a mean between the condition that F is a cubic and that F_* is a cubic.

Finally, we shall characterize the metrised Jordan algebras which correspond to the canonical barrier on symmetric cones.

Lemma 1.5.23. *Let A be an Euclidean Jordan algebra and $K \subset \mathbb{R}^n$ its cone of squares. Let $F : K^o \to \mathbb{R}$ be the canonical barrier on K, and let e be the unit element of A. Then F defines on $T_e K^o$ the metrised Jordan algebra (A, τ), where τ is the trace form of A.*

Proof. Since the canonical barrier on a symmetric cone is of the form (1.47), we have by virtue of Lemma 1.5.20 that the algebra generated by F is again A. In order to compute the invariant form $\sigma = F''(e)$ generated by F, we shall differentiate (1.21). We get $F^{,\beta\gamma} F_{,\alpha\beta\gamma} = 2F_{,\alpha}$.

The trace form is then given by

$$\begin{aligned}\tau(u,v) = tr\, L_{u \bullet v} &= K^\delta_{\gamma\delta} K^\gamma_{\alpha\beta} u^\alpha v^\beta = \frac{1}{4} F^{,\delta\rho} F_{,\gamma\delta\rho} F^{,\gamma\sigma} F_{,\alpha\beta\sigma} u^\alpha v^\beta = \frac{1}{2} F_{,\gamma} F^{,\gamma\sigma} F_{,\alpha\beta\sigma} u^\alpha v^\beta \\ &= F_{,\alpha\beta} u^\alpha v^\beta = F''(e)[u,v].\end{aligned}$$

Here we used (1.30) to express the structure tensor K of A and (1.31) in the fifth equality. □

1.5.6 Classification of affine spheres with parallel cubic corm

In this subsection we apply the connection between Jordan algebras and the parallelism of the cubic form to a problem in affine differential geometry, namely the classification of all affine hyperspheres satisfying the condition $\hat{\nabla} C = 0$. This result has been published in [96].

Since the affine metric is parallel with respect to $\hat{\nabla}$, the conditions $\hat{\nabla} C = 0$ and $\hat{\nabla} K = 0$ are equivalent. A Blaschke immersion satisfying $\hat{\nabla} C = 0$ must be an affine hypersphere [21]. Thus both the classification of affine spheres satisfying $\hat{\nabla} K = 0$ and of Blaschke immersions satisfying $\hat{\nabla} C = 0$ or $\hat{\nabla} K = 0$ are equivalent to the classification problem considered in this subsection.

In [141] all Blaschke immersions into $\mathbb{R}^3$ satisfying $\hat{\nabla} C = 0$ have been classified. In [59, 103, 104] all such Blaschke immersions into $\mathbb{R}^4$ with definite, Lorentzian, and general affine metric, respectively, have been classified. In [61] all such Blaschke immersions into $\mathbb{R}^5$ with definite affine metric have been classified, and it has been shown that in arbitrary dimension, definiteness of the affine metric implies that the immersion is either a quadric or a locally homogeneous affine hypersphere. In [106] all such immersions into $\mathbb{R}^k$, $k \leq 8$, with definite affine metric have been classified. In [60, 107] it has been observed that the *Calabi product* (a procedure for constructing higher-dimensional affine spheres from lower-dimensional ones) of two affine hyperspheres with parallel cubic form or of such a hypersphere with a point are again affine hyperspheres with parallel cubic form, and hence one can speak of decomposable or irreducible such immersions. In a classification, one then only needs to consider the irreducible immersions. Finally, in [108, 105] a classification of all irreducible Blaschke hypersurface immersions with parallel cubic form whose affine metric is definite or Lorentzian, respectively, has been achieved.

A closer look at the classification in [108] reveals that the locally strongly convex hyperbolic affine hyperspheres with parallel cubic form are exactly those hyperspheres which are asymptotic to symmetric cones. Now the interiors of the symmetric cones are exactly the convex ω-domains of Koecher [123], and it is not hard to verify that the hyperspheres in question are exactly the level surfaces of the ω-function in these ω-domains.

Our result is that this relation holds in general, i.e., independently of the convexity assumption. Namely, every non-degenerate proper affine hypersphere with center in the origin satisfying $\hat{\nabla}C = 0$ can be represented as a level surface of the ω-function in some ω-domain, and conversely, every such level surface is a non-degenerate proper affine hypersphere with center in the origin satisfying $\hat{\nabla}C = 0$. The ω-function of Koecher is a homogeneous polynomial. The non-convex analog of the canonical barrier is the *logarithmic potential* Φ, which is defined as a multiple of the logarithm of the ω-function. The affine spheres with parallel cubic form are then also level surfaces of the potential Φ.

The ω-domains of Koecher are closely linked to real semi-simple Jordan algebras J. Namely, every ω-domain can be represented as a connected component of the set of invertible elements in J, and every such connected component is an ω-domain. The potential Φ generates the metrised algebra (J, τ) as in Lemma 1.5.23, where τ is the trace form of J.

The classification of proper affine hyperspheres with parallel cubic form then reduces to the classification of real semi-simple Jordan algebras. Much like in the case of semi-simple Lie algebras, any semi-simple Jordan algebra breaks down into a direct sum of a finite number of simple algebras [123, Theorem III.11], each of which is in turn a member of one of finitely many infinite series, or one of finitely many exceptional algebras. The Calabi product of affine hyperspheres with parallel cubic form corresponds to the decomposition of semi-simple Jordan algebras into simple factors. This allows to characterize the proper affine hyperspheres with parallel cubic form as Calabi products of irreducible such hyperspheres. The irreducible proper affine hyperspheres with parallel cubic can in turn be classified using the classification of simple real Jordan algebras.

In the table below we list the non-convex analogs of the objects appearing in the classification of convex hyperbolic affine spheres.

convex case	general case
symmetric cone	ω-domain
Euclidean Jordan algebra	semi-simple Jordan algebra
irreducible Euclidean Jordan algebra	simple Jordan algebra
canonical barrier	logarithmic potential Φ
determinant of Jordan algebra	ω-function

In the table below we present an exhaustive list of simple Jordan algebras along with the corresponding irreducible affine spheres with parallel cubic form. In the first column we list the ambient vector space of the ω-domain, and in the second column its real dimension. Here M_m, S_m, A_m, H_m, SH_m stands for full, symmetric, skew-symmetric, Hermitian and skew-Hermitian matrices of size $m \times m$, respectively. Most of the classes of real simple Jordan algebras constitute infinite series parameterized by an integer. We give the range of this parameter in the third column. In the fourth column we give an expression for the local potential Φ, parameterized by a nonzero complex number c for complex Jordan algebras, and by a nonzero real number α for real central-simple algebras. In the last two columns we provide the ω-function of the corresponding ω-domains and a description of the affine hyperspheres associated with these domains. The constants in the last column are assumed to be nonzero. Note that in the case of a matrix space over the quaternions $\mathbb{H}$, the matrix S is the complex representation $\begin{pmatrix} Z & W \\ -\bar{W} & \bar{Z} \end{pmatrix}$ of the quaternionic matrix and has twice the size. In the row corresponding to the vector space $\mathbb{R}^m$, Q denotes a non-degenerate quadratic form on $\mathbb{R}^m$. The symbol $\mathbb{O}$ stands for the octonions, and O for the split octonions. The first group of rows corresponds to complex Jordan algebras considered as real vector spaces, and the second group corresponds to real central-simple Jordan algebras.

vector space	real dimension	range	Φ	ω	affine sphere
$\mathbb{C}$	2		$Re(c \log x)$	$\|x\|^2$	$\|x\| = const$
$\mathbb{C}^m$	$2m$	$m \geq 3$	$Re(c \log x^T x)$	$\|x^T x\|^m$	$\|x^T x\| = const$
$S_m(\mathbb{C})$	$m(m+1)$	$m \geq 3$	$Re(c \log \det A)$	$\|\det A\|^{m+1}$	$\|\det A\| = const$
$M_m(\mathbb{C})$	$2m^2$	$m \geq 3$	$Re(c \log \det A)$	$\|\det A\|^{2m}$	$\|\det A\| = const$
$A_{2m}(\mathbb{C})$	$2m(2m-1)$	$m \geq 3$	$Re(c \log \mathrm{pf}\, A)$	$\|\mathrm{pf}\, A\|^{2(2m-1)}$	$\|\mathrm{pf}\, A\| = const$
$H_3(O, \mathbb{C})$	54		$Re(c \log \det A)$	$\|\det A\|^{18}$	$\|\det A\| = const$
$\mathbb{R}$	1		$\log \|x\|$	$\|x\|$	point
$\mathbb{R}^m$	m	$m \geq 3$	$\log \|x^T Q x\|$	$\|x^T Q x\|^{m/2}$	quadric
$M_m(\mathbb{R})$	m^2	$m \geq 3$	$\log \|\det A\|$	$\|\det A\|^m$	$\det A = const$
$M_m(\mathbb{H})$	$4m^2$	$m \geq 2$	$\log \det S$	$(\det S)^{2m}$	$\det S = const$
$S_m(\mathbb{R})$	$\frac{m(m+1)}{2}$	$m \geq 3$	$\log \|\det A\|$	$\|\det A\|^{(m+1)/2}$	$\det A = const$
$H_m(\mathbb{C})$	m^2	$m \geq 3$	$\log \|\det A\|$	$\|\det A\|^m$	$\det A = const$
$H_m(\mathbb{H})$	$m(2m-1)$	$m \geq 3$	$\log \det S$	$(\det S)^{m-1/2}$	$\det S = const$
$A_{2m}(\mathbb{R})$	$m(2m-1)$	$m \geq 3$	$\log \|\mathrm{pf}\, A\|$	$\|\mathrm{pf}\, A\|^{2m-1}$	$\mathrm{pf}\, A = const$
$SH_m(\mathbb{H})$	$m(2m+1)$	$m \geq 2$	$\log \det S$	$(\det S)^{m+1/2}$	$\det S = const$
$H_3(\mathbb{O})$	27		$\log \|\det A\|$	$\|\det A\|^9$	$\det A = const$
$H_3(O, \mathbb{R})$	27		$\log \|\det A\|$	$\|\det A\|^9$	$\det A = const$

Our classification result can then be summarized as follows.

Theorem 1.5.24. *[96] Let $M \subset \mathbb{R}^n$ be a proper affine hypersphere with parallel cubic form and with center in the origin. Then $\mathbb{R}^n$ can be decomposed into a direct product of vector spaces $V_1, \dots, V_r$, where each of the V_k is one of the spaces indicated in the first column of the above table, and M is a Calabi product of proper affine hyperspheres $M_k \subset V_k$ which have the form indicated in the last column of the above table.*

On the other hand, all affine hyperspheres listed in the last column of the table have parallel cubic form.

Chapter 2

Copositive cones

2.1 Introduction

Copositive matrices appear to have been introduced in 1952 by Motzkin [152]. A real symmetric $n \times n$ matrix A is called *copositive* if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n_+$. The set of copositive matrices forms a convex cone, the *copositive cone* $\mathcal{C}^n$. In this section we first give a general overview over this cone and its relevance in applications, and then explain the more specific context of our work on the extreme rays of $\mathcal{C}^n$.

2.1.1 Copositivity in optimization

The matrix cone $\mathcal{C}^n$ is of interest for optimization, as various difficult non-convex optimization problems can be reformulated as conic programs over the copositive cone, so-called *copositive programs*. Among these are combinatorial problems such as the bandwidth problem [179], graph partitioning [180], computing the stability number [48], clique number [215], and chromatic number [80] of graphs, and the quadratic assignment problem [181]. Copositive formulations have been derived for quadratic programming problems [182, 25, 22] and mixed-integer programs [36]. The connection of the copositive cone with sufficient optimality conditions for quadratic programming, i.e., the problem of minimizing a quadratic function under linear constraints, has been recognized already in the 70s [109, Theorem 3.2.3]. For quadratically constrained quadratic programming problems with additional linear constraints copositive relaxations are tighter than standard Lagrangian semi-definite relaxations [24]. In [142, 120, 35, 19] copositive matrices are used for determining Lyapunov functions for switched linear dynamical systems with state confined to the positive orthant or, more generally, to a polyhedral cone. More applications of copositive programming can be found in the surveys [63, 23].

Verifying copositivity of a given matrix is a co-NP-complete problem [153]. Likewise, verifying whether a given linear hyperplane in the space $\mathcal{S}^n$ of $n \times n$ real symmetric matrices is supporting to $\mathcal{C}^n$ at the zero matrix is NP-hard [56]. This is not surprising given the extraordinary descriptive power of copositive programs. Therefore much research has been focussed on finding tractable approximations of the copositive cone, in particular, semi-definite approximations.

The commonest approximation of the cone $\mathcal{C}^n$ is that by the sum of the cone $\mathcal{S}^n_+$ of positive semi-definite matrices and the cone $\mathcal{N}^n$ of element-wise nonnegative symmetric matrices. In [109] the matrices in this sum are called *stochastically copositive*. It is a classical result by Diananda [51, Theorem 2] that for $n \leq 4$ the relation $\mathcal{C}^n = \mathcal{S}^n_+ + \mathcal{N}^n$ holds, i.e., copositivity and stochastic copositivity are equivalent. In general, stochastic copositivity merely implies copositivity, and $\mathcal{S}^n_+ + \mathcal{N}^n \subset \mathcal{C}^n$. A. Horn showed that for $n \geq 5$ this inclusion is indeed strict [51, p.25]. Matrices which are copositive but not stochastically copositive are called *exceptional*, a term that has been coined in [111].

With the appearance of semi-definite programming more sophisticated approximations of $\mathcal{C}^n$ have been elaborated in order to solve copositive programs. In [175] a hierarchy of inner semi-definite approximations for $\mathcal{C}^n$ has been constructed, with the sum $\mathcal{S}^n_+ + \mathcal{N}^n$ being its simplest member. It is based on representing the copositive cone as a cone of positive polynomials and applying sum of squares approximations. In [22] this hierarchy has been relaxed to a hierarchy of polyhedral inner approximations. In [131] a hierarchy of outer semi-definite approximations of $\mathcal{C}^n$ has been proposed based on moments involving the exponential measure on $\mathbb{R}^n_+$. All these hierarchies are asymptotically exact, i.e., the approximating cones tend to $\mathcal{C}^n$ as the order of the approximation tends to infinity. The complexity of the approximating cones grows exponentially with the order, however.

There exist also methods which deal directly with the data of the copositive program under consideration. In [34, 35, 215] branch-and-bound methods based on a tree of polyhedral approximations of the copositive cone have been proposed to check membership in this cone and to solve copositive programs. In [27] a local descent method was proposed which works with the conic dual to the copositive program. In [26, 64] copositivity is checked by a decomposition of a non-convex function as a difference of two convex functions.

For further surveys on copositive matrices see [99, 28], for a list of open problems see [17]. Closely related to the copositive cone $\mathcal{C}^n$ is its dual $\mathcal{C}_n^*$, the *completely positive cone*, which is, however, outside of the scope of this thesis. For surveys on completely positive matrices see, e.g., [18, 28, 53].

2.1.2 Extreme copositive matrices

Our work on copositive cones mainly focusses on a particular topic, namely the extreme rays of $\mathcal{C}^n$. An element $x \in K$ is called an *extremal* element of a regular convex cone K if a decomposition $x = x_1 + x_2$ of x into elements $x_1, x_2 \in K$ is only possible if $x_1 = \lambda x$, $x_2 = (1 - \lambda)x$ for some $\lambda \in [0, 1]$. The set of positive multiples of an extremal element is called an *extreme ray* of K. The set of extreme rays is an important characteristic of a convex cone. Its structure, first of all its stratification into a union of manifolds of different dimension, yields much information about the shape of the cone. The extreme rays of a difficult cone are especially important if one wishes to check the tightness of inner convex approximations of the cone. Namely, an inner approximation is exact if and only if it contains all extreme rays. Since the extreme rays of a cone determine the facets of its dual cone, they are also important tools for the study of this dual cone [52, 194, 29, 30, 193, 192].

It is therefore not surprising that the extreme rays of $\mathcal{C}^n$ have been the subject already of many of the first papers on copositive matrices. The extreme rays of $\mathcal{C}^n$ which are elements of the sum $\mathcal{S}^n_+ + \mathcal{N}^n$ have been completely classified in [82]. Since $\mathcal{C}^n = \mathcal{S}^n_+ + \mathcal{N}^n$ for $n \leq 4$, this yields also a complete classification of the extreme rays of $\mathcal{C}^n$ for $n \leq 4$. The first exceptional extreme copositive form has been found by A. Horn, according to [51, p.25]. This *Horn form* is a circulant 5×5 matrix with entries in $\{-1, +1\}$. In [11, Theorem 3.8] Baumert gave a procedure to construct an extreme ray of $\mathcal{C}^{n+1}$ from an extreme ray of $\mathcal{C}^n$, by duplicating a row and the corresponding column of the original matrix. Starting with the Horn form, he was then able to construct explicit exceptional extreme copositive matrices of every size $n \geq 5$. Extreme copositive matrices which cannot be obtained by this procedure have been called *basic* in [9].

In his thesis [10] and his paper [11] Baumert laid the foundation of a theory of extremal exceptional copositive forms. He recognized the importance of the symmetry group $\mathcal{G}_n$ of the cone $\mathcal{C}^n$, which consists of maps of the form $A \mapsto PDADP^T$, where D is a positive definite diagonal matrix, and $P \in S_n$ is a permutation matrix. The elements of this symmetry group preserve the sum $\mathcal{S}^n_+ + \mathcal{N}^n$ and hence also the property of a copositive matrix of being exceptional. Baumert showed that an exceptional extreme copositive matrix has positive diagonal elements and hence can be scaled to a matrix with all diagonal elements equal to 1 by the action of $\mathcal{G}_n$. By a result from [82] he concluded that the off-diagonal elements of the scaled extremal exceptional matrix have all to be in the interval $[-1, +1]$.

The extremal exceptional matrices of $\mathcal{C}^n$ with elements in $\{-1, +1\}$ have been classified completely in [12] for $n \leq 7$, where it has been shown that they can all be obtained from the Horn form by a group action and the above-mentioned procedure of duplicating rows and columns, a result which does not hold anymore for $n = 8$ [9]. For general n the extremal exceptional matrices with elements in $\{-1, +1\}$ have been characterized independently in [88, 9]. The extreme exceptional matrices in $\mathcal{C}^n$ with elements from the set $\{-1, 0, +1\}$ have been characterized in [101].

Since an exceptional copositive matrix cannot be a multiple of an element in the sum $\mathcal{S}^n_+ + \mathcal{N}^n$, subtraction of a non-zero such element from an extreme exceptional copositive matrix will lead to a matrix which is no more copositive. This fact has early been recognized and led to a number of conditions on exceptional copositive matrices which are weaker than extremality but more tractable.

Baumert called a copositive matrix *reduced* if one cannot subtract a non-zero nonnegative matrix from it without leaving the copositive cone [11], a condition which has been initially introduced and put to use in [51]. Baumert refined this condition by requiring the subtracted nonnegative matrix to be proportional to the extremal element E_{ij} of $\mathcal{N}^n$, where E_{ij} is the symmetric $n \times n$ matrix having a 1 at positions (i,j) and (j,i) and whose other elements all equal zero. He furnished a necessary and sufficient condition on a copositive matrix to be reduced with respect to E_{ii} [11, Theorem 3.4] and conjectured a similar condition for reducedness with respect to E_{ij} with $i \neq j$ [12, Conjecture 4.1], refuted later in [101] by a counterexample of order $n = 7$.

These conditions are expressed in terms of the presence or absence of zeros with certain properties. The importance of the concept of zeros of a copositive matrix has been recognized already by Diananda who introduced it in [51]. A nonzero vector $u \in \mathbb{R}^n_+$ is called a *zero* of a copositive matrix $A \in \mathcal{C}^n$ if $u^T A u = 0$. For a vector $u \in \mathbb{R}^n$ we define its *support* as $\operatorname{supp} u = \{i \in \{1,\dots,n\} \mid u_i \neq 0\}$, i.e., as the index set of the non-zero elements of u. The possible supports of a nonnegative vector are in one-to-one correspondence with the faces of the nonnegative orthant where this vector may be situated. However, a zero u of a copositive form represents a global minimum of this form on the nonnegative orthant. Therefore the first and second order optimality conditions at u are determined by its support. The set of supports of the zeros of a copositive matrix is hence an informative combinatorial characteristic of this matrix which has attracted a lot of attention and is an important mathematical tool in the analysis of copositive matrices and the copositive cone. We shall call this set the *support set* of the copositive matrix in question. In [51, 82, 10, 11, 12] many necessary conditions on the support set of an extremal or a reduced exceptional copositive matrix have been found, and on the other hand, many conditions on the matrix have been established which are determined by its support set. Let us remark that instead of the support as defined here, Baumert defined and used the equivalent notion of the *pattern* of a zero. This notion turned out to be less convenient than that of the support, by which it has been superseded nowadays. Properties of zeros and algorithms to find the zero set of copositive matrices have been recently considered in [52] in application to a study of the faces of the copositive cone and its dual.

In [10, 12] Baumert discovered that the cone $\mathcal{C}^5$ possessed a family of exceptional extreme elements with a support set which is different from that of the Horn form, and gave an explicit matrix from this family. Key to this finding was the introduction of the concept of *maximal zero*. A maximal zero u of a copositive matrix A is a zero such that there does not exist another zero v of A such that $\operatorname{supp} u \subset \operatorname{supp} v$ strictly.

After the paper [101] from the early 70s research on the extreme elements of the copositive cone came to a halt for many years, until the revival which occurred in the current decade.

2.1.3 Overview of our work

In this subsection we give a short summary of our work on extreme copositive matrices and related concepts, and place it into the larger context described in the previous subsections.

While the extreme elements of $\mathcal{C}^n$ for $n \leq 4$ have been completely understood by the work of Diananda [51] and Hall and Newman [82], the structure of $\mathcal{C}^5$ remained a mystery until recently. It was known that $\mathcal{C}^5$ contained exceptional extreme matrices, namely the orbit of the Horn form with respect to the action of the symmetry group $\mathcal{G}_5$, and a family of matrices with 5 isolated zeros with supports of cardinality three [12]. Here we call a zero u of a copositive form A *isolated* if there are no other zeros of A in the neighbourhood of u other than the multiples of u.

Our work on copositive matrices started with a complete description of the extreme rays of the cone $\mathcal{C}^5$, published in [90] and described in more detail in Section 2.2 below. Our strategy follows the one outlined by Baumert [10], by replacing extremality by the weaker condition of reducedness with respect to nonnegative matrices, which is easier to handle. However, two new ideas have been necessary for a successful implementation.

The first one has been to introduce a trigonometric parametrization of the extreme matrices with all diagonal elements equal to 1. As mentioned above, such matrices have their off-diagonal elements in the interval $[-1,+1]$, which can be parameterized by $\cos\varphi$ with the angle φ running through the interval $[0,\pi]$. It turns out that the family of extreme elements discovered by Baumert becomes affine in these angles and its range is delimited by linear inequalities on the angles. As a result, the manifold of these exceptional extreme 5×5 matrices, which have initially been called T-matrices in [90] but are nowadays called *Hildebrand matrices*, can be described in a closed analytic form. The reason for this to happen is the special structure of Cayleys nodal cubic surface which models the zero set of the determinant of real symmetric 3×3 matrices with diagonal elements equal to 1. This surface decomposes into a union of four planes when undergoing the above trigonometric transformation. However, the optimality conditions associated with the isolated zeros of the extreme forms of $\mathcal{C}^5$ in question force the 3×3 principal submatrices of the forms corresponding to the supports of the zeros to be singular. This will happen anytime a zero of a copositive form has a support of cardinality less or equal to three. Thus the proposed trigonometric approach will lead to similar results for any family of extreme rays of $\mathcal{C}^n$ whose zeros have supports with cardinality less or equal to three, independently of the order n. We shall apply this method to the cone $\mathcal{C}^6$ in Section 2.4.

The second critical ingredient was to derive a necessary and sufficient condition on a copositive matrix to be reduced with respect to the extreme element E_{ij} of the nonnegative cone for $i \neq j$. Baumert has conjectured such a condition in [12, Conjecture 4.1] and was able to prove that his families of extreme elements of $\mathcal{C}^5$ were indeed exhaustive, assuming the conjecture. Namely, he provided a partial classification of the support sets of matrices in $\mathcal{C}^5$ which are reduced with respect to the cone $\mathcal{N}^5$, which would have been complete were the conjecture true. In collaboration with M. Dür, P. Dickinson, and L. Gijben we completed this classification in [54], after having derived the correct condition for reducedness with respect to E_{ij}. It turned out that this led to additional families of reduced matrices, but none of them were extremal.

The study of the cone $\mathcal{C}^5$ was completed in the joint paper [55], where it was shown that the second relaxation in Parrilos hierarchy [175] was exact in describing the subset of 5×5 copositive matrices with all diagonal elements equal to 1. In the same paper, we showed that none of Parrilos relaxations is exact for the complete cone $\mathcal{C}^5$. We describe these results in more detail in Section 2.2.

The classification of the extreme rays of $\mathcal{C}^5$ was based on a tedious classification of the possible support sets of copositive 5×5 matrices which are reduced with respect to the nonnegative cone $\mathcal{N}^5$, initiated by Baumert in [12] and completed in [54]. An extension of these results to copositive cones of order $n > 5$ seemed impossible without a more systematic study of support sets of exceptional extremal copositive matrices, due to the expected extraordinary complexity. Our efforts in this direction resulted in the paper [95] on support sets of copositive matrices. We present these results in Section 2.3 below.

In [95] we introduced and investigated the concept of minimal zeros, as opposed to the maximal zeros studied by Baumert in [10]. Here a zero u of a copositive form A is called *minimal* if for no other zero v of A, the support of v is a strict subset of the support of u. In contrast to maximal zeros, or zeros in general, a minimal zero of a copositive matrix is determined up to scaling by a positive constant only by its support and by the matrix itself. Thus a copositive matrix can essentially have only a finite number of minimal zeros, which opens the way to a combinatorial approach. The set of supports of all minimal zeros of a copositive matrix A is called the *minimal support set* of A.

The second innovation presented in [95] was the extension of the concept of reducedness. An exceptional extreme copositive matrix $A \in \mathcal{C}^n$ is not only reduced with respect to the nonnegative cone, but for the same reasons must also be reduced with respect to the positive semi-definite cone, i.e., it cannot be decomposed into a non-trivial sum $A = C + P$, where C is copositive and P is positive semi-definite. This reducedness requirement leads to additional conditions on the support set of the extremal matrix. In fact, we were able to derive a necessary and sufficient condition for reducedness with respect to $\mathcal{S}_+^n$ in terms of the minimal zeros.

The main result of [95] is a set of necessary conditions on the minimal support set of an exceptional copositive matrix which is reduced with respect to both $\mathcal{S}_+^n$ and $\mathcal{N}^n$. When applied retrospectively to the cone $\mathcal{C}^5$, these conditions are strong enough to single out exactly the two support sets which correspond to the two types of exceptional extreme rays of $\mathcal{C}^5$, namely the orbits of the Horn form and the Hildebrand matrices, thus making the classification in [10] and [54] obsolete. For $n = 6$, the conditions reduce the number of potential minimal support sets to 44, which makes the classification of the extreme rays of $\mathcal{C}^6$ possible with a manageable effort. Surprisingly, for some applications the list of support sets itself suffices, without explicit knowledge of the extreme rays [192]. We present some preliminary results on $\mathcal{C}^6$ in Section 2.4.

Our next step in the study of copositive matrices has been to tackle the condition of extremality. As mentioned above, in previous work this condition was substituted by the weaker condition of reducedness, because the latter is easier to handle. However, it is a trivial observation that extremality itself can also be described by a reducedness condition. Namely, a copositive matrix is extremal if and only if one cannot subtract another copositive matrix from it without leaving the copositive cone, except when this other matrix is a multiple of the original matrix. This motivated a study of the reducedness condition with respect to general convex cones and resulted in the paper [57] which was a joint work with P. Dickinson. Those results of this paper which pertain to extremality are described in Section 2.5 below.

The concept of reducedness is generalized in the following way. A copositive matrix $A \in \mathcal{C}^n$ is called *reduced* with respect to another copositive matrix C if for every $\delta > 0$, we have $A - \delta C \not\in \mathcal{C}^n$, and it is called reduced with respect to a subset $\mathcal{M} \subset \mathcal{C}^n$ if it is irreducible with respect to all nonzero elements $C \in \mathcal{M}$.

The paper [57] has a strong convex analysis flavour. Its main result is a necessary and sufficient condition on a pair (A, B), where $A \in \mathcal{C}^n$ and $B \in \mathcal{S}^n$, for the existence of a scalar $\delta > 0$ such that $A + \delta B \in \mathcal{C}^n$. For fixed A, the set of all such matrices $B \in \mathcal{S}^n$ forms a convex cone $\mathcal{K}^A$, which is referred to as the *cone of feasible directions* [177]. We express this cone in terms of the zeros of A and their supports.

The obtained description of the cone $\mathcal{K}^A$ is a powerful tool. It allows to compute the minimal face of A, see [16, 186] for further information on faces of a convex set or cone. In particular, we obtain a simple test of extremality of A, which amounts to checking the rank of a certain matrix constructed from the minimal zeros of A. The necessary and sufficient conditions for the reducedness of A with respect to a nonnegative matrix $C \in \mathcal{N}^n$ or a positive semi-definite matrix $C \in \mathcal{S}_+^n$, which have been given in [54] and [95], respectively, are generalized to the case of arbitrary matrices $C \in \mathcal{C}^n$. The conditions in [54] and [95] follow as particular cases.

Our latest paper on copositive matrices is the article [97], whose results are described in Section 2.6. On the one hand, it complements the trigonometric approach which served to study matrices with zeros having small supports, in that it considers copositive matrices in $\mathcal{C}^n$ with large supports of size $n-2$. On the other hand, it generalizes the Horn form and the Hildebrand matrices, which are of order $n = 5$, to families of basic exceptional extreme copositive forms of arbitrary order $n \geq 5$.

The defining property of the copositive matrices studied in [97] is that their support set contains n zero supports of cardinality $n-2$ which form the orbit of the index set $\{1, \dots, n-2\}$ under the action of cyclic permutations of the indices $\{1, \dots, n\}$. Two questions related to such matrices are considered. Firstly, the n zeros having the requested supports are fixed and the set of copositive forms having these zeros is studied. This set must be a face of the copositive cone $\mathcal{C}^n$. Surprisingly, the considered condition on the support set is restrictive enough to determine the structure of this face in most cases. Secondly, the whole variety of copositive matrices with support set having the considered property is studied. This variety is shown to contain large families of exceptional extreme rays of $\mathcal{C}^n$. We give explicit examples of circulant exceptional extreme matrices from this variety for every $n \geq 5$.

The proof of these results has been made possible by establishing a link between the properties of the copositive matrices in question and the behaviour of a certain periodic discrete time-varying linear dynamical system whose coefficients are given by the elements of the n defining zeros. Parts of the theory developed in [97] can also be applied to copositive matrices with zeros having smaller support, given the set of the supports still has the cyclic structure described in the previous paragraph.

Let us now summarize the elaborated approach to exceptional extremal copositive matrices. We divide our study in two steps. First we look at the possible support sets of extremal copositive matrices, constrained by necessary conditions on the zeros. This step can be characterized as a qualitative analysis, because the main object is of a combinatorial nature. Then we consider which extremal copositive matrices exist with a given support set. This step is of a quantitative nature, and essentially boils down to solving underdetermined systems of algebraic equations. Both steps encounter difficulties when the order of the copositive matrices increases. One problem is the exploding number of possible support sets, and the other is the increasing complexity of the system of equations. There are two regimes where these problems seem manageable. If the supports of the zeros are small, of cardinality 2 or 3, then the trigonometric parametrization of the extremal matrices scaled such that their diagonal elements equal 1 yields a linear system on the parameterizing angles, and the corresponding families of extremal matrices can explicitly be written down. If the supports are large, then the corresponding system of equations is rigid enough to prevent a too complex structure of the extremal matrices.

2.1.4 Notations and preliminaries

In this subsection we introduce notations and provide definitions which are common for the subsequent sections. We also provide the first and second order optimality conditions which a zero u imposes on a copositive matrix A.

We shall denote vectors with lower-case letters and matrices with upper-case letters. Individual entries of a vector u or a matrix A will be denoted by u_i, A_{ij}, respectively. For a matrix A and a vector u of compatible size, the i-th element of the vector Au will be denoted by $(Au)_i$. Inequalities $u \geq 0$ on vectors will be meant element-wise. We denote by $\mathbf{1} = (1, \dots, 1)^T$ the all-ones vector.

For a subset $I \subset \{1, \dots, n\}$ we denote by A_I the principal submatrix of A whose elements have row and column indices in I, i.e. $A_I = (A_{ij})_{i,j \in I}$. Similarly for a vector $u \in \mathbb{R}^n$ we define the subvector $u_I = (u_i)_{i \in I}$.

The vector space of real symmetric matrices will be denoted by $\mathcal{S}^n$. The cones of positive semi-definite matrices, element-wise nonnegative matrices, element-wise nonnegative matrices with zero diagonal, and copositive matrices will be denoted by $\mathcal{S}_+^n$, $\mathcal{N}^n$, $\mathcal{N}_0^n$, and $\mathcal{C}^n$, respectively. Here a real symmetric $n \times n$ matrix A is *positive semi-definite* (PSD), denoted $A \succeq 0$, if $x^T A x \geq 0$ for all $x \in \mathbb{R}^n$, and *copositive* if $x^T A x \geq 0$ for all $x \in \mathbb{R}_+^n$. A copositive matrix $A \in \mathcal{C}^n$ will be called *exceptional* if $A \notin \mathcal{S}_+^n + \mathcal{N}^n$.

Definition 2.1.1. Let $K \subset \mathbb{R}^n$ be a closed convex cone. An element $x \in K$ is called *extremal* if for every $x_1, x_2 \in K$ such that $x_1 + x_2 = x$ there exists $\lambda \in [0, 1]$ such that $x_1 = \lambda x$, $x_2 = (1 - \lambda)x$. The conic hull of an extremal element is called *extreme ray* of K.

Let $C \subset \mathbb{R}^n$ be a closed convex set. An element $x \in C$ is called *extremal* if for every $x_1, x_2 \in C$ and $\lambda \in (0, 1)$ such that $\lambda x_1 + (1 - \lambda)x_2 = x$ we have that $x_1 = x_2 = x$.

An extreme ray or an extreme element is a special case of a face of a convex cone or set, respectively.

Definition 2.1.2. Let $K \subset \mathbb{R}^n$ be a closed convex cone. A convex subset $\mathcal{F} \subset K$ is a *face* of K if every closed line segment in K with a relative interior point in $\mathcal{F}$ must have both end points in $\mathcal{F}$. For $x \in K$ we let $\mathcal{F}^x$ equal the intersection of all faces of K containing x. This is itself a face, and is referred to as the *minimal face* of K containing x.

We shall deal almost exclusively with extreme elements and faces of the copositive cone $\mathcal{C}^n$.

For a given $n \geq 1$, denote by $E_{ij} = E_{ji}$, $i, j = 1, \dots, n$, the generators of the extreme rays of the cone $\mathcal{N}_n$, normalized such that their elements are from the set $\{0, 1\}$. Let e_i, $i = 1, \dots, n$ be the canonical basis vectors of $\mathbb{R}^n$, and let $\Delta_n = \{x \in \mathbb{R}_+^n \mid \sum_{j=1}^n x_j = 1\}$ be their convex hull.

Let $\mathrm{Aut}(\mathbb{R}_+^n)$ be the automorphism group of the positive orthant. It is generated by all $n \times n$ permutation matrices and by all $n \times n$ diagonal matrices with positive diagonal elements. This group generates a group $\mathcal{G}_n$ of automorphisms of the cones $\mathcal{S}_+^n$, $\mathcal{N}^n$, $\mathcal{C}^n$ by $A \mapsto GAG^T$, $G \in \mathrm{Aut}(\mathbb{R}_+^n)$.

We call a nonzero vector $u \in \mathbb{R}_+^n$ a *zero* of a copositive matrix $A \in \mathcal{C}^n$ if $u^T A u = 0$. We denote the set of zeros of A by $\mathcal{V}^A = \{u \in \mathbb{R}_+^n \setminus \{0\} \mid u^T A u = 0\}$. For a vector $u \in \mathbb{R}^n$ we define its *support* as $\operatorname{supp} u = \{i \in \{1, \dots, n\} \mid u_i \neq 0\}$. A zero u of a copositive matrix A is called *minimal* if there exists no zero v of A such that the inclusion $\operatorname{supp} v \subset \operatorname{supp} u$ holds strictly. We shall denote the set of minimal zeros of a copositive matrix A by $\mathcal{V}_{\min}^A$. The *support set* of A is the set $\operatorname{supp} \mathcal{V}^A = \{\operatorname{supp} u \mid u \in \mathcal{V}^A\}$, and the *minimal support set* is the set $\operatorname{supp} \mathcal{V}_{\min}^A = \{\operatorname{supp} u \mid u \in \mathcal{V}_{\min}^A\}$.

Definition 2.1.3. [54, Definition 1.1] For a matrix $A \in \mathcal{C}^n$ and a subset $\mathcal{M} \subset \mathcal{C}^n$, we say that A is *reduced with respect to* $\mathcal{M}$ if there do not exist $\gamma > 0$ and $M \in \mathcal{M} \setminus \{0\}$ such that $A - \gamma M \in \mathcal{C}^n$.

For simplicity we speak about reducedness with respect to M when $\mathcal{M} = \{M\}$. Note that if a matrix A is on an exceptional extreme ray of $\mathcal{C}^n$, then A must be reduced with respect to both $\mathcal{S}_+^n$ and $\mathcal{N}^n$.

Let now u be a zero of a copositive matrix A. Then $x = u$ is a global minimum of the quadratic function $x^T A x$ on the nonnegative orthant, and this function fulfills the necessary optimality conditions at this point. These conditions translate to the following result.

Lemma 2.1.4. *Let $u \in \mathbb{R}^n_+$ with support $I = \operatorname{supp} u \subset \{1, \dots, n\}$ be a zero of a copositive matrix $A \in \mathcal{C}^n$. Define $I' = \{1, \dots, n\} \setminus \operatorname{supp} Au$. Then the following conditions hold:*

first-order conditions: $Au \geq 0$, $I \subset I'$;

second-order conditions: the submatrix $A_{I'}$ can be written as a sum $P + C$, where P is positive semi-definite, and C is copositive such that its non-zero elements are contained in the subblock $C_{I' \setminus I}$.

In particular, the submatrix A_I is positive semi-definite.

The first order condition and the condition $A_I \succeq 0$ are in [51, Lemma 7], the full second-order condition is in [11, Lemma 3.1]. Note that the nonnegative vector Au is precisely the vector λ of Lagrange multipliers corresponding to the constraints $x \geq 0$. The inclusion $I \subset I'$ is then nothing else than the complementarity conditions $\lambda_i u_i = 0$.

These conditions enforce positive semi-definiteness of A in the presence of zeros with large supports. Clearly, if there is a zero u of A with $\operatorname{supp} u = \{1, \dots, n\}$, then A is positive semi-definite. However, we also have the following result [11, Corollary 3.2].

Corollary 2.1.5. *Let $A \in \mathcal{C}^n$ and let $u \in \mathcal{V}^A$ such that $|\operatorname{supp}(u)| = n - 1$ and $Au = 0$. Then $A \in \mathcal{S}^n_+$.*

2.2 The cone $\mathcal{C}^5$

2.2.1 Introduction

In this section we study the extreme rays of the copositive cone $\mathcal{C}^5$. We present a synthesis of the papers [54, 90]. The outline of the section is as follows. First we derive a necessary and sufficient condition on a copositive matrix to be reduced with respect to the extremal matrix E_{ij} of the cone of nonnegative matrices, for $i \neq j$. This will be accomplished in Subsection 2.2.2. Next we introduce the trigonometric parametrization of reduced copositive matrices with diagonal elements equal to 1. This will be done in Subsection 2.2.3. Then we study the support set of an exceptional copositive matrix in $\mathcal{C}^5$ which is reduced with respect to the cone of nonnegative matrices with zero diagonal. This step will be accomplished in Subsection 2.2.4. Next we shall investigate which support sets give rise to exceptional extremal matrices, and parameterize these matrices with the help of the trigonometric transformation. This will be accomplished in Subsection 2.2.5. Finally, we consider the affine section of $\mathcal{C}^5$ which consists of the matrices with all diagonal elements equal to 1, and give a semi-definite description of this section. This will be the subject of Subsection 2.2.6.

The value $n = 5$ is the smallest order for which there exist matrices in $\mathcal{C}^n$ which cannot be represented as a sum of a positive semi-definite matrix and a nonnegative matrix. An example of such a matrix is the *Horn form* [82]

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}. \tag{2.1}$$

The Horn form has been characterized as an exceptional extreme ray of $\mathcal{C}^5$. It follows that all forms that can be obtained from the Horn form by a permutation of the indices and a scaling with a positive diagonal matrix, i.e., the $\mathcal{G}_5$-orbit of the Horn form, are also extreme rays of $\mathcal{C}^5$ which do not belong to $\mathcal{S}^5_+ + \mathcal{N}_5$.

Much work has also been devoted to characterize the difference between the completely positive cone $\mathcal{C}^*_n$ and the intersection $\mathcal{S}^n_+ \cap \mathcal{N}_n$, which are the dual cones to $\mathcal{C}^n$ and $\mathcal{S}^n_+ + \mathcal{N}_n$, respectively. Special emphasis has been made on the 5×5 case. In [227] the extreme rays of $\mathcal{S}^n_+ \cap \mathcal{N}_n$ for $n = 5, 6$ are characterized, and a procedure for general n is given. An earlier paper with a partial characterization of the 5×5 completely positive cone is [224]. In [37] extreme rays of $\mathcal{S}^5_+ \cap \mathcal{N}_5$ which do not belong to $\mathcal{C}^*_5$ are characterized and it is shown how to separate them from $\mathcal{C}^*_5$ by a copositive matrix.

2.2.2 Copositive matrices reduced with respect to E_{ij}

We now consider weaker properties than extremality, namely reducedness with respect to the cone $\mathcal{N}^n$ of nonnegative matrices, and reducedness with respect to the cone $\mathcal{N}_0^n$ of nonnegative matrices with zero diagonal. The first of these properties has been utilized and recognized as being more convenient than extremality already in the early work on copositive matrices [51],[82],[12]. In particular, it was studied by Baumert who gave a characterisation of copositive matrices which are reduced with respect to E_{ii} [11, Theorem 3.4].

Lemma 2.2.1. *A matrix $A \in \mathcal{C}^n$ is reduced with respect to the matrix E_{ii}, $i = 1, \dots, n$, if and only if there exists a zero u of A such that $u_i > 0$.*

It follows for a copositive matrix which is reduced with respect to $\mathcal{N}^n$ that for every $i = 1, \dots, n$ there exists a zero such that $u_i > 0$. This condition is not strong enough to reasonably restrict the support set of a reduced matrix. However, a matrix which is reduced with respect to $\mathcal{N}^n$ is also reduced with respect to E_{ij} for $i \neq j$, which gives another source of information on the support set. Our key result is the following analog of Lemma 2.2.1 [54, Theorem 2.6].

Theorem 2.2.2. *Let $A \in \mathcal{C}^n$, $n \geq 2$, and let $1 \leq i, j \leq n$. Then the following conditions are equivalent.*

(i) A is reduced with respect to E_{ij},

(ii) there exists $u \in \mathcal{V}^A$ such that $(Au)_i = (Au)_j = 0$ and $u_i + u_j > 0$.

The theorem shows that reducedness with respect to E_{ij} is tied to the presence of a zero u with certain properties involving both the support of the zero u and the support of the Lagrange multiplier $\lambda = Au$. Clearly a copositive matrix A is reduced with respect to $\mathcal{N}_0^n$ if and only if it is reduced with respect to all E_{ij}, $i \neq j$. This property has strong implications, especially in the presence of zeros with large support.

We have the following result [54, Lemma 4.12].

Lemma 2.2.3. *Let $A \in \mathcal{C}^n$ be reduced with respect to $\mathcal{N}_0^n$, and assume there is a $(n-1) \times (n-1)$ principal submatrix B of A which is positive semi-definite. Then $A \in \mathcal{S}_+^n$.*

In conjunction with Corollary 2.1.5 this gives the following [54, Corollary 4.15].

Corollary 2.2.4. *Let $A \in \mathcal{C}^n$ be reduced with respect to $\mathcal{N}_0^n$, and let u be a zero of A with $|\operatorname{supp}(u)| \geq n-2$. If $|\operatorname{supp} Au| < 2$, then $A \in \mathcal{S}_+^n$.*

Clearly an exceptional copositive matrix $A \in \mathcal{C}^n$ cannot have a zero with support of cardinality n, because in this case A is positive semi-definite by Lemma 2.1.4. If the matrix is in addition reduced with respect to $\mathcal{N}_0^n$, then it cannot have even a zero with cardinality $n-1$, because it must again be positive semi-definite by Lemma 2.2.3. On the other hand, if it has a zero with support of cardinality 1, then it must have a zero row and is essentially given by a copositive matrix form $\mathcal{C}^{n-1}$. This leads to the following result.

Lemma 2.2.5. *Let $A \in \mathcal{C}^n$ be an exceptional copositive matrix with positive diagonal elements which is reduced with respect to $\mathcal{N}_0^n$. Then the support of any zero of A has cardinality between 2 and $n-2$.*

The following result is evident.

Lemma 2.2.6. *Let $A \in \mathcal{S}_+^n + \mathcal{N}^n$ be reduced with respect to $\mathcal{N}_0^n$. Then $A \in \mathcal{S}_+^n$.*

From work done on the copositive completion problem [102] we have also the following result [54, Lemma 4.5].

Lemma 2.2.7. *Let $A \in \mathcal{C}^n$ with $\operatorname{diag} A = \mathbf{1}$ be reduced with respect to $\mathcal{N}_0^n$. Then $a_{ij} \in [-1, 1]$ for all i, j.*

This result allows us to apply the trigonometric parametrization introduced in the next subsection.

2.2.3 The trigonometric parametrization

Let $A \in \mathcal{S}^n$ have diagonal elements equal to 1 and assume its off-diagonal elements are contained in the interval $[-1,1]$. Then A_{ij} can be written as $-\cos\varphi_{ij}$ for some angle $\varphi_{ij} \in [0,\pi]$. To appreciate the benefits of this parametrization, we shall first consider copositive matrices of order $n=3$.

The cone $\mathcal{C}^3$ has been characterized in [81, Theorem 4]. A reformulation of this result in terms of the angles leads to the following.

Lemma 2.2.8. *Let*

$$A = \begin{pmatrix} 1 & -\cos\varphi_{12} & -\cos\varphi_{13} \\ -\cos\varphi_{12} & 1 & -\cos\varphi_{23} \\ -\cos\varphi_{13} & -\cos\varphi_{23} & 1 \end{pmatrix} \tag{2.2}$$

for some angles $\varphi_{ij} \in [0,\pi]$. Then A is copositive if and only if $\varphi_{12}+\varphi_{13}+\varphi_{23} \geq \pi$.

The algebraic constraint $\det A \geq 0$ from [81] has thus been converted into a *linear* constraint on the angles φ_{ij}. Define the vector $\varphi = (\varphi_{12},\varphi_{13},\varphi_{23})^T$ and let $\Delta = \{\varphi \in [0,\pi]^3 \,|\, \mathbf{1}^T\varphi = \pi\}$. Then we have for $A \in \mathcal{C}^3$ as in (2.2):

- A is reduced with respect to $\mathcal{N}_0^3$ if and only if $\varphi \in \Delta$;
- φ is a vertex of Δ if and only if $\operatorname{supp}\mathcal{V}^A = \{\{i,j\},\{j,k\},\{1,2,3\}\}$;
- $\{i,j\},\{j,k\} \in \operatorname{supp}\mathcal{V}^A$ if and only if $\{1,2,3\} \in \operatorname{supp}\mathcal{V}^A$ and $\varphi_{ik} = \pi$;
- $\operatorname{supp}\mathcal{V}^A = \{\{1,2,3\}\}$ if and only if φ is in the relative interior of Δ, in this case the zero is proportional to $(\sin\varphi_{23},\sin\varphi_{13},\sin\varphi_{12})^T$;
- $\{i,j\} \in \operatorname{supp}\left(\mathcal{V}^A\right)$ if and only if $\varphi_{ij} = 0$, in this case $e_i + e_j$ is a zero;
- if $\{i,j\},\{1,2,3\} \in \operatorname{supp}\left(\mathcal{V}^A\right)$, then either $\{i,k\}$ or $\{j,k\}$ are in $\operatorname{supp}\left(\mathcal{V}^A\right)$.

Here (i,j,k) stands for some permutation of $(1,2,3)$.

Conditions on the support set of A hence translate into linear equality and inequality constraints on the angle vector φ. If we consider copositive matrices of general order n, then the above relations hold for every 3×3 principal submatrix of A.

The parametrization $A_{ij} = -\cos\varphi_{ij}$ has close connections to the semi-definite approximation of the MAXCUT problem by Goemans and Williamson [75] and to Nesterovs $\frac{\pi}{2}$-theorem in the semi-definite approximation of nonconvex quadratic optimization problems [164].

Definition 2.2.9. The *MAXCUT polytope* $\mathcal{MC}_n \subset \mathcal{S}_+^n$ is the convex hull of all matrices $A \in \mathcal{S}_+^n$ such that $A_{ij} \in \{-1,+1\}$ for all $i,j = 1,\dots,n$, i.e., all matrices of the form vv^T, $v \in \{-1,+1\}^n$.

The following lemma is a consequence of [75, Lemma 3.2].

Lemma 2.2.10. *[100, Corollary 4.3] Let $A \in \mathcal{S}_+^n$ be a positive semi-definite matrix with $A_{ii} = 1$, $i = 1,\dots,n$. Let B be the real symmetric $n\times n$ matrix defined entry-wise by $B_{ij} = \frac{2}{\pi}\arcsin A_{ij}$, $i,j = 1,\dots,n$. Then $B \in \mathcal{MC}_n$.*

The function $f(x) = \frac{2}{\pi}\arcsin x$ maps the interval $[-1,+1]$ monotonically onto itself and plays an important role in the results cited above when applied element-wise to positive semi-definite matrices with diagonal elements equal to 1. If we introduce the affine transformation $[0,\pi] \ni \varphi_{ij} \mapsto \beta_{ij} = \frac{2}{\pi}\varphi_{ij} - 1$, then we obtain $\beta_{ij} = \frac{2}{\pi}\arcsin A_{ij}$, i.e., the transformation used in our trigonometric parametrization equals the function f up to an affine scaling. We may define the following analog of the MAXCUT polytope for copositive matrices with unit diagonal.

Definition 2.2.11. The *triangle-free polytope* $\mathcal{TF}_n \subset \mathcal{S}^n$ is the convex hull of all matrices $A \in \mathcal{S}^n$ such that $A_{ij} \in \{-1,+1\}$ for all $i,j = 1,\dots,n$, $\operatorname{diag} A = \mathbf{1}$, and the incidence graph of the -1 entries is triangle-free.

We have the obvious inclusion $\mathcal{MC}_n \subset \mathcal{TF}_n$. Moreover, by [88] the extreme copositive matrices of $\mathcal{C}^n$ with elements in $\{-1,+1\}$ are exactly those vertices of $\mathcal{TF}_n$ which are reduced with respect to $\mathcal{N}_0^n$. The above characterization of the unit diagonal section of $\mathcal{C}^3$ can be reformulated as follows.

Corollary 2.2.12. *A matrix $A \in \mathcal{S}^3$ with unit diagonal is in $\mathcal{C}^3$ if and only if it is in the sum $f^{-1}[\mathcal{TF}_3] + \mathcal{N}_0^3$, where the function $f^{-1}(\varphi) = \sin\frac{\pi}{2}\varphi$ is applied element-wise.*

Thus portions of the boundary of $\mathcal{C}^3$ are mapped to facets of $\mathcal{TF}_3$ by the function f.

2.2.4 Copositive matrices reduced with respect to $\mathcal{N}_0^5$

In this subsection we restrict the support sets of exceptional copositive matrices $A \in \mathcal{C}^5$ which are reduced with respect to the cone of nonnegative matrices with zero diagonal.

An exceptional copositive matrix $A \in \mathcal{C}^5$ which is reduced with respect to $\mathcal{N}_0^5$ can only have zeros with supports of cardinality 2 or 3 by Lemma 2.2.5. This gives still $\sim 10^4$ possible support sets, up to permutation of the indices $1,\dots,5$. We can, however, further constrain the support set of A. In addition to the constraints from Subsection 2.2.3, which apply to every 3×3 principal submatrix of A, we have the following restrictions:

- For every index i there exist distinct indices j,k such that there is no zero u with $j,k \in \operatorname{supp} u$ and $i \notin \operatorname{supp} u$. Indeed, if for some i such vertices j,k do not exist, then by Theorem 2.2.2 the 4×4 submatrix $A_{\{1,\dots,5\}\setminus\{i\}}$ is a copositive matrix which is reduced with respect to $\mathcal{N}_0^4$. But this submatrix is in $\mathcal{S}_+^4 + \mathcal{N}^4$, and hence must be positive semi-definite by Lemma 2.2.6. Hence A is positive semi-definite by Lemma 2.2.3, leading to a contradiction with exceptionality.

- For every pair (i,j) of indices, $i \neq j$, there either exists a zero u with $i,j \in \operatorname{supp} u$, or there exists a zero u with $|\operatorname{supp} u| = 2$ and $\{i,j\} \cap \operatorname{supp} u \neq \emptyset$. Indeed, by Theorem 2.2.2 for every pair (i,j) there exists a zero u with $\{i,j\} \cap \operatorname{supp} u \neq \emptyset$, and $(Au)_i = (Au)_j = 0$ if $u_i u_j = 0$. Hence if the condition does not hold for some pair (i,j), then there exists a zero u with $|\operatorname{supp} u| = 3$, $\{i,j\} \not\subset \operatorname{supp} u$, $(Au)_i = (Au)_j = 0$. Then $A \in \mathcal{S}_+^5$ by Corollary 2.2.4, a contradiction.

Supports with cardinality 2 or 3 can conveniently be represented by edges in a graph on 5 vertices. We will represent a support $\{i,j\}$ by a dashed edge between the vertices i and j, whilst we will represent a support $\{1,\dots,5\} \setminus \{i,j\}$ by a solid edge between the vertices i and j. There are 17 support sets satisfying above conditions, up to permutation of the vertices. They give rise to the graphs in Fig. 2.1.

In order to describe the exceptional matrices $A \in \mathcal{C}^5$ which are reduced with respect to $\mathcal{N}_0^5$ we have to consider each of these 17 cases of support sets. We assume without loss of generality that $\operatorname{diag} A = \mathbf{1}$, because every such matrix A has a positive diagonal which can be scaled to $\mathbf{1}$ by a symmetry from $\mathcal{G}_5$. We may then parameterize the off-diagonal elements $A_{ij} = -\cos\varphi_{ij}$ by angles $\varphi_{ij} \in [0,\pi]$. The support set yields linear conditions on these angles by the relations established in Subsection 2.2.3. Using these conditions to eliminate variables and applying the reducedness conditions in Theorem 2.2.2, we obtain that

- the support sets given by the graphs (a),(b),(c),(d),(e),(f),(k),(l),(q) do not correspond to an exceptional reduced copositive matrix;

- the support sets given by the graphs (g),(h),(i),(j),(m),(n),(o),(p) lead to the matrices

$$T(\psi) = \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix}, \qquad (2.3)$$

where $\psi = (\psi_1,\dots,\psi_5)^T$ is a quintuple of angles satisfying $\psi_i \in [0,\pi)$, $i = 1,\dots,5$, and $\sum_{i=1}^5 \psi_i < \pi$. Here the individual cases correspond to

(g) $\psi_2,\psi_3,\psi_5 > 0$, $\psi_1 = \psi_4 = 0$;

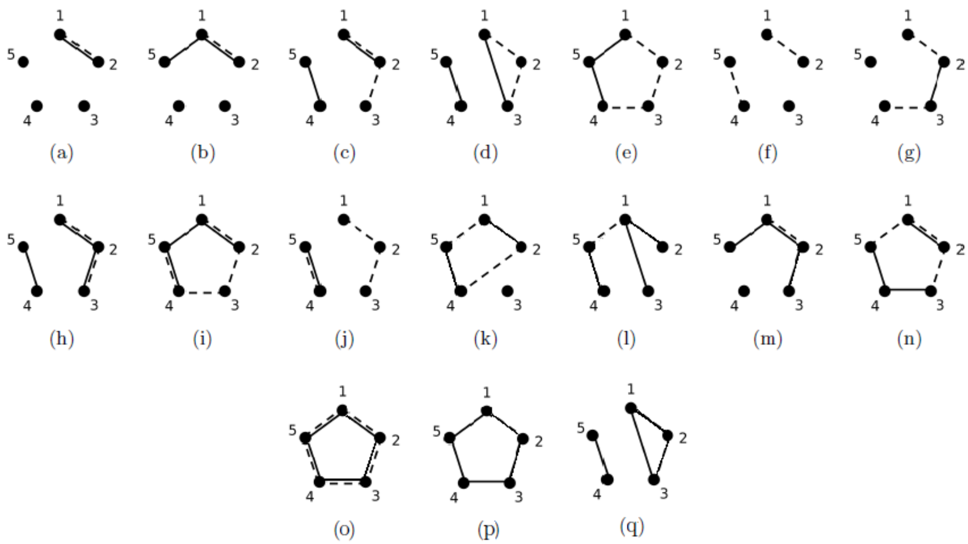

Figure 2.1: Graphs of possible support sets of an exceptional copositive 5×5 matrix which is reduced with respect to $\mathcal{N}_0^5$. A dashed edge between vertices i and j represents a zero with support $\{i, j\}$, whilst a solid edge between the vertices i and j represents a zero with support $\{1, \dots, 5\} \setminus \{i, j\}$.

(h) $\psi_1, \psi_2, \psi_3 > 0$, $\psi_4 = \psi_5 = 0$;

(i) $\psi_3 > 0$, $\psi_1 = \psi_2 = \psi_4 = \psi_5 = 0$;

(j) $\psi_1, \psi_3 > 0$, $\psi_2 = \psi_4 = \psi_5 = 0$;

(m) $\psi_1, \psi_2, \psi_3, \psi_5 > 0$, $\psi_4 = 0$;

(n) $\psi_1, \psi_2 > 0$, $\psi_3 = \psi_4 = \psi_5 = 0$;

(o) $\psi = 0$;

(p) $\psi > 0$.

The cases (o),(p),(q) have already been considered by Baumert [10], who determined that case (o) leads to the Horn form, (p) leads to extremal exceptional copositive matrices of some new type, and (q) does not correspond to any exceptional copositive matrices which are reduced with respect to $\mathcal{N}^5$.

Each support set in Fig. 2.1 is hence represented by matrices $T(\psi)$ in the relative interior of some face of the simplex

$$\Psi = \{\psi \in [0, \pi]^5 \mid \mathbf{1}^T \psi \leq \pi\}. \tag{2.4}$$

If we consider also the support sets which are obtained from those in Fig. 2.1 by cyclic permutations of the indices $1, \dots, 5$, we obtain all faces of Ψ with the exception of those in the facet $\{\psi \in [0, \pi]^5 \mid \mathbf{1}^T \psi = \pi\}$.

In fact, the matrices $T(\psi)$ for ψ in this facet are positive semi-definite. This can be easily seen by the factorization

$$T(\psi) = \begin{pmatrix} \cos(\psi_4 + \psi_5) \\ -\cos\psi_5 \\ 1 \\ -\cos\psi_1 \\ \cos(\psi_1 + \psi_2) \end{pmatrix} \begin{pmatrix} \cos(\psi_4 + \psi_5) \\ -\cos\psi_5 \\ 1 \\ -\cos\psi_1 \\ \cos(\psi_1 + \psi_2) \end{pmatrix}^T + \begin{pmatrix} \sin(\psi_4 + \psi_5) \\ -\sin\psi_5 \\ 0 \\ \sin\psi_1 \\ -\sin(\psi_1 + \psi_2) \end{pmatrix} \begin{pmatrix} \sin(\psi_4 + \psi_5) \\ -\sin\psi_5 \\ 0 \\ \sin\psi_1 \\ -\sin(\psi_1 + \psi_2) \end{pmatrix}^T,$$

where $\psi_3 = \pi - \psi_1 - \psi_2 - \psi_4 - \psi_5$.

In order to demonstrate that the matrices $T(\psi)$ for ψ in the other facets of Ψ are indeed copositive, we can decompose them into a sum of a positive semi-definite matrix and a matrix in the $\mathcal{G}_5$-orbit of the Horn form (2.1). For the facet $\{\psi \in [0,\pi]^5 \mid \mathbf{1}^T\psi < \pi,\ \psi_4 = 0\}$ we get for example

$$T(\psi) = vv^T + \operatorname{diag}(d) H \operatorname{diag}(d)$$

with

$$v = \begin{pmatrix} -\sin(\frac{1}{2}(\ \ \psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ \sin(\frac{1}{2}(\ \ \psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ -\sin(\frac{1}{2}(-\psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ \sin(\frac{1}{2}(-\psi_5 - \psi_1 + \psi_2 + \psi_3)) \\ -\sin(\frac{1}{2}(-\psi_5 - \psi_1 - \psi_2 + \psi_3)) \end{pmatrix}, \qquad d = \begin{pmatrix} \cos(\frac{1}{2}(\ \ \psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ \cos(\frac{1}{2}(\ \ \psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ \cos(\frac{1}{2}(-\psi_5 + \psi_1 + \psi_2 + \psi_3)) \\ \cos(\frac{1}{2}(-\psi_5 - \psi_1 + \psi_2 + \psi_3)) \\ \cos(\frac{1}{2}(-\psi_5 - \psi_1 - \psi_2 + \psi_3)) \end{pmatrix}.$$

Note that $v = 0$ if and only if $\psi = 0$, and $d > 0$ if $\mathbf{1}^T\psi < \pi$. These decompositions are due to P. Dickinson and L. Gijben. That these matrices are indeed reduced with respect to $\mathcal{N}_0^5$ can be checked directly by applying the criterion in Theorem 2.2.2. We hence get the following result.

Lemma 2.2.13. *Let $\psi \in [0,\pi)^5$ be such that $\mathbf{1}^T\psi < \pi$ and $\min_i \psi_i = 0$. Then the matrix $T(\psi)$ is copositive and reduced with respect to $\mathcal{N}_0^5$. It is extremal if and only if $\psi = 0$, in which case it equals the Horn form. In all other cases it can be represented as a non-trivial sum of a rank 1 positive semi-definite matrix and a matrix in the $\mathcal{G}_5$-orbit of the Horn form.*

The case when ψ is in the interior of the simplex Ψ, which corresponds to the support set represented by the graph (p) in Fig. 2.1, is more complicated and treated in the next subsection.

2.2.5 Exceptional extreme rays of $\mathcal{C}^5$

In the previous subsection we characterized all support sets of exceptional copositive matrices in $\mathcal{C}^5$ which are reduced with respect to $\mathcal{N}_0^5$. This is a necessary, but not a sufficient condition for extremality. Indeed, not all matrices $T(\psi)$ are extremal, as demonstrated in Lemma 2.2.13. We described the families of reduced copositive matrices corresponding to all support sets except case (p) in Fig. 2.1. In this subsection we show that this support set corresponds to the matrices $T(\psi)$ with ψ in the interior of the simplex Ψ defined in (2.4). We will give only a sketch of the proof, which is to some extent simpler than the original proof in [90].

Lemma 2.2.14. *Let ψ be a vector in the interior of Ψ. Then $T(\psi)$ is copositive and extremal in $\mathcal{C}^5$.*

The proof of copositivity is in two steps. First we prove that $T(\psi)$ is nonnegative on all vectors on the boundary of $\mathbb{R}_+^5$, and then we prove copositivity by a standard determinantal criterion.

Let ψ be in the interior of Ψ and introduce positive quantities $t_1 = \cos(\psi_5+\psi_1+\psi_2)+\cos(\psi_3+\psi_4) > 0$, and $t_2,\dots,t_5$ defined in a similar way after cyclic permutation of the indices. Then the upper left 4×4 principal submatrix of $T(\psi)$ can be written as

$$\begin{aligned}(T(\psi))_{\{1,2,3,4\}} &= \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & -\cos(\psi_4+\psi_5+\psi_1)+t_5 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 \\ -\cos(\psi_4+\psi_5+\psi_1)+t_5 & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \sin\psi_4 & -\cos\psi_4 \\ 0 & 1 \\ -\sin\psi_5 & -\cos\psi_5 \\ \sin(\psi_1+\psi_5) & \cos(\psi_1+\psi_5) \end{pmatrix} \begin{pmatrix} \sin\psi_4 & -\cos\psi_4 \\ 0 & 1 \\ -\sin\psi_5 & -\cos\psi_5 \\ \sin(\psi_1+\psi_5) & \cos(\psi_1+\psi_5) \end{pmatrix}^T + t_5E_{14},\end{aligned}$$

which shows that this submatrix is in $\mathcal{S}_+^4 + \mathcal{N}^4$. The other 4×4 principal submatrices are copositive by a similar argument.

Next we show that $\det T(\psi) > 0$. The proof is by direct calculation, which is most easily done by introducing complex variables $z_j = e^{i\psi_j}$, $j = 1,\dots,5$. Then

$$\det T(\psi) = \frac{t_1t_2t_3t_4t_5}{1+\cos(\psi_1+\psi_2+\psi_3+\psi_4+\psi_5)} > 0.$$

It follows that $T(\psi)$ is copositive by [44, Theorem 3.1].

Finally, let $u^1,\dots,u^5$ be the zeros of $T(\psi)$, which are given by the columns of the matrix

$$\begin{pmatrix} \sin(\psi_3+\psi_4) & \sin\psi_5 & 0 & 0 & \sin\psi_2 \\ \sin\psi_3 & \sin(\psi_4+\psi_5) & \sin\psi_1 & 0 & 0 \\ 0 & \sin\psi_4 & \sin(\psi_5+\psi_1) & \sin\psi_2 & 0 \\ 0 & 0 & \sin\psi_5 & \sin(\psi_1+\psi_2) & \sin\psi_3 \\ \sin\psi_4 & 0 & 0 & \sin\psi_1 & \sin(\psi_2+\psi_3) \end{pmatrix}.$$

Every matrix A in the minimal face of $T(\psi)$ must satisfy the linear conditions $(Au^j)_{\operatorname{supp} u^j} = 0$. This gives a linear system of 15 equations on the 15 coefficients of A. By passing again to the complex variables $z_j = e^{i\psi_j}$, the minors of the coefficient matrix can be factorized into components which are of small degree in the z_j. It is then easily seen that this coefficient matrix has corank 1, and hence the only solutions of the system are the multiples of $T(\psi)$ itself. This shows that $T(\psi)$ is extremal.

We may formalize this result as follows.

Theorem 2.2.15. *A matrix $A \in \mathcal{C}^5$ is an exceptional copositive matrix that is reduced with respect to $\mathcal{N}_0^5$ if and only if it is in the $\mathcal{G}_5$-orbit of a matrix $T(\psi)$ as given by (2.3) with $\psi = (\psi_1,\dots,\psi_5)^T$ satisfying $\psi_i \in [0,\pi)$, $i=1,\dots,5$, and $\sum_{i=1}^5 \psi_i < \pi$.*

A matrix $A \in \mathcal{C}^5$ is an exceptional extremal copositive matrix if and only if it is in the $\mathcal{G}_5$-orbit of a matrix $T(\psi)$ with either $\psi = 0$ (A is in the $\mathcal{G}_5$-orbit of the Horn form) or ψ in the interior of the simplex Ψ given by (2.4) (A is a Hildebrand matrix).

Every exceptional copositive matrix $A \in \mathcal{C}^5$ can be written as a sum $C+N$, where N is nonnegative with zero diagonal, and C is in the $\mathcal{G}_5$-orbit of a matrix $T(\psi)$ with $\psi_i \in [0,\pi)$, $i=1,\dots,5$, and $\sum_{i=1}^5 \psi_i < \pi$.

While the orbit of the Horn form represents a 5-dimensional variety, the Hildebrand matrices form a 10-dimensional variety, parameterized by the diagonal elements of D in the scaling element of $\mathcal{G}_5$ and the quintuple of angles ψ in the normal form $T(\psi)$. Here for each permutation $P \in S_5$ we obtain a smooth component of this variety. Cyclic permutations of the indices and a complete reversal of order leave the support set of the Horn form and of the matrices $T(\psi)$, ψ from the interior of Ψ, invariant. Hence the smooth component of these matrices is also invariant with respect to this subgroup. Thus there exist $5!/10 = 12$ such smooth components.

2.2.6 The diagonal 1 section of $\mathcal{C}^5$

In this subsection we consider those copositive 5×5 matrices whose diagonal elements equal 1. Denote the subset of these matrices by $\mathcal{C}_{\mathbf{1}}^5$. It is a 10-dimensional subset of $\mathcal{S}^5$. The action of a general element of the group $\mathcal{G}_5$ does not preserve $\mathcal{C}_{\mathbf{1}}^5$, it is, however, still invariant under simultaneous permutations of the row and column indices. In contrast to the diagonal 1 section of the positive semi-definite cone the set $\mathcal{C}_{\mathbf{1}}^5$ is not compact. Its recession cone has, however, a simple description.

Lemma 2.2.16. *The recession cone of $\mathcal{C}_{\mathbf{1}}^5$ is given by the cone $\mathcal{N}_0^5$ of nonnegative matrices with zero diagonal.*

This follows from the evident fact that the recession cone of $\mathcal{C}_{\mathbf{1}}^5$ equals the intersection of $\mathcal{C}^5$ with the subspace of real symmetric matrices with zero diagonal.

In general, an extreme element of an affine section of a convex cone does not need to lie on an extreme ray of this cone, and the set of extreme elements of the section can be much more complex than the set of extreme rays of the cone. However, in the case of $\mathcal{C}_{\mathbf{1}}^5$ we have the following result.

Lemma 2.2.17. *Let A be an extreme element of $\mathcal{C}_{\mathbf{1}}^5$. Then either $A \in \mathcal{S}_+^5 + \mathcal{N}^5$, or there exists a permutation matrix $P \in S_5$ and a quintuple of angles $\psi \in \Psi$, $\mathbf{1}^T\psi < \pi$, such that $A = PT(\psi)P^T$, where Ψ is the simplex given by (2.4), and $T(\psi)$ is given by (2.3).*

This lemma is a direct consequence of Theorem 2.2.15. It allows to deduce a semi-definite description of $\mathcal{C}_{\mathbf{1}}^5$ by virtue of Parrilos hierarchy of inner semi-definite approximations of the copositive cone [175].

Here for an integer $r \geq 0$ the r-th Parrilos semi-definite approximation of $\mathcal{C}^n$ is given by the cone $\mathcal{K}_r^n$ of matrices $A \in \mathcal{S}^n$ such that the polynomial $p(x) = \sum_{i,j=1}^5 A_{ij}x_i^2x_j^2$ equals the ratio $\frac{\Sigma(x)}{(\sum_{i=1}^5 x_i^2)^r}$, where $\Sigma(x)$ is a sum of squares of polynomials of degree $r+2$ in x. We have the chain of inclusions $\mathcal{K}_r^n \subset \mathcal{K}_{r'}^n$ for $r \leq r'$, and $\mathcal{C}^n$ equals the closure of the union $\bigcup_{r\geq 0} \mathcal{K}_r^n$. Moreover, the simplest relaxation equals $\mathcal{K}_0^n = \mathcal{S}_+^n + \mathcal{N}^n$. It has been checked by P. Dickinson and L. Gijben that for every $\psi \in \Psi$ we have $T(\psi) \in \mathcal{K}_1^5$, and hence also $PT(\psi)P^T \in \mathcal{K}_1^5$ for every permutation matrix $P \in S_5$. By virtue of the preceding lemma we then get the following result, proven in [55].

Theorem 2.2.18. *A matrix $A \in \mathcal{S}^5$ with all diagonal elements equal to 1 is copositive if and only if it is an element of $\mathcal{K}_1^5$.*

In order to check whether a given matrix $A \in \mathcal{S}^5$ with positive diagonal is copositive it hence suffices to check whether the matrix DAD is in $\mathcal{K}_1^5$, where D is a positive definite diagonal matrix chosen such that the diagonal elements of the product DAD all equal 1.

On the other hand, we have the following result [55].

Lemma 2.2.19. *Let $\mathcal{D}_n$ be the set of positive definite diagonal $n \times n$ matrices. Then for every $r \geq 0$ we have*

$$\bigcap_{D\in\mathcal{D}_n} D\mathcal{K}_r^n D = \mathcal{S}_+^n + \mathcal{N}^n.$$

Thus for $n \geq 5$ none of Parrilos relaxations of the copositive cone will be exact.

Finally we shall consider the image of $\mathcal{C}_1^5$ under the map $f(x) = \frac{2}{\pi} \arcsin x$ when applied element-wise. This map sends the set $\{T(\psi) \,|\, \psi \in \Psi\}$ to a simplex with vertex set $\{T(\psi) \,|\, \psi \text{ is a vertex of } \Psi\}$. This simplex is a 5-dimensional face of the triangle-free polytope $\mathcal{TF}_5$, but its relative interior is outside of the MAXCUT polytope $\mathcal{MC}_5$. In fact, we have the following result.

Lemma 2.2.20. *The image of the set $\mathcal{C}_1^5$ under the map $f(x) = \frac{2}{\pi} \arcsin x$ when applied element-wise is contained in the sum $\mathcal{TF}_5 + \mathcal{N}_0^5$.*

Note that for the cone $\mathcal{C}^3$ the analogous statement Corollary 2.2.12 is valid with equality.

2.3 Minimal zeros of copositive matrices

2.3.1 Introduction

In this section we consider a modification of the support set of a copositive matrix, namely the *minimal support set*. This set was introduced in [95] along with the notion of minimal zero. Since the minimal support set is a subset of the support set, the former is a coarser characteristic of the copositive matrix than the latter. This has the advantage that the number of possible minimal support sets for certain subclasses of copositive matrices is smaller than the number of possible support sets. The downside is, of course, some loss of information on the copositive matrix. The main motivation of introducing this characteristic is that the decrease in complexity outweighs this loss.

In Subsection 2.3.2 we elaborate some properties of minimal zeros and their supports. In Subsection 2.3.3 we shall show that reducedness of a copositive matrix $A \in \mathcal{C}^n$ with respect to the cones $\mathcal{N}^n$ and $\mathcal{S}_+^n$ can be expressed in terms of minimal zeros and entails constraints on its minimal support set. In Subsection 2.3.4 we apply the results in order to restrict the combinations of minimal zeros that can occur in exceptional extreme copositive matrices.

2.3.2 Minimal zeros of copositive matrices

In this subsection we describe some basic properties of minimal zeros and their relation to general zeros of a copositive matrix.

The following result follows from the optimality conditions in Lemma 2.1.4.

Corollary 2.3.1. *[95, Corollary 3.4] Let A be a copositive matrix and u a zero of A. Then u can be represented as a finite sum of minimal zeros of A.*

This means that the convex hull of the minimal zeros is an upper bound on the set of all zeros. The following result shows that up to multiplication by a constant, a minimal zero is defined by its support.

Lemma 2.3.2. *[95, Lemma 3.5] Let A be a copositive matrix and $u \in \mathcal{V}^A$. Then the following are equivalent.*

(a) u is a minimal zero of A,

(b) if v is another zero of A with support $\operatorname{supp} v \subset \operatorname{supp} u$, then there exists $\mu > 0$ such that $v = \mu u$.

The number of equivalence classes of minimal zeros with respect to multiplication by a positive constant is hence finite, and the classes of minimal zeros are in a one-to-one correspondence with the minimal support set $\operatorname{supp} \mathcal{V}^A_{\min}$. Next we give a characterization of minimal zeros in terms of principal submatrices.

Lemma 2.3.3. *[95, Lemma 3.7] Let $A \in \mathcal{C}^n$ be a copositive matrix and let $I \subset \{1, \dots, n\}$ be a nonempty index set. Then the following are equivalent.*

(a) A has a minimal zero with support I,

(b) the principal submatrix A_I is positive semi-definite with corank 1, and the generator of the kernel of A_I can be chosen such that all its elements are positive.

This lemma has an important consequence. If the index subset $I \subset \{1, \dots, n\}$ belongs to the minimal support set of some copositive matrix $A \in \mathcal{C}^n$, then every proper principal submatrix of A_I is positive definite. This implies, e.g., the following non-trivial result.

Theorem 2.3.4. *[95, Theorem 3.11] Let $A \in \mathcal{C}^n$ be a copositive matrix and $I \subset \{1, \dots, n\}$ an index set such that the principal submatrix A_I is positive definite. Let $u^1, \dots, u^m$ be zeros of A such that $(\operatorname{supp} u^l) \setminus I = \{k^l\}$ consists of exactly one element, and let u^l be normalized such that $u^l_{k^l} = 1$, $l = 1, \dots, m$. Suppose that the zeros $u^1, \dots, u^m$ are mutually different after normalization. Suppose further that $\operatorname{supp} u^r_I \subset \operatorname{supp} u^{r+1}_I$ for all $r = 1, \dots, m-1$.*

Then the indices $k^1, \dots, k^m$ are mutually different, and $u^1, \dots, u^m$ are minimal zeros. Moreover, if $v \in \mathcal{V}^A$ is a zero satisfying $\operatorname{supp} v \subset I \cup \{k^1, \dots, k^m\}$, then $v = \sum_{i=1}^m \alpha_i u^i$ for some nonnegative scalars α^i. If in addition v is minimal, then there exists $l \in \{1, \dots, m\}$ and $\alpha > 0$ such that $v = \alpha u^l$.

Theorem 2.3.4 restricts the ensemble of minimal zeros that a copositive matrix can have. For example, we have the following restriction on pairs of minimal zeros with overlapping supports.

Corollary 2.3.5. *[95, Corollary 3.12] Let A be a copositive matrix and u, v minimal zeros of A with supports $\operatorname{supp} u = I$, $\operatorname{supp} v = J$. Assume that $J \setminus I = \{k\}$ consists of one element. Then every zero w of A with support $\operatorname{supp} w \subset I \cup J$ can be represented as a convex conic combination $w = \alpha u + \beta v$ with $\alpha, \beta \geq 0$. In particular, up to multiplication by a positive constant, there are no minimal zeros w with $\operatorname{supp} w \subset I \cup J$ other than u and v.*

2.3.3 Minimal zeros of reduced copositive matrices

In this subsection we establish necessary and sufficient criteria for the reducedness of a copositive matrix $A \in \mathcal{C}^n$ with respect to the cones $\mathcal{N}^n$ and $\mathcal{S}^n_+$, respectively.

First we give a slightly stronger version of Theorem 2.2.2, by requiring the zero u to be *minimal*.

Lemma 2.3.6. *[95, Lemma 4.1] Let $A \in \mathcal{C}^n$, and let $i, j \in \{1, \dots, n\}$. Then A is reduced with respect to E_{ij} if and only if there exists a minimal zero u of A such that $(Au)_i = (Au)_j = 0$ and $u_i + u_j > 0$.*

This yields a necessary and sufficient condition on the reducedness of a copositive matrix with respect to the cones $\mathcal{N}^n$ and $\mathcal{N}^n_0$ in terms of minimal zeros only.

We shall now consider reducedness with respect to the cone of positive semi-definite matrices.

Lemma 2.3.7. *[95, Corollary 4.4] Let $A \in \mathcal{C}^n$ be a copositive matrix and let $w \in \mathbb{R}^n$ be a nonzero vector. Then A is reduced with respect to ww^T if and only if there exists a minimal zero u of A with $w^T u \neq 0$.*

This allows us to characterize reducedness with respect to the cone of positive semi-definite matrices in terms of minimal zeros.

Theorem 2.3.8. *[95, Theorem 4.5] A copositive matrix $A \in \mathcal{C}^n$ is reduced with respect to the cone $\mathcal{S}_+^n$ if and only if the linear span of the minimal zeros of A equals $\mathbb{R}^n$. In particular, the number of linearly independent minimal zeros, and hence also the cardinality of the minimal support set, has to be at least n.*

2.3.4 Minimal support sets of reduced copositive matrices

In this subsection we present necessary conditions for a collection $\mathcal{I} = \{I_1, \dots, I_m\}$ of index subsets $I_i \subset \{1, \dots, n\}$ to represent the minimal support set $\operatorname{supp} \mathcal{V}_{\min}^A$ of a copositive matrix $A \in \mathcal{C}^n$ which is reduced with respect to both $\mathcal{S}_+^n$ and $\mathcal{N}_n$ and satisfies $A_{ii} = 1$ for all i. The obtained results are to be applied to the classification of the extreme rays of $\mathcal{C}^n$, by limiting the number of possible minimal support sets of an exceptional extreme element with unit diagonal. The restrictions of the minimal support set fall into several categories.

One set of conditions has its origin in the trigonometric parametrization presented in Subsection 2.2.3. Let $A \in \mathcal{C}^n$ have unit diagonal and be reduced with respect to $\mathcal{N}_0^n$. Let $B = f[A]$ be its image under the element-wise application of the function $f(x) = \frac{2}{\pi} \arcsin x$. Due to Lemma 2.2.10, Corollary 2.2.12, Lemma 2.2.20, and the results in Subsection 2.2.3 the principal submatrices of B of orders 3 and 5 satisfy some strict or non-strict inclusion properties in the polytopes $\mathcal{MC}_j, \mathcal{TF}_j$ for $j = 3, 5$, respectively, depending on whether the corresponding submatrices of A are positive (semi-)definite or merely copositive, and whether there exist minimal zeros with supports in the index set of these submatrices. These properties translate into linear inequalities and equalities on the elements of B. We summarize these in the following result.

Lemma 2.3.9. *[95, Lemma 5.6] Let $A \in \mathcal{C}^n$ be irreducible with respect to $\mathcal{N}_n$ and such that $A_{ii} = 1$ for every $i = 1, \dots, n$. For $i, j = 1, \dots, n$, let $\alpha_{ij} \in [0, 1]$ be such that $A_{ij} = -\cos(\alpha_{ij}\pi)$. Let further B be a real symmetric $n \times n$ matrix defined element-wise by $B_{ij} = \frac{2}{\pi} \arcsin A_{ij} = 2\alpha_{ij} - 1$. Then the following relations hold, where the indices i, j, k are assumed to be pairwise distinct:*

(a) if $\{i, j\} \in \operatorname{supp} \mathcal{V}_{\min}^A$, then $\alpha_{ij} = 0$;

(b) if $\{i, j\} \notin \operatorname{supp} \mathcal{V}_{\min}^A$, then $\alpha_{ij} > 0$;

(c) if $I \in \operatorname{supp} \mathcal{V}_{\min}^A$, then $B_I \in \mathcal{MC}_{|I|}$;

(d) if $I \subset J$ strictly and $J \in \operatorname{supp} \mathcal{V}_{\min}^A$, then $B_I \in \operatorname{relint} \mathcal{MC}_{|I|}$;

(e) if $\{i, j, k\} \in \operatorname{supp} \mathcal{V}_{\min}^A$, then $\alpha_{ij} + \alpha_{ik} + \alpha_{jk} = 1$;

(f) if there does not exist $I \in \operatorname{supp} \mathcal{V}_{\min}^A$ such that $I \subset \{i, j, k\}$, then $\alpha_{ij} + \alpha_{ik} + \alpha_{jk} > 1$;

(g) if $\{i, j\} \in \operatorname{supp} \mathcal{V}_{\min}^A$, then $\alpha_{ik} + \alpha_{jk} \geq 1$ for all k;

(h) for every pairwise distinct indices $i_1, \dots, i_5 \in \{1, \dots, n\}$ we have $\sum_{1 \leq j < k \leq 5} \alpha_{i_j i_k} \geq 4$.

Another set of conditions comes from the reducedness of A with respect to $\mathcal{S}_+^n$, which was characterized in Theorem 2.3.8 in terms of the minimal zeros of A. The next result presents a necessary condition in terms of the minimal support set. We shall need the following construction. Let $I_1, \dots, I_m \subset \{1, \dots, n\}$ be the elements of $\mathcal{I} = \operatorname{supp} \mathcal{V}_{\min}^A$, sorted by their cardinality. Let m_2 be the number of support sets of cardinality 2. We construct two graphs $G_2(\mathcal{I}), G_{>2}(\mathcal{I})$ from $I_1, \dots, I_m$. The graph $G_2(\mathcal{I})$ has n vertices $1, \dots, n$ and m_2 edges $I_1, \dots, I_{m_2}$. The graph $G_{>2}(\mathcal{I})$ is bipartite, with the two vertex subsets being defined as $V = \{1, \dots, n\}$, $W = \{m_2 + 1, \dots, m\}$. A pair $(v, w) \in V \times W$ is an edge of $G_{>2}(\mathcal{I})$ if and only if $v \in I_w$. Let $G_{2,1}, \dots, G_{2,r}$ be the connected components of $G_2(\mathcal{I})$ which are bipartite.

Lemma 2.3.10. *[95, Lemma 5.2] Let $A \in \mathcal{C}^n$ be a copositive matrix with unit diagonal. Let $I_1, \dots, I_m$ be the elements of its minimal support set $\mathcal{I} = \operatorname{supp} \mathcal{V}_{\min}^A$, ordered by cardinality, and let m_2 be the number of supports with cardinality 2. Define the two graphs $G_2(\mathcal{I}), G_{>2}(\mathcal{I})$ as above, and let $G_{2,1}, \dots, G_{2,r}$ be the connected components of $G_2(\mathcal{I})$ which are bipartite.*

If the linear span of the minimal zero set $\mathcal{V}^A_{\min}$ is the whole space $\mathbb{R}^n$, then there exist edges $(v_1, w_1), \dots, (v_r, w_r)$ of $G_{>2}(\mathcal{I})$ such that v_j is a vertex of $G_{2,j}$ for all $j = 1, \dots, r$, and the vertices $w_1, \dots, w_r$ are mutually different.

The third set of conditions on the minimal support set is of a combinatorial nature and comes from Theorem 2.3.4, Lemma 2.2.5, and from the definition of minimal zeros.

We summarize all these conditions in the following theorem.

Theorem 2.3.11. *[95, Theorem 5.7] Let $A \in \mathcal{C}^n$ be a copositive matrix with unit diagonal. Suppose that A is reduced with respect to both $\mathcal{S}^n_+$ and $\mathcal{N}^n$. Let $I_1, \dots, I_m$ be the supports in the minimal support set $\mathcal{I} = \operatorname{supp} \mathcal{V}^A_{\min}$ of A, ordered by their cardinality. Then $\mathcal{I}$ satisfies the following conditions.*

(i) Every index set I_i contains $2 \le |I_i| \le n-2$ indices.

(ii) There do not exist i, j such that $I_i \subset I_j$ strictly.

(iii) For every index set $I \subset \{1, \dots, n\}$ and indices $i, i^1, \dots, i^l, j$ satisfying the conditions

- *$I \subset I_i$ strictly,*
- *$I_{i^r} \setminus I = \{k^r\}$ consists of exactly one element for $r = 1, \dots, l$,*
- *$(I_{i^r} \cap I) \subset (I_{i^{r+1}} \cap I)$ for $r = 1, \dots, l-1$,*
- *$I_j \subset I \cup \{k^1, \dots, k^l\}$,*

there exists $r \in \{1, \dots, l\}$ such that $j = i^r$.

(iv) Let $G_2(\mathcal{I})$, $G_{>2}(\mathcal{I})$ be the graphs constructed from $\mathcal{I}$ as in Lemma 2.3.10, and let $G_{2,1}, \dots, G_{2,r}$ be the bipartite connected components of $G_2(\mathcal{I})$. Then there exist edges $(v_1, w_1), \dots, (v_r, w_r)$ of $G_{>2}(\mathcal{I})$ such that v_j is a vertex of $G_{2,j}$ for all $j = 1, \dots, r$, and the vertices $w_1, \dots, w_r$ are mutually different.

(v) The system of linear equations and strict and nonstrict inequalities which is defined by (a)–(h) of Lemma 2.3.9 on the variables $\alpha_{ij} = \alpha_{ji} \in [0, 1]$, $1 \le i, j \le n$, has a solution.

An exceptional extremal matrix $A \in \mathcal{C}^n$ is irreducible with respect to both $\mathcal{S}^n_+$ and $\mathcal{N}^n$. Hence conditions (i)–(v) of Theorem 2.3.11 are necessary conditions for the minimal support set of an exceptional extremal copositive matrix.

For given n it can be checked algorithmically whether a collection $I_1, \dots, I_m \subset \{1, \dots, n\}$ of index sets satisfies conditions (i)–(v) of Theorem 2.3.11. While this is evident for conditions (i)–(iii), condition (iv) can be reduced to a matching problem, and condition (v) to a linear program with integer coefficients.

Two collections $I_1, \dots, I_m$ and $J_1, \dots, J_m$ satisfying conditions (i)–(v) of Theorem 2.3.11 can be considered being equivalent if there exists a permutation $\pi \in S_n$ of the indices $1, \dots, n$ such that $\{\pi(I_1), \dots, \pi(I_m)\} = \{J_1, \dots, J_m\}$. We have computed all such collections for $n \le 7$. The number of equivalence classes is 0 for $n \le 4$, 2 for $n = 5$, 44 for $n = 6$, and 12378 for $n = 7$. The classification of the extreme rays at least for $\mathcal{C}^6$ thus comes within reach. The results imply that $\mathcal{C}^n$ cannot have exceptional extreme rays for $n \le 4$, which yields a quick proof of Dianandas identity $\mathcal{C}^n = \mathcal{S}^n_+ + \mathcal{N}^n$ for $n \le 4$. The two equivalence classes for the case $n = 5$, with representatives $\{\{1,2\},\{2,3\},\{3,4\},\{4,5\},\{1,5\}\}$ and $\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{1,4,5\},\{1,2,5\}\}$, are realized by the $\mathcal{G}_5$-orbit of the Horn form (2.1) and the Hildebrand matrices, respectively, which indeed exhaust the types of exceptional extreme rays of $\mathcal{C}^5$. In the next section we consider the implications of Theorem 2.3.11 for the extreme rays of the cone $\mathcal{C}^6$.

2.4 Extreme elements of the cone $\mathcal{C}^6$

In this section we apply the approach to extreme copositive matrices which was developed in the previous section to the cone $\mathcal{C}^6$. There are, up to permutation of the indices, 44 possible minimal support sets which an extremal exceptional copositive 6×6 matrix can have [95]. These are listed in

Table 2.1. As of now the classification of the extreme rays of $\mathcal{C}^6$ has not been completed. However, a number of possible minimal support sets has been examined in collaboration with P. Dickinson, and the corresponding families of exceptional extreme copositive matrices and exceptional reduced copositive matrices have been found. Reducedness is considered not with respect to the cone of nonnegative matrices, but with respect to the larger cone $\mathcal{S}_+^6 + \mathcal{N}^6$, and is hence stronger and closer to the condition of extremality. Below we list the examined support sets along with its families of extreme and reduced exceptional copositive matrices $A \in \mathcal{C}^6$ with diagonal elements equal to 1.

No.	supp $\mathcal{V}^A_{\min}$
1	{1,2},{1,3},{1,4},{2,5},{3,6},{5,6}
2	{1,2},{1,3},{1,4},{2,5},{3,6},{4,5,6}
3	{1,2},{1,3},{1,4},{2,5},{3,5,6},{4,5,6}
4	{1,2},{1,3},{1,4},{2,5,6},{3,5,6},{4,5,6}
5	{1,2},{1,3},{2,4},{3,4,5},{1,5,6},{4,5,6}
6	{1,2},{1,3},{1,4,5},{2,4,6},{3,4,6},{4,5,6}
7	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,4,6}
8	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,5,6}
9	{1,2},{3,4},{1,3,5},{2,4,6},{1,5,6},{4,5,6}
10	{1,2},{1,3,4},{1,3,5},{2,3,6},{3,4,6},{3,5,6}
11	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6}
12	{1,2},{1,3,4},{1,3,5},{1,4,6},{3,5,6},{4,5,6}
13	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6}
14	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{3,5,6}
15	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{4,5,6}
16	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,5,6},{4,5,6}
17	{1,2},{1,3,4},{2,3,5},{3,4,5},{2,4,6},{3,4,6}
18	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{1,5,6}
19	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6}
20	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6}
21	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6}
22	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6}
23	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,5,6}
24	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{3,5,6}
25	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{4,5,6}
26	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6}
27	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{3,4,6}
28	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,5},{2,3,6}
29	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{2,3,6},{2,5,6}
30	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,6},{3,5,6}
31	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{1,5,6},{2,5,6}
32	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{1,5,6},{4,5,6}
33	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,5,6},{4,5,6}
34	{1,2,3},{1,2,4},{1,3,5},{2,4,6},{3,5,6},{4,5,6}
35	{1,2,3,4},{1,2,3,5},{1,2,4,6},{1,3,5,6},{2,4,5,6},{3,4,5,6}
36	{1,2},{1,3},{1,4},{2,5},{4,5},{3,6},{5,6}
37	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6},{4,5,6}
38	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6},{3,5,6}
39	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6},{3,5,6}
40	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6},{4,5,6}
41	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6},{3,5,6}
42	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6},{4,5,6}
43	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6},{3,5,6},{4,5,6}
44	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6},{3,5,6},{4,5,6}

Table 2.1: Candidate minimal support sets of exceptional extreme matrices in $\mathcal{C}^6$

supp $(\mathcal{V}^A) = \{\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,6\},\{5,6\}\}$. The reduced matrices with this support set are given by

$$A = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & \lambda & -\lambda \\ 1 & -1 & 1 & \lambda & 1 & -1 \\ 1 & 1 & -1 & -\lambda & -1 & 1 \end{pmatrix},$$

where $\lambda \in (-1,1)$. These matrices are not extremal.

$\operatorname{supp}(\mathcal{V}^A) = \{\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,6\},\{4,5,6\}\}$. The reduced matrices with this support set are given by

$$A = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_3 \\ -1 & 1 & 1 & 1 & \cos\phi_3 & -1 \\ -1 & 1 & 1 & 1 & -\cos\phi_1 & -\cos\phi_2 \\ 1 & -1 & \cos\phi_3 & -\cos\phi_1 & 1 & -\cos\phi_3 \\ 1 & \cos\phi_3 & -1 & -\cos\phi_2 & -\cos\phi_3 & 1 \end{pmatrix},$$

where $\phi_1, \phi_2, \phi_3 > 0$, $\phi_1 + \phi_2 + \phi_3 = \pi$. All these matrices are extremal.

$\operatorname{supp}(\mathcal{V}^A) = \{\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{3,5,6\},\{4,5,6\}\}$. The reduced matrices with this support set are given by

$$A = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & \cos\phi_1 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_3 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_1 \\ -1 & 1 & 1 & 1 & \cos(\phi_2+\phi_3) & -\cos\phi_2 \\ 1 & -1 & \cos(\phi_1+\phi_3) & \cos(\phi_2+\phi_3) & 1 & -\cos\phi_3 \\ \cos\phi_1 & \cos\phi_3 & -\cos\phi_1 & -\cos\phi_2 & -\cos\phi_3 & 1 \end{pmatrix}$$

and those matrices which are obtained from the above by an exchange of the row and column indices 3 and 4, where $0 < \phi_1 < \phi_2 < \pi - \phi_3 < \pi$. All these matrices are extremal. This support set has been examined by P. Dickinson.

$\operatorname{supp}(\mathcal{V}^A) = \{\{1,2\},\{1,3\},\{1,4\},\{2,5,6\},\{3,5,6\},\{4,5,6\}\}$. The reduced matrices with this support set are given by

$$A = \begin{pmatrix} 1 & -1 & -1 & -1 & -\cos(\phi_1+\phi_4) & \cos\phi_3 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_4) & -\cos\phi_1 \\ -1 & 1 & 1 & 1 & \cos(\phi_2+\phi_4) & -\cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos(\phi_3+\phi_4) & -\cos\phi_3 \\ -\cos(\phi_1+\phi_4) & \cos(\phi_1+\phi_4) & \cos(\phi_2+\phi_4) & \cos(\phi_3+\phi_4) & 1 & -\cos\phi_4 \\ \cos\phi_3 & -\cos\phi_1 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_4 & 1 \end{pmatrix}$$

and those matrices which are obtained from the above by a permutation of the row and column indices 2,3, and 4, where $0 < \phi_3 < \phi_2 < \phi_1 < \pi - \phi_4 < \pi$. All these matrices are extremal. This support set has been examined by P. Dickinson.

$\operatorname{supp}(\mathcal{V}^A) = \{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,6\},\{5,6,1\},\{6,1,2\}\}$. The reduced matrices with this support set are given by

$$A = \begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & a & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & b & \cos(\phi_1+\phi_6) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & c \\ a & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ \cos(\phi_5+\phi_6) & b & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ -\cos\phi_6 & \cos(\phi_1+\phi_6) & c & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix} \quad (2.5)$$

with $\phi_1,\dots,\phi_6 > 0$; $\phi_j + \phi_{j+1} < \pi$, $j = 1,\dots,5$; $\phi_1 + \phi_6 < \pi$; $\sum_{j=1}^6 \phi_j < 2\pi$;

$$\begin{aligned} a &= -\min\{\cos(\phi_1+\phi_2+\phi_3), \cos(\phi_4+\phi_5+\phi_6)\}, \\ b &= -\min\{\cos(\phi_2+\phi_3+\phi_4), \cos(\phi_1+\phi_5+\phi_6)\}, \\ c &= -\min\{\cos(\phi_3+\phi_4+\phi_5), \cos(\phi_1+\phi_2+\phi_6)\}. \end{aligned}$$

A matrix of this form is extremal if and only if either $\sum_{j=1}^6 \phi_j \neq \pi$, or at least four of the sums $\phi_1+\phi_2+\phi_3, \phi_2+\phi_3+\phi_4, \dots, \phi_1+\phi_2+\phi_6$ appearing in the expressions for a, b, c equal $\frac{\pi}{2}$.

supp $(\mathcal{V}^A) = \{\{1,2\},\{1,3\},\{1,4\},\{2,5\},\{4,5\},\{3,6\},\{5,6\}\}$. The support set uniquely determines the extremal exceptional copositive matrix

$$A = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix}.$$

This matrix is non-basic, and an equivalent matrix has been obtained by Baumert [12] by duplicating a row and a column of the Horn form.

supp $(\mathcal{V}^A) = \{\{1,2,5\},\{1,2,3\}, \{2,3,4\},\{3,4,5\},\{1,4,5\},\{3,4,6\},\{1,2,6\},\{1,4,6\}\}$. The variety of reduced matrices corresponding to this support set is given by

$$\begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & -\cos(\phi_3+\phi) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & \cos(\phi_3+\phi_4+\phi) \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_2-\phi) \\ \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & -\cos\phi_1 & 1 & -\cos\phi_2 & -\cos(\phi_2-\phi) \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & \cos\phi \\ -\cos(\phi_3+\phi) & \cos(\phi_3+\phi_4+\phi) & \cos(\phi_1+\phi_2-\phi) & -\cos(\phi_2-\phi) & \cos\phi & 1 \end{pmatrix}$$

with $\phi_i > 0$, $\sum_{i=1}^5 \phi_i < \pi$, $\phi \in (-\phi_3, \phi_2)$. All of them are extremal.

These preliminary results indicate that the number of types of exceptional extreme rays is an order of magnitude larger for $\mathcal{C}^6$ than for $\mathcal{C}^5$. However, it appears that the extreme rays of $\mathcal{C}^6$ can still be described by the trigonometric approach elaborated in Subsection 2.2.3. This is no more the case for the cone $\mathcal{C}^7$, because there are extremal elements of $\mathcal{C}^7$ which have minimal zeros with a support of cardinality 5.

2.5 Local properties of the boundary

2.5.1 Introduction

In this section we describe results which have been obtained in collaboration with P. Dickinson and have been published in [57]. We present necessary and sufficient criteria when a copositive matrix is reduced with respect to another matrix. This allows to compute the minimal face of a copositive matrix and to characterize extremality of a copositive matrix in terms of its minimal zeros. These results greatly simplify the proof or refutation of extremality of the families of reduced matrices which can be found by virtue of the classification of minimal support sets in Section 2.3.

In Subsection 2.5.2 we provide the main result of [57], the description of the cone $\mathcal{K}^A$ of feasible directions of $\mathcal{C}^n$ at A. We also compute its closure, the *tangent cone* $\mathrm{cl}(\mathcal{K}^A)$. In Section 2.5.3 we deduce the descriptions of the minimal face of a copositive matrix. In Section 2.5.4 we consider when a copositive matrix is reduced with respect to another copositive matrix.

2.5.2 Reducedness with respect to arbitrary matrices

For a matrix $A \in \mathcal{C}^n$ we consider the convex cone $\mathcal{K}^A = \{B \in \mathcal{S}^n \mid \exists \delta > 0 \text{ s.t. } A + \delta B \in \mathcal{C}^n\}$, which is called *cone of feasible directions* in [177]. By definition it consists of all matrices $B \in \mathcal{S}^n$ such that A is not reduced with respect to $-B$. Clearly we have $\mathcal{C}^n \subset \mathcal{K}^A$. However, $\mathcal{K}^A$ is not pointed, unless $A = 0$, as we always have $\pm A \in \mathcal{K}^A$. It is also in general not closed. The results in this section are based on the following theorem.

Theorem 2.5.1. *[57, Theorem 6] Let $A \in \mathcal{C}^n$, then*

$$\mathcal{K}^A = \left\{ B \in \mathcal{S}^n \;\middle|\; \begin{array}{l} v^T B v \geq 0 \text{ for all } v \in \mathcal{V}^A, \\ (Bv)_i \geq 0 \text{ for all } v \in \mathcal{V}^A \cap \mathcal{V}^B,\ i \in \{1,\dots,n\} \setminus \operatorname{supp}(Av) \end{array} \right\},$$

where $\mathcal{V}^B = \{v \in \mathbb{R}^n_+ \setminus \{0\} \mid v^T B v = 0\}$.

In convex analysis there exists the notion of the *(solid) tangent cone* to some closed convex set $C \subset \mathbb{R}^n$ at a boundary point $x \in \partial C$ [98, 177]. By definition the tangent cone to $\mathcal{C}^n$ at a boundary point $A \in \partial\mathcal{C}^n$ is given by the closure of the cone of feasible directions $\mathcal{K}^A$. The next result gives a simple characterization of the tangent cone in our case.

Theorem 2.5.2. *[57, Theorem 9] For $A \in \mathcal{C}^n$ we have $\operatorname{cl}(\mathcal{K}^A) = \{B \in \mathcal{S}^n \mid v^T B v \geq 0$ for all $v \in \mathcal{V}^A\}$.*

2.5.3 Minimal Faces

In this subsection we apply Theorem 2.5.1 to determine the linear span of the minimal face $\mathcal{F}^A$ of the copositive cone containing a matrix $A \in \mathcal{C}^n$.

For $A \in \mathcal{C}^n$ denote the linear span of $\mathcal{F}^A$ by $\mathcal{L}^A$. We have $\mathcal{K}^A = \mathcal{C}^n + \mathcal{L}^A$, following from the general result [177, Lemma 3.2.1] which is valid for arbitrary cones. Application of Theorem 2.5.1 then yields

$$\mathcal{L}^A = \mathcal{K}^A \cap (-\mathcal{K}^A) = \{B \in \mathcal{S}^n \mid (Bv)_i = 0 \ \forall\ v \in \mathcal{V}^A,\ i \in \{1,\dots,n\} \setminus \operatorname{supp} Av\}.$$

In contrast to the characterization of $\mathcal{K}^A$ in Theorem 2.5.1, the characterization of $\mathcal{L}^A$ involves only expressions which are *linear* in the zeros $v \in \mathcal{V}^A$. Therefore it is sufficient to consider only the set of minimal zeros of A by Corollary 2.3.1. We therefore get [57, Theorem 17]

Theorem 2.5.3. *Let $A \in \mathcal{C}^n$. The linear span of the minimal face of A is given by*

$$\mathcal{L}^A = \{B \in \mathcal{S}^n \mid (Bv)_i = 0 \ \forall\ v \in \mathcal{V}^A_{\min},\ i \in \{1,\dots,n\} \setminus \operatorname{supp} Av\}.$$

Since $\mathcal{V}^A_{\min}$ is a finite set up to multiplication of the minimal zeros by positive scalars, the system of linear equations in Theorem 2.5.3 is finite. We can thus algorithmically compute the dimension of $\mathcal{L}^A$ by finding the rank of the coefficient matrix of this system of linear equations. This then allows us to determine if the copositive matrix A lies on an extreme ray.

Corollary 2.5.4. *Let $A \in \mathcal{C}^n$ be a non-zero matrix. Then A is extremal if and only if the system of linear equations*

$$(Bv)_i = 0, \qquad v \in \mathcal{V}^A_{\min},\ i \in \{1,\dots,n\} \setminus \operatorname{supp} Av$$

on $B \in \mathcal{S}^n$ has a 1-dimensional solution space.

2.5.4 Reducedness with respect to copositive matrices

In this subsection we describe when a copositive matrix A is reduced with respect to another *copositive* matrix C. This allows us to recover Lemmas 2.3.6 and 2.3.7 as special cases. By definition A is not reduced with respect to C if and only if $B = -C \in \mathcal{K}^A$. By Theorem 2.5.1 we have in this case that for every $v \in \mathcal{V}^A$ also $v \in \mathcal{V}^C$ and further $\operatorname{supp}(Cv) \subset \operatorname{supp}(Av)$. Here we used the first order optimality conditions from Lemma 2.1.4 for C at v. As in the previous subsection, we then need to consider only the minimal zeros of A, which leads to the following result.

Theorem 2.5.5. *[57, Theorem 23] Let $A, C \in \mathcal{C}^n$. Then A is not reduced with respect to C if and only if for all $v \in \mathcal{V}^A_{\min}$ we have $\operatorname{supp}(Cv) \subset \operatorname{supp}(Av)$.*

Alternatively we could have stated this theorem as follows:

Theorem 2.5.6. *[57, Theorem 24] Let $A, C \in \mathcal{C}^n$. Then A is reduced with respect to C if and only if there exist $v \in \mathcal{V}^A_{\min}$, $i \in \{1, \dots, n\}$ such that $(Av)_i = 0 \neq (Cv)_i$.*

2.6 Copositive matrices with circulant support set

2.6.1 Introduction

In this section we consider copositive matrices with zeros having very specific supports. The prototypes of these matrices are the exceptional extremal elements of the cone $\mathcal{C}^5$, which have been classified in Section 2.2 above. Both the Horn form H given by (2.1) and the matrices $T(\theta)$ given by (2.3) possess zeros with supports $\{1,2,3\}, \{2,3,4\}, \{3,4,5\}, \{4,5,1\}, \{5,1,2\}$, respectively. These supports are exactly the vertex subsets obtained by removing the vertices of a single edge in the cycle graph C_5. In this section we show that the presence of zeros with this kind of supports is sufficient to explain many of the properties of the Horn form and the matrices $T(\psi)$, including their being exceptional and extremal. Moreover, these relations hold for copositive matrices of arbitrary order $n \geq 5$, thus giving rise to families of basic exceptional extremal copositive matrices for every $n \geq 5$.

We shall generalize the exceptional extremal elements of $\mathcal{C}^5$ to arbitrary order $n \geq 5$ by taking the above property of the supports as our point of departure. Fix a set $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ of nonnegative vectors with supports $\{1, 2, \dots, n-2\}$, $\{2, 3, \dots, n-1\}, \dots, \{n, 1, \dots, n-3\}$, respectively, i.e., the supports of the vectors u^j are the vertex subsets obtained by removing the vertices of a single edge in the cycle graph C_n. We consider the faces

$$F_{\mathbf{u}} = \{A \in \mathcal{C}^n \mid (u^j)^T A u^j = 0 \ \forall\ j = 1, \dots, n\}, \quad P_{\mathbf{u}} = \{A \in \mathcal{S}^n_+ \mid (u^j)^T A u^j = 0 \ \forall\ j = 1, \dots, n\} \quad (2.6)$$

of the copositive cone and the positive semi-definite cone, respectively. Note that $P_{\mathbf{u}} \subset F_{\mathbf{u}}$. For $n \geq 5$ a copositive matrix having zeros $u^1, \dots, u^n$ satisfies the conditions of Theorem 2.2.2 and hence must be reduced with respect to $\mathcal{N}^n$. It follows that every matrix in $F_{\mathbf{u}} \setminus P_{\mathbf{u}}$ is exceptional.

One of our main results is an explicit semi-definite description of the faces $F_{\mathbf{u}}$ and $P_{\mathbf{u}}$ (Theorem 2.6.4). In order to obtain this description, we associate the set $\mathbf{u}$ with a discrete-time linear dynamical system $\mathbf{S}_{\mathbf{u}}$ of order $d = n - 3$ and with time-dependent coefficients having period n. If $\mathcal{L}_{\mathbf{u}}$ is the d-dimensional solution space of this system, then there exists a canonical bijective linear map between $F_{\mathbf{u}}$ and the set of positive semi-definite symmetric bilinear forms on the dual space $\mathcal{L}^*_{\mathbf{u}}$ satisfying certain additional homogeneous linear equalities and inequalities. For an arbitrary collection $\mathbf{u}$ in general only the zero form satisfies the corresponding linear matrix inequality (LMI) and the face $F_{\mathbf{u}}$ consists of the zero matrix only. However, for every $n \geq 5$ there exist collections $\mathbf{u}$ for which the LMI has non-trivial feasible sets.

The properties of the copositive matrices in $F_{\mathbf{u}}$ are closely linked to the properties of the periodic linear dynamical system $\mathbf{S}_{\mathbf{u}}$. Such systems are the subject of *Floquet theory*, see, e.g., [66, Section 3.4]. We need only the concept of the *monodromy operator* and its eigenvalues, the *Floquet multipliers*, which we shall review in Subsection 2.6.3. It turns out that the face $P_{\mathbf{u}}$ is isomorphic to $\mathcal{S}^{d_1}_+$, where d_1 is the geometric multiplicity of the Floquet multiplier 1, or equivalently, the dimension of the subspace of n-periodic solutions of $\mathbf{S}_{\mathbf{u}}$. For the existence of exceptional copositive matrices in $F_{\mathbf{u}}$ it is necessary that all or all but one Floquet multiplier are located on the unit circle (Corollary 2.6.7).

We are able to describe the structure of $F_{\mathbf{u}}$ explicitly in general. Exceptional matrices $A \in F_{\mathbf{u}}$ can be divided in two categories, defined as follows.

Definition 2.6.1. Let $A \in \mathcal{C}^n$ be an exceptional copositive matrix possessing zeros $u^1, \dots, u^n \in \mathbb{R}^n_+$ such that $\operatorname{supp} u^j = I_j$, $j = 1, \dots, n$. We say the matrix A has *minimal circulant zero support set* if every zero v of A is proportional to one of the zeros $u^1, \dots, u^n$, and *non-minimal circulant zero support set* otherwise.

Matrices with non-minimal circulant zero support set are always extremal, while matrices with minimal circulant zero support set can be extremal only for odd n. For even n a matrix with minimal circulant zero support set can be represented as a non-trivial sum of a matrix with non-minimal circulant zero support set and a positive semi-definite rank 1 matrix, the corresponding face $F_{\mathbf{u}}$ is then isomorphic to $\mathbb{R}_+^2$ (Lemma 2.6.9). For odd n a sufficient condition for extremality of a matrix with minimal circulant zero support set is that -1 does not appear among the Floquet multipliers (Theorem 2.6.11). For every $n \geq 5$ the matrices with non-minimal circulant zero support set constitute an algebraic submanifold of $\mathcal{S}^n$ of codimension $2n$ (Theorem 2.6.14), while the matrices with minimal circulant zero support set form an algebraic submanifold of codimension n (Theorem 2.6.12), in which the extremal matrices form an open subset (Theorem 2.6.13). In Subsection 2.6.8 we construct explicit examples of circulant (i.e., invariant with respect to simultaneous circular shifts of row and column indices) exceptional extremal copositive matrices, both with minimal and non-minimal circulant zero support set. The results in this section have been published in the paper [97].

For $n \geq 5$ an integer, define the ordered index sets $I_1 = (1, 2, \dots, n-2)$, $I_2 = (2, 3, \dots, n-1), \dots, I_n = (n, 1, \dots, n-3)$ of cardinality $n-2$, each obtained by a circular shift of the indices from the previous one. We will need also the index sets $I'_1 = (1, 2, \dots, n-3), \dots, I'_n = (n, 1, \dots, n-4)$ defined similarly.

In order to distinguish it from the index sets $I_1, \dots, I_n$ defined above, we shall denote the identity matrix or the identity operator by Id or Id_k if it is necessary to indicate the size of the matrix. For a real number r, we denote by $\lfloor r \rfloor$ the largest integer not exceeding r and by $\lceil r \rceil$ the smallest integer not smaller than r.

2.6.2 Conditions for copositivity

In this subsection we consider matrices $A \in \mathcal{S}^n$ such that the submatrices $A_{I_1}, \dots, A_{I_n}$ are all positive semi-definite and possess element-wise positive kernel vectors. We derive necessary and sufficient conditions for such a matrix to be copositive.

Theorem 2.6.2. *[97, Theorem 2.9] Let $n \geq 5$ and let $A \in \mathcal{S}^n$ be such that for every $j = 1, \dots, n$ there exists a nonnegative vector u^j with $\operatorname{supp} u^j = I_j$ satisfying $(u^j)^T A u^j = 0$. Then the following are equivalent:*

(i) A is copositive;
(ii) every principal submatrix of A of size $n-1$ is copositive;
(iii) every principal submatrix of A of size $n-1$ is in $\mathcal{S}_+^{n-1} + \mathcal{N}^{n-1}$;
(iv) A_{I_j} is positive semi-definite for $j = 1, \dots, n$, $(u^n)^T A u^1 \geq 0$, and $(u^j)^T A u^{j+1} \geq 0$ for $j = 1, \dots, n-1$.

Moreover, given above conditions (i)—(iv), the following are equivalent:

(a) A is positive semi-definite;
(b) at least one of the n numbers $(u^n)^T A u^1$ and $(u^j)^T A u^{j+1}$, $j = 1, \dots, n-1$, is zero;
(c) all n numbers $(u^n)^T A u^1$ and $(u^j)^T A u^{j+1}$, $j = 1, \dots, n-1$, are zero;
(d) A is not exceptional.

The theorem states that the presence of n zeros with supports I_j, $j = 1, \dots, n$ places stringent constraints on a copositive matrix $A \in \mathcal{C}^n$. Such a matrix must either be exceptional or positive semi-definite. Which of these two cases arises is determined by any of the n numbers in condition (iv) of the theorem, which are either simultaneously positive or simultaneously zero. Note also that condition (iv) is easy to check, as it represents an LMI on the coefficients of A. We shall, however, derive an equivalent and much simpler LMI below.

2.6.3 Linear systems with periodic coefficients

In this subsection we investigate the solution spaces of linear periodic dynamical systems and perform some linear algebraic constructions on them. These will be later put in correspondence to copositive forms. First we shall introduce the monodromy and the Floquet multipliers associated with such systems, for further reading about these and related concepts see, e.g., [66, Section 3.4].

We consider real scalar discrete-time homogeneous linear dynamical systems governed by the equation

$$x_{t+d} + \sum_{i=0}^{d-1} c_i^t x_{t+i} = \sum_{i=0}^{d} c_i^t x_{t+i} = 0, \qquad t = 1, 2, \dots \tag{2.7}$$

where $x_t \in \mathbb{R}$ is the value of the solution x at time instant t, $d > 0$ is the order, and $c^t = (c_0^t, \dots, c_d^t)^T \in \mathbb{R}^{d+1}$, $t \geq 1$, are the coefficient vectors of the system. For convenience we have set $c_d^t = 1$ for all $t \geq 1$. We assume that the coefficients are periodic with period $n > d$, i.e., $c^{t+n} = c^t$ for all $t \geq 1$. Denote by $\mathcal{L}$ the linear space of all solutions $x = (x_t)_{t \geq 1}$. This space has dimension d and can be parameterized, e.g., by the vector $(x_1, \dots, x_d) \in \mathbb{R}^d$ of initial conditions.

If $x = (x_t)_{t \geq 1}$ is a solution of the system, then $y = (x_{t+n})_{t \geq 1}$ is also a solution by the periodicity of the coefficients. The corresponding linear map $\mathfrak{M} : \mathcal{L} \to \mathcal{L}$ taking x to y is called the *monodromy* of the periodic system. Its eigenvalues are called *Floquet multipliers*. The following result is a trivial consequence of this definition.

Lemma 2.6.3. *Let $\mathcal{L}_{per} \subset \mathcal{L}$ be the subspace of n-periodic solutions of system* (2.7). *Then $x \in \mathcal{L}_{per}$ if and only if x is an eigenvector of the monodromy operator $\mathfrak{M}$ with eigenvalue 1. In particular,* $\dim \mathcal{L}_{per}$ *equals the geometric multiplicity of the eigenvalue 1 of $\mathfrak{M}$.* □

Let us now consider the space $\mathcal{L}^*$ of linear functionals on the solution space $\mathcal{L}$. For every $t \geq 1$, the map taking a solution $x = (x_s)_{s \geq 1}$ to its value x_t at time instant t is such a linear functional. We shall denote this evaluation functional by $\mathbf{e}_t \in \mathcal{L}^*$. By definition of the monodromy we have $\mathbf{e}_{t+n} = \mathfrak{M}^* \mathbf{e}_t$ for all $t \geq 1$, where $\mathfrak{M}^* : \mathcal{L}^* \to \mathcal{L}^*$ is the adjoint of $\mathfrak{M}$. Our main tool in the study of copositive forms are positive semi-definite symmetric bilinear forms B on $\mathcal{L}^*$ which are invariant with respect to a time shift by the period n, i.e.,

$$B(\mathbf{e}_{t+n}, \mathbf{e}_{s+n}) = B(\mathbf{e}_t, \mathbf{e}_s) \qquad \forall\, t, s \geq 1. \tag{2.8}$$

An equivalent condition is $B(w, w') = B(\mathfrak{M}^* w, \mathfrak{M}^* w')$ for all $w, w' \in \mathcal{L}^*$.

2.6.4 Copositive matrices and linear periodic systems

In this subsection we establish a relation between the objects considered in the preceding two subsections. Throughout this and the next section, we fix a collection $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}_+^n$ of nonnegative vectors such that $\operatorname{supp} u^j = I_j$, $j = 1, \dots, n$. Moreover, we assume these vectors are normalized such that the last elements of their positive subvectors $u_{I_j}^j$ all equal 1. With the collection $\mathbf{u}$ we associate a discrete-time linear periodic system $\mathbf{S_u}$ of order $d = n - 3$ and with period n, given by (2.7) with coefficient vectors $c^t = u_{I_t}^t$, $t = 1, \dots, n$. The coefficient vectors c^t for all other time instants $t > n$ are then determined by the periodicity relation $c^{t+n} = c^t$. Denote by $\mathcal{L}_\mathbf{u}$ the space of solutions of $\mathbf{S_u}$.

Let $\mathcal{A}_\mathbf{u} \subset \mathcal{S}^n$ be the linear subspace of matrices A satisfying $A_{I_j} u_{I_j}^j = A_{I_j} c^j = 0$ for all $j = 1, \dots, n$. With $A \in \mathcal{A}_\mathbf{u}$ we associate a symmetric bilinear form B on the dual space $\mathcal{L}_\mathbf{u}^*$ by setting $B(\mathbf{e}_t, \mathbf{e}_s) = A_{ts}$ for every $t, s = 1, \dots, d$ and defining the value of B on arbitrary vectors in $\mathcal{L}_\mathbf{u}^*$ by linear extension. In other words, in the basis $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ of $\mathcal{L}_\mathbf{u}^*$ the coefficient matrix of B is given by the submatrix $A_{I_1'}$. Let $\Lambda : A \mapsto B$ be the so-defined linear map from $\mathcal{A}_\mathbf{u}$ into the space of symmetric bilinear forms on $\mathcal{L}_\mathbf{u}^*$. It can be shown that the map Λ is injective [97, Lemma 4.4].

Now we are in a position to describe the face $F_\mathbf{u}$ of the copositive cone and the face $P_\mathbf{u}$ of the positive semi-definite cone which are defined by virtue of (2.6) by the zeros u^j, $j = 1, \dots, n$. The description will be by linear matrix inequalities on the images of these faces under the map Λ, which is much more convenient than to describe these faces directly in terms of the elements of the matrices. The map Λ translates conditions on bilinear forms on the dual space $\mathcal{L}_\mathbf{u}^*$ into conditions on matrices in $\mathcal{S}^n$.

Theorem 2.6.4. *[97, Theorem 4.8] Let $n \geq 5$, and let $\mathcal{F}_\mathbf{u}$ be the set of positive semi-definite symmetric bilinear forms B on $\mathcal{L}_\mathbf{u}^*$ satisfying the linear equality relations*

$$\begin{aligned} B(\mathbf{e}_t, \mathbf{e}_s) &= B(\mathfrak{M}^* \mathbf{e}_t, \mathfrak{M}^* \mathbf{e}_s), && t, s = 1, \dots, n-3; \\ B(\mathbf{e}_t, \mathbf{e}_s) &= B(\mathfrak{M}^* \mathbf{e}_t, \mathbf{e}_s), && 1 \leq t < s \leq n : \ 3 \leq s - t \leq n-3 \end{aligned}$$

and the linear inequalities

$$B(\mathbf{e}_t, \mathbf{e}_{t+2}) \geq B(\mathfrak{M}^*\mathbf{e}_t, \mathbf{e}_{t+2}), \qquad t = 1, \dots, n.$$

Let $\mathcal{P}_\mathbf{u} \subset \mathcal{F}_\mathbf{u}$ be the subset of forms B which satisfy all linear inequalities with equality.

The set $\mathcal{F}_\mathbf{u}$ is a subset of the image of Λ. The face of $\mathcal{C}^n$ defined by the zeros u^j, $j = 1, \dots, n$, satisfies $F_\mathbf{u} = \Lambda^{-1}[\mathcal{F}_\mathbf{u}]$, and the face of $\mathcal{S}_+^n$ defined by these zeros satisfies $P_\mathbf{u} = \Lambda^{-1}[\mathcal{P}_\mathbf{u}]$. Moreover, for all forms $B \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$ the linear inequalities are satisfied strictly, and $F_\mathbf{u} \setminus P_\mathbf{u}$ consists of exceptional matrices.

This theorem yields an algorithmic procedure to determine the faces $F_\mathbf{u}$ and $P_\mathbf{u}$ for a given collection $\mathbf{u}$ of zeros. From the zeros u^j one obtains the coefficients of the linear periodic dynamical system $\mathbf{S}_\mathbf{u}$. The monodromy of this system then yields the linear constraints for the LMI that describes these faces. If the vectors in the collection $\mathbf{u}$ are in generic position, then the set $\mathcal{F}_\mathbf{u}$ defined in Theorem 2.6.4 consists of the zero form only. In the next section we investigate the consequences of a non-trivial set $\mathcal{F}_\mathbf{u}$.

2.6.5 Structure of the faces $\mathcal{F}_\mathbf{u}$ and $\mathcal{P}_\mathbf{u}$

As was mentioned in the introduction, the eigenvalues of the monodromy $\mathfrak{M}$, the Floquet multipliers, largely determine the properties of the matrices in the face $F_\mathbf{u}$ of $\mathcal{C}^n$. In this section we shall investigate these connections in detail. In particular, we will be interested in the structure of the cones $P_\mathbf{u}$ and $\mathcal{P}_\mathbf{u} = \Lambda[P_\mathbf{u}]$ defined by the positive semi-definite matrices in the face $F_\mathbf{u} \subset \mathcal{C}^n$ and its connections to the periodic solutions of the system $\mathbf{S}_\mathbf{u}$. We also investigate the properties of the exceptional copositive matrices with minimal and non-minimal circulant zero support set as defined in Definition 2.6.1.

Denote by $\mathcal{L}_{per} \subset \mathcal{L}_\mathbf{u}$ the subspace of n-periodic solutions. We have the following characterization of $\mathcal{L}_{per}$.

Lemma 2.6.5. *[97, Lemma 5.1] An n-periodic infinite sequence $x = (x_1, x_2, \dots)$ is a solution of $\mathbf{S}_\mathbf{u}$ if and only if the vector $(x_1, \dots, x_n)^T \in \mathbb{R}^n$ is orthogonal to all vectors u^j, $j = 1, \dots, n$. In particular, the dimension of $\mathcal{L}_{per}$ equals the corank of the $n \times n$ matrix U composed of the column vectors $u^1, \dots, u^n$.*

This means the periodic solutions of the system $\mathbf{S}_\mathbf{u}$ are given directly by the kernel of the matrix U^T. On the other hand, a positive semi-definite matrix has the vectors in $\mathbf{u}$ as zeros if and only if it is in the face of $\mathcal{S}_+^n$ which is orthogonal to the column span of U. This yields the following connection between the subspace $\mathcal{L}_{per}$ of periodic solutions and the face $P_\mathbf{u}$.

Lemma 2.6.6. *[97, Lemma 5.2] Suppose that $n \geq 5$. Then $\mathcal{P}_\mathbf{u}$ equals the convex hull of all tensor products $x \otimes x$, $x \in \mathcal{L}_{per}$. In particular, $\mathcal{P}_\mathbf{u} \simeq \mathcal{S}_+^{\dim \mathcal{L}_{per}}$, and for every $B \in \mathcal{P}_\mathbf{u}$ we have $Im\, B \subset \mathcal{L}_{per}$. Moreover, for every $B \in \mathcal{P}_\mathbf{u}$ the preimage $A = \Lambda^{-1}(B) \in P_\mathbf{u}$ is given by $A = (B(\mathbf{e}_t, \mathbf{e}_s))_{t,s=1,\dots,n}$.*

The positive semi-definite face $P_\mathbf{u}$ is hence closely connected to the eigenvalue 1 of the monodromy operator $\mathfrak{M}$. In particular, the rank of this face is equal to the dimension of the eigenspace to this eigenvalue.

The existence of exceptional copositive matrices with zeros $u^1, \dots, u^n$ has much more stringent consequences on the structure and the eigenvalues of the monodromy operator.

Lemma 2.6.7. *[97, Corollary 5.5] Let $n \geq 5$, and let $B \in \mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$. Then the bilinear form on $\mathcal{L}_\mathbf{u}^*$ given by $(w, w') \mapsto B((Id - \mathfrak{M}^*)w, w')$ has corank at most 1. In particular, both B and $Id - \mathfrak{M}^*$ have corank at most 1. Moreover, $\mathfrak{M}$ has at least $n - 4$ linearly independent eigenvectors with eigenvalues on the unit circle.*

A trivial consequence is that if the face $F_\mathbf{u}$ contains exceptional copositive matrices, then the positive semi-definite matrices in this face can have rank at most 1. The forms B in the set $\mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$ can have either full rank or have corank 1. The following results describe the structure of $F_\mathbf{u}$ in dependence on whether there exist positive definite forms in $\mathcal{F}_\mathbf{u} \setminus \mathcal{P}_\mathbf{u}$ or not.

Lemma 2.6.8. *[97, Lemma 5.7] Suppose $n \geq 5$ and assume that every form $B \in \mathcal{F}_\mathbf{u}$ is degenerate. Then either $F_\mathbf{u}$ consists of positive semi-definite matrices only, or $F_\mathbf{u}$ is 1-dimensional and generated by an extremal exceptional copositive matrix A. In the latter case the submatrices A_{I_j} of this exceptional matrix have corank 2 for all $j = 1, \dots, n$.*

Lemma 2.6.9. *[97, Lemma 5.9] Let $n > 5$ be even, and suppose that there exist positive definite forms $B \in \mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$. Then $F_{\mathbf{u}}$ is linearly isomorphic to $\mathbb{R}^2_+$, where one boundary ray of $F_{\mathbf{u}}$ is generated by a rank 1 positive semi-definite matrix, and the other boundary ray is generated by an extremal exceptional copositive matrix A. The submatrices A_{I_j} of this exceptional matrix have corank 2 for all $j = 1, \dots, n$.*

Lemma 2.6.10. *[97, Lemma 5.10] Let $n \geq 5$ be odd, and suppose that there exist positive definite forms $B \in \mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$. Then $F_{\mathbf{u}}$ does not contain non-zero positive semi-definite matrices.*

If $F_{\mathbf{u}}$ is 1-dimensional, then it is generated by an extremal exceptional copositive matrix A such that the submatrices A_{I_j} have corank 1 for all $j = 1, \dots, n$.

If $\dim F_{\mathbf{u}} > 1$, then the monodromy operator $\mathfrak{M}$ of the system $\mathbf{S_u}$ possesses the eigenvalue -1, and all boundary rays of $F_{\mathbf{u}}$ are generated by extremal exceptional copositive matrices. For any such boundary matrix $A \neq 0$, its submatrices A_{I_j} have corank 2 for all $j = 1, \dots, n$.

The previous results described the face $F_{\mathbf{u}}$. The next theorem gives more details on the structure of the exceptional copositive matrices in this face, in dependence on whether their support set is minimal circulant or not.

Theorem 2.6.11. *[97, Theorem 5.12] Let $A \in F_{\mathbf{u}}$ be an exceptional copositive matrix and set $B = \Lambda(A)$. Then either*

- *(i.a) A has minimal circulant zero support set;*
- *(i.b) B is positive definite;*
- *(i.c) the corank of the submatrices A_{I_j} equals 1, $j = 1, \dots, n$;*
- *(i.d) the minimal zero support set of A is $\{I_1, \dots, I_n\}$, with minimal zeros $u^1, \dots, u^n$;*
- *(i.e) for even n the matrix A is the sum of an exceptional copositive matrix with non-minimal circulant zero support set and a rank 1 positive semi-definite matrix;*
- *(i.f) if n is odd and the monodromy operator $\mathfrak{M}$ has no eigenvalue equal to -1, then A is extremal;*

or

- *(ii.a) A has non-minimal circulant zero support set;*
- *(ii.b) the corank of B equals 1;*
- *(ii.c) the corank of the submatrices A_{I_j} equals 2, $j = 1, \dots, n$;*
- *(ii.d) the support of any minimal zero of A is a strict subset of one of the index sets $I_1, \dots, I_n$, and every index set I_j has exactly two subsets which are supports of minimal zeros of A;*
- *(ii.e) every non-minimal zero of A has support equal to I_j for some $j = 1, \dots, n$ and is a sum of two minimal zeros;*
- *(ii.f) A is extremal.*

The prototype of exceptional copositive matrices satisfying conditions (i.a)—(i.f) are the matrices (2.3) for ψ in the interior of the simplex Ψ given by (2.4), while the prototype of those satisfying (ii.a)—(ii.f) is the Horn form (2.1).

2.6.6 Submanifolds of extremal exceptional copositive matrices

In the previous two subsections we considered the face $F_{\mathbf{u}} \subset \mathcal{C}^n$ for a fixed collection $\mathbf{u}$ of zeros. In Theorem 2.6.11 we have shown that there are two potential possibilities for an exceptional copositive matrix A in such a face $F_{\mathbf{u}}$. Namely, either A has minimal, or A has non-minimal circulant zero support set, either case imposing its own set of conditions on A. In this section we show that in each of these cases, the matrix A is embedded in a submanifold of $\mathcal{S}^n$ of codimension n or $2n$, respectively, which consists of exceptional copositive matrices with similar properties. However, different matrices in this submanifold may belong to faces $F_{\mathbf{u}}$ corresponding to different collections $\mathbf{u}$.

Theorem 2.6.12. *[97, Theorem 6.1] Let $n \geq 5$, and let $\hat{A} \in \mathcal{C}^n$ be an exceptional matrix with minimal circulant zero support set and with zeros $\hat{u}^1, \dots, \hat{u}^n \in \mathbb{R}^n_+$ such that $\operatorname{supp} \hat{u}^j = I_j$. Then there exists a neighbourhood $\mathcal{U} \subset \mathcal{S}^n$ of $\hat{A}$ with the following properties:*

- *(i) if $A \in \mathcal{U}$ and $\det A_{I_j} = 0$ for all $j = 1, \dots, n$, then A is an exceptional copositive matrix with minimal circulant zero support set;*

(ii) the set of matrices $A \in \mathcal{U}$ satisfying the conditions in (i) is an algebraic submanifold of codimension n in $\mathcal{S}^n$.

The matrices in the manifold described in this theorem can be extremal only if n is odd. The next result states that if there are any extremal matrices, then they form a submanifold of codimension n too.

Theorem 2.6.13. *[97, Theorem 6.2] The extremal exceptional copositive matrices with minimal circulant zero support set form an open subset of the manifold of all exceptional matrices with minimal circulant zero support set.*

The simplest manifold of the type described in Theorem 2.6.13 is the 10-dimensional union of the $\mathcal{G}_5$-orbits of the matrices (2.3) for ψ in the interior of Ψ. Matrices (2.3) themselves depend on 5 parameters, while the action of $\mathcal{G}_5$ adds another 5 parameters.

Theorem 2.6.14. *[97, Theorem 6.3] Let $n \geq 5$, and let $\hat{A} \in \mathcal{C}^n$ be an exceptional matrix with non-minimal circulant zero support set and having zeros $\hat{u}^1, \dots, \hat{u}^n \in \mathbb{R}^n_+$ such that $\operatorname{supp} \hat{u}^j = I_j$. Then there exists a neighbourhood $\mathcal{U} \subset \mathcal{S}^n$ of $\hat{A}$ with the following properties:*

(i) if $A \in \mathcal{U}$ and $\operatorname{rk} A_{I_j} = n - 4$ for all $j = 1, \dots, n$, then A is an exceptional extremal copositive matrix with non-minimal circulant zero support set;

(ii) the set of matrices $A \in \mathcal{U}$ satisfying the conditions in (i) is an algebraic submanifold of codimension $2n$ in $\mathcal{S}^n$.

The simplest manifold of the type described in Theorem 2.6.14 is the 5-dimensional $\mathcal{G}_5$-orbit of the Horn form (2.1). Another example is the 9-dimensional variety composed of the $\mathcal{G}_6$-orbits of matrices (2.5) with $\phi_{j+3} = \phi_j$, $j = 1, 2, 3$.

In both Theorem 2.6.12 and 2.6.14 the polynomials defining the algebraic submanifold are minors of the matrix $A \in \mathcal{S}^n$.

2.6.7 Faces consisting of positive semi-definite matrices

So far we have always supposed that the feasible sets $\mathcal{F}_{\mathbf{u}}$ or $\mathcal{P}_{\mathbf{u}}$ of the LMIs in Theorem 2.6.4 contain non-zero forms. We have not yet shown that non-trivial faces $F_{\mathbf{u}}$ and $P_{\mathbf{u}}$ actually exist. In this subsection we construct non-zero faces $F_{\mathbf{u}}$ of $\mathcal{C}^n$ which contain only positive semi-definite matrices, i.e., which satisfy $F_{\mathbf{u}} = P_{\mathbf{u}}$.

We shall need the following concept of a *slack matrix*, which has been introduced in [225] for convex polytopes. Let $K \subset \mathbb{R}^m$ be a regular polyhedral convex cone, and let $K^* = \{f \in \mathbb{R}_m \mid \langle f, x \rangle \geq 0 \ \forall \ x \in K\}$ be its dual cone, where $\mathbb{R}_m$ is the space of linear functionals on $\mathbb{R}^m$. Then K^* is also a regular convex polyhedral cone. Let $x_1, \dots, x_r$ be generators of the extreme rays of K, and $f_1, \dots, f_s$ generators of the extreme rays of K^*.

Definition 2.6.15. Assume the notations of the previous paragraph. The *slack matrix* of K is the nonnegative $s \times r$ matrix $(\langle f_i, x_j \rangle)_{i=1,\dots,s;j=1,\dots,r}$.

Theorem 2.6.16. *Assume $n \geq 5$, and let $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ be such that $\operatorname{supp} u^j = I_j$ for all $j = 1, \dots, n$. Let U be the $n \times n$ matrix with columns $u^1, \dots, u^n$. Then the face $F_{\mathbf{u}}$ consists of positive semi-definite matrices up to rank $n-3$ inclusive if and only if U is the slack matrix of a convex polyhedral cone $K \subset \mathbb{R}^3$ with n extreme rays.*

Theorem 2.6.16 provides a way to construct all collections $\mathbf{u} \subset \mathbb{R}^n_+$ of vectors $u^1, \dots, u^n$ satisfying $\operatorname{supp} u^j = I_j$, $j = 1, \dots, n$, such that the face $F_{\mathbf{u}}$ of $\mathcal{C}^n$ consists of positive semi-definite matrices only and is linearly isomorphic to $\mathcal{S}^{n-3}_+$.

Let now $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ be an arbitrary collection such that $\operatorname{supp} u^j = I_j$ for all $j = 1, \dots, n$. Let again U be the $n \times n$ matrix with columns $u^1, \dots, u^n$. By Lemmas 2.6.5 and 2.6.6 we have $\mathcal{P}_{\mathbf{u}} \simeq \mathcal{S}^k_+$, where k is the corank of U. We have shown that there exist collections $\mathbf{u}$ such that U has corank $n-3$. By perturbing some of the zeros u^j in such a collection, the corank of U can be decreased and may assume an arbitrary value between 0 and $n-3$. In this way we obtain faces $F_{\mathbf{u}}$ of $\mathcal{C}^n$ for which the subset $P_{\mathbf{u}}$ of positive semi-definite matrices is isomorphic to $\mathcal{S}^k_+$ with arbitrary rank $k = 0, \dots, n-3$. Here for $k \geq 2$ we must have that $F_{\mathbf{u}} = P_{\mathbf{u}}$.

2.6.8 Circulant matrices

In this subsection we shall explicitly construct non-zero faces $\mathcal{F}_{\mathbf{u}} \neq \mathcal{P}_{\mathbf{u}}$ for arbitrary matrix sizes $n \geq 5$. We consider faces $F_{\mathbf{u}}$ defined by special collections $\mathbf{u}$. Let $u \in \mathbb{R}^{n-2}_{++}$ be *palindromic*, i.e., with positive entries and invariant with respect to inversion of the order of its entries. Define $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ such that $\operatorname{supp} u^j = I_j$ and $u^j_{I_j} = u$ for all $j = 1, \dots, n$. By construction, the linear dynamical system $\mathbf{S_u}$ defined by $\mathbf{u}$ has constant coefficients, namely the entries of u. Set $p(x) = \sum_{k=0}^{n-3} u_{k+1}x^k$.

We provide necessary and sufficient conditions on $\mathbf{u}$ such that the corresponding face $F_{\mathbf{u}} \subset \mathcal{C}^n$ contains exceptional copositive matrices, and construct explicit collections $\mathbf{u}$ which satisfy these conditions. We show that the copositive matrices in these faces must be circulant, i.e., invariant with respect to simultaneous circular shifts of its row and column indices.

The next two lemmas provide necessary conditions on the entries of u by virtue of constraints on the roots of the polynomial $p(x)$, and give an explicit expression of the matrices in the corresponding face $F_{\mathbf{u}}$.

Lemma 2.6.17. *[97, Lemma 7.6] Let $n > 5$ be even, let $\mathbf{u}$ be as above, and let $A \in F_{\mathbf{u}}$ be an exceptional copositive circulant matrix. Then there exist $m = \frac{n}{2} - 2$ distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi)$, arranged in increasing order, with the following properties:*
(a) the fractional part of $\frac{n\zeta_j}{4\pi}$ is in $(0, \frac{1}{2})$ for odd j and in $(\frac{1}{2}, 1)$ for even j;
(b) the polynomial $p(x)$ is a positive multiple of $(x+1) \cdot \prod_{j=1}^{m}(x^2 - 2x\cos\zeta_j + 1)$;
(c) there exist $c > 0$, $\lambda \geq 0$ such that for all $k = 1, \dots, \frac{n}{2} + 1$ we have

$$A_{1k} = (-1)^{k-1}\lambda + c \cdot \sum_{j=1}^{m} \frac{\cos(k-1)\zeta_j}{\sin\zeta_j \sin\frac{n\zeta_j}{2} \prod_{l\neq j}(\cos\zeta_j - \cos\zeta_l)}. \tag{2.9}$$

If $\lambda = 0$, then A is extremal with non-minimal circulant zero support set. If $\lambda > 0$, then A has minimal circulant zero support set and is not extremal.

Lemma 2.6.18. *[97, Lemma 7.7] Let $n \geq 5$ be odd, let $\mathbf{u}$ be as above, and let $A \in F_{\mathbf{u}}$ be an exceptional copositive circulant matrix. Then there exist $m = \frac{n-3}{2}$ distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi]$, arranged in increasing order, with the following properties:*
(a) the fractional part of $\frac{n\zeta_j}{4\pi}$ is in $(0, \frac{1}{2})$ for odd j and in $(\frac{1}{2}, 1)$ for even j;
(b) the polynomial $p(x)$ is a positive multiple of $\prod_{j=1}^{m}(x^2 - 2x\cos\zeta_j + 1)$;
(c) there exists $c > 0$ such that for all $k = 1, \dots, \frac{n+1}{2}$ we have

$$A_{1k} = c \cdot \sum_{j=1}^{m} \frac{\cos(k-1)\zeta_j}{\sin\frac{\zeta_j}{2} \sin\frac{n\zeta_j}{2} \prod_{l\neq j}(\cos\zeta_j - \cos\zeta_l)}. \tag{2.10}$$

The matrix A has non-minimal circulant zero support set if $\zeta_m = \pi$ and minimal circulant zero support set if $\zeta_m < \pi$. In both cases A is extremal.

In contrast to item (i.f) in Theorem 2.6.11 item (c) in Lemma 2.6.18 states the extremality of A unconditionally. This allows us to prove below that extremal exceptional copositive matrices with minimal circulant zero support set actually exist for every odd order $n \geq 5$. Note that the elements A_{1k}, $k = 1, \dots, \lceil \frac{n+1}{2} \rceil$, determine the matrix A completely by its circulant property. We obtain the following characterization of collections $\mathbf{u}$ defining faces $F_{\mathbf{u}}$ which contain exceptional matrices.

Theorem 2.6.19. *[97, Lemma 7.8] Let $n > 5$ be even, $m = \frac{n}{2} - 2$, and let $\mathbf{u}$ and $p(x)$ be as in the first paragraph of this section. Then $F_{\mathbf{u}} \neq P_{\mathbf{u}}$ if and only if there exist distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi)$, arranged in increasing order, such that conditions (a),(b) of Lemma 2.6.17 hold. In this case the face $F_{\mathbf{u}}$ is linearly isomorphic to $\mathbb{R}^2_+$ and consists of the circulant matrices A with entries A_{1k}, $k = 1, \dots, \frac{n}{2} + 1$, given by (2.9) with $c, \lambda \geq 0$. The subset $P_{\mathbf{u}} \subset F_{\mathbf{u}}$ is given by those A with $c = 0$.*

Theorem 2.6.20. *[97, Lemma 7.9] Let $n \geq 5$ be odd, $m = \frac{n-3}{2}$, and let $\mathbf{u}$ and $p(x)$ be as in the first paragraph of this section. Then $F_{\mathbf{u}} \neq P_{\mathbf{u}}$ if and only if there exist distinct angles $\zeta_1, \dots, \zeta_m \in (0, \pi]$, arranged in increasing order, such that conditions (a),(b) of Lemma 2.6.18 hold. In this case the face*

$F_{\mathbf{u}}$ is an extreme ray of $\mathcal{C}^n$ and consists of the circulant matrices A with entries A_{1k}, $k = 1, \dots, \frac{n+1}{2}$, given by (2.10) *with $c \geq 0$.*

The question which collections $\mathbf{u}$, of the type described at the beginning of this subsection, yield faces $F_{\mathbf{u}}$ containing exceptional copositive matrices hence reduces to the characterization of real polynomials of the form given in (b) of Lemmas 2.6.17 or 2.6.18, with positive coefficients and satisfying condition (a) of these lemmas. This is seemingly a difficult question, and only limited results are known. However, the existence of faces $F_{\mathbf{u}}$ containing exceptional copositive matrices is guaranteed for every $n \geq 5$ by the following result on polynomials with equally spaced roots on the unit circle.

Lemma 2.6.21. *[67, Theorem 2] Let $m \geq 1$ be an integer, and let $\alpha > 0$, $\theta \geq 0$ be such that $\frac{\pi}{2} \leq \theta + \frac{(m-1)\alpha}{2} \leq \pi$ and $0 < \alpha < \frac{\pi}{m}$. Then the polynomial $q(x) = \prod_{j=1}^m (x^2 - 2x\cos(\theta + (j-1)\alpha) + 1)$ has positive coefficients.*

Based on this result we are able to construct the following explicit examples of extremal exceptional circulant matrices.

Degenerate extremal matrices. Let $n \geq 5$, $m = \lceil \frac{n}{2} \rceil - 2$, and $p(x) = \frac{(x^n+1)(x+1)}{(x^2-2x\cos\frac{\pi}{n}+1)(x^2-2x\cos\frac{3\pi}{n}+1)}$. Then $p(x)$ is a palindromic polynomial of degree $n-3$. Set also $q(x) = p(x)$ for odd n and $q(x) = \frac{p(x)}{x+1}$ for even n. Then $q(x)$ is of degree $2m$ and has positive coefficients by virtue of Lemma 2.6.21 with $\alpha = \frac{2\pi}{n}$, $\theta = \frac{5\pi}{n}$. It follows that also $p(x)$ has positive coefficients. Let $u \in \mathbb{R}_+^{n-2}$ be the vector of its coefficients, and let $\mathbf{u}$ be the collection of nonnegative vectors constructed from u as in the first paragraph of this section. Then the angles $\zeta_j = \frac{(2j+3)\pi}{n}$, $j = 1, \dots, m$, satisfy conditions (a),(b) of Lemmas 2.6.17 and 2.6.18, for even and odd n, respectively. By Theorems 2.6.19 and 2.6.20 we obtain that $F_{\mathbf{u}} \simeq \mathbb{R}_+^2$ for even n and $F_{\mathbf{u}} \simeq \mathbb{R}_+$ for odd n, their elements being circulant matrices given by (2.9) and (2.10), respectively. One extreme ray of $F_{\mathbf{u}}$ is then generated by an extremal copositive circulant matrix A with non-minimal circulant zero support set. For even n the other extreme ray is generated by a circulant positive semi-definite rank 1 matrix P. Their elements are given by $P_{ij} = (-1)^{i-j}$ and

$$A_{ij} = \begin{cases} 2(1 + 2\cos\frac{\pi}{n}\cos\frac{3\pi}{n}), & i = j, \\ -2(\cos\frac{\pi}{n} + \cos\frac{3\pi}{n}), & |i-j| \in \{1, n-1\}, \\ 1, & |i-j| \in \{2, n-2\}, \\ 0, & |i-j| \in \{3, \dots, n-3\}, \end{cases} \tag{2.11}$$

$i, j = 1, \dots, n$. For $n = 5$ we obtain the Horn form.

Regular extremal matrices. Let $n \geq 5$ be odd, and set $p(x) = \frac{x^{n+1}+1}{(x^2-2x\cos\frac{\pi}{n+1}+1)(x^2-2x\cos\frac{3\pi}{n+1}+1)}$, $m = \frac{n-3}{2}$. Then $p(x)$ is a palindromic polynomial of degree $2m = n-3$, and it has positive coefficients by virtue of Lemma 2.6.21 with $\alpha = \frac{2\pi}{n+1}$, $\theta = \frac{5\pi}{n+1}$. Construct $u \in \mathbb{R}_+^{n-2}$ and $\mathbf{u} \subset \mathbb{R}_+^n$ as above from the coefficients of $p(x)$. Then the angles $\zeta_j = \frac{(2j+3)\pi}{n+1}$, $j = 1, \dots, m$, satisfy conditions (a),(b) of Lemma 2.6.18. By Theorem 2.6.20 $F_{\mathbf{u}}$ is one-dimensional and generated by a circulant extremal copositive matrix with minimal circulant zero support set whose elements are given by (2.10). The elements of A are explicitly given by

$$A_{ij} = \begin{cases} 2(1 + 2\cos\frac{\pi}{n+1}\cos\frac{3\pi}{n+1}), & i = j, \\ -2(\cos\frac{\pi}{n+1} + \cos\frac{3\pi}{n+1}), & |i-j| \in \{1, n-1\}, \\ 1, & |i-j| \in \{2, n-2\}, \\ 0, & |i-j| \in \{3, \dots, n-3\}, \end{cases} \tag{2.12}$$

$i, j = 1, \dots, n$. For $n = 5$ we obtain a multiple of matrix (2.3) with $\psi = \frac{\pi}{6} \cdot \mathbf{1}$.

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