Chapter 7

Approximation under equality constraints

In this chapter we consider the following problem of *least squares approximation under equality (linear) constraints*.

Considering a (n, p) matrix F $(p \leq n)$ of maximal rank p and a vector y in $\mathbb{R}^n$, we are looking for a vector $x \in \mathbb{R}^p$ that minimizes

$$f(x) = \left|\left|F\,x - y\right|\right|^2 \tag{1}$$

subject to m linear constraints $(m \leq p)$ defined by the linear system

$$A\,x = b \tag{2}$$

where A is a (m, p) matrix of maximal rank m and b a vector in $\mathbb{R}^m$.

That is, we consider the problem

$$\min_{A\,x = b} \left|\left|F\,x - y\right|\right|^2 \tag{3}$$

with $A = \left(a_{ij}\right)_{1 \leq i \leq m,\, 1 \leq j \leq p}$ and $b = (b_1, \ldots, b_m)^T$.

Denoting by v_j the column vectors of matrix F, we reformulate this problem as follows.

Problem P

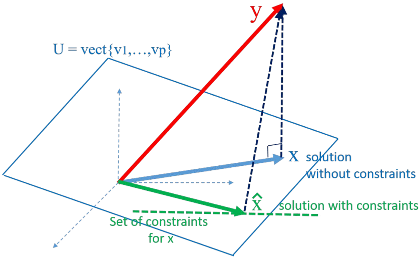
Given a vector $y \in \mathbb{R}^n$ and a subspace $U = \text{Vect}\{v_1, \ldots, v_p\}$ of $\mathbb{R}^n$ (where vectors v_j are linearly independant) we consider the following problem :

find a vector $x = \sum_{j=1}^{p} x_j v_j \in U$ that minimizes

$$f(x) = \left|\left| \sum_{j=1}^{p} x_j v_j - y \right|\right|^2 \quad (4)$$

subject to the m linear constraints $(m \leq p)$

$$\sum_{j=1}^{p} a_{ij} x_j = b_i \quad \text{for} \quad i = 1, \ldots, m \quad (5)$$



More generally, this optimization problem can be stated as follows.

Problem G

Let $f\ : U \subset \mathbb{R}^p \longrightarrow \mathbb{R}$ and $g\ : U \subset \mathbb{R}^p \longrightarrow \mathbb{R}^m$ two C^1 functions defined on an open set U of $\mathbb{R}^p$.

We consider the problem :

$$\min_{x \in U,\, g(x)=0} f(x) \qquad \text{or} \qquad \max_{x \in U,\, g(x)=0} f(x) \tag{6}$$

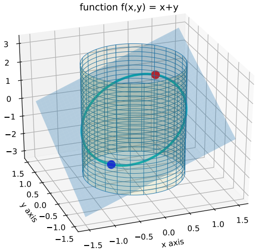
In this statement, the constraints are not necessarily linear, but are equality constraints nonetheless.

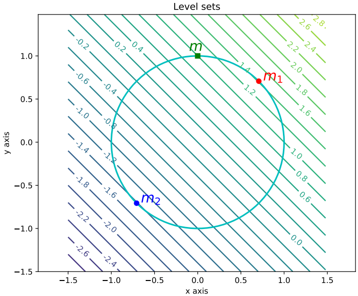
f is the *objective* function and $g = (g_1, \ldots, g_m)$ is the *constraint* function.

The method of Lagrange multipliers is a strategy for finding the local extrema of a function subject to equality constraints.

Preliminary example. Find extrema of the objective function $f(x,y) = x + y$ subject to the non linear equality constraint $g(x,y) = x^2 + y^2 - 1 = 0$.

$$\min_{(x,y)\in\Gamma} f(x,y) \qquad \text{where } \Gamma \text{ is the unit circle.}$$





• 3D analysis : the objective function defines a plane and the constraint a circular cylinder, so that we are looking for the extrema of the 3D intersection curve of these two surfaces in the 3D space.

• However, in practice, the analysis of this optimization problem will be based on 2D tools , and essentially on the level sets of the objective function , which are here straight lines.

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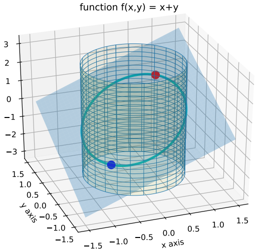
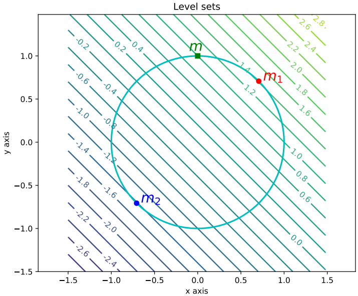




2D Geometric analysis

→ Situation at point $m = (x,y)$ shows that a small displacement $m \pm dm$ on the curve Γ will increase or decrease the value of the objective function.

→ Situation at point m_1 is different : any small displacement on the curve constraint Γ can only decrease the value of the objective function which shows that the curve Γ is tangent to the level set $\{(x,y), f(x,y) = f(m_1)\}$ at point m_1 .

Notation :

Let $h : \mathbb{R}^n \to \mathbb{R}$, $x = (x_1, \ldots, x_n) \mapsto h(x_1, \ldots, x_n)$ be a C^1 function.
The derivative (or differential) of h at point $a = (a_1, \ldots, a_n)$ is the linear form on $\mathbb{R}^n$ defined by the Jacobian matrix (equal to the transpose of the gradient of h at point a)

$$Dh(a) = \left(\frac{\partial h}{\partial x_1}(a), \frac{\partial h}{\partial x_2}(a), \ldots, \frac{\partial h}{\partial x_n}(a)\right) = \nabla h(a)^T \quad \in \mathbb{R}^n$$

Proposition 7.1 (Lagrange multipliers)

Let U be an open set of $\mathbb{R}^p$ and functions $f, g_1, \ldots, g_m \in C^1(U, \mathbb{R})$.
Let $\Gamma = \{x \in U,\ g_1(x) = g_2(x) = \cdots = g_m(x) = 0\}$ and let f_Γ be the restriction of f to Γ.
If the function f_Γ has a local extremum at a point $a \in \Gamma$, and if the differential $Dg_1(a), \ldots, Dg_m(a)$ are linearly independent, then there exist real numbers $\lambda_1, \ldots, \lambda_m$, called the Lagrange multipliers, such that

$$Df(a) = \lambda_1 Dg_1(a) + \cdots + \lambda_m Dg_m(a) \tag{7}$$

In other words, if gradient vectors $\nabla g_i(a)$ are linearly independent,

$$a \in \Gamma,\ f(a) = \min_{x \in \Gamma} f(x) \quad \Rightarrow \quad \exists\, \lambda_1, \ldots, \lambda_m, \quad \nabla f(a) = \sum_{i=1}^{m} \lambda_i \nabla g_i(a) \tag{8}$$

Solution to Problem G

With hypothesis of proposition 7.1, solutions of the optimization problems G

$$\min_{x \in U,\, g(x)=0} f(x) \qquad \text{or} \qquad \max_{x \in U,\, g(x)=0} f(x)$$

are solutions (but not necessarily all the solutions) of the following system in the variables $x = (x_1, \ldots, x_p)$ and $\lambda = (\lambda_1, \ldots, \lambda_m)$

$$\begin{cases} \nabla f(x) &= \sum_{i=1}^{m} \lambda_i \nabla g_i(x) \\ g(x) &= 0 \end{cases} \tag{9}$$

Lagrangian — another formulation of the solution

Relation between the gradient of the objective function f and the gradients of the constraint functions g_i naturally leads to introduce a new function known as the *Lagrangian function*

$$L(x,\lambda) = f(x) - \sum_{i=1}^{m} \lambda_i \, g_i(x)\,, \qquad \lambda = (\lambda_1, \ldots, \lambda_m) \tag{10}$$

Therefore, solutions of the optimization problem G are stationary points of the Lagrangian function $L(x,\lambda)$ and can be expressed as the vanishing of the differential of the Lagrangian :

$$DL(x,\lambda) = 0 \quad \Leftrightarrow \quad \begin{cases} \dfrac{\partial L}{\partial x}(x,\lambda) &= 0 \\ \dfrac{\partial L}{\partial \lambda}(x,\lambda) &= 0 \end{cases} \quad \Leftrightarrow \quad \begin{cases} \nabla f(x) &= \displaystyle\sum_{i=1}^{m} \lambda_i \nabla g_i(x) \\ g(x) &= 0 \end{cases} \tag{11}$$

Example

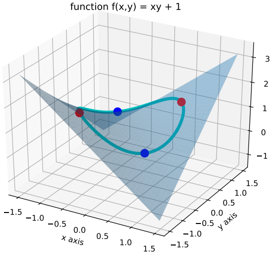
Find extrema of the function $f(x,y) = xy + 1$ with the non linear equality constraint $g(x,y) = x^2 + y^2 - 1 = 0$.

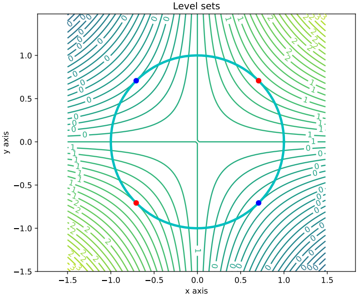
$$\left\{ \begin{array}{l} \left\{ \begin{array}{rcl} \dfrac{\partial f}{\partial x}(x,y) & = & \lambda \, \dfrac{\partial g}{\partial x}(x,y) \\ \dfrac{\partial f}{\partial x}(x,y) & = & \lambda \, \dfrac{\partial g}{\partial x}(x,y) \end{array} \right. \\ g(x,y) = 0 \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \left\{ \begin{array}{rcl} y & = & \lambda \, 2\, x \\ x & = & \lambda \, 2\, y \end{array} \right. \\ x^2 + y^2 - 1 = 0 \end{array} \right.$$

which leads to $\lambda = \pm\frac{1}{2}$ and to four solutions :

– two maximum at $(\sqrt{2}/2, \sqrt{2}/2)$ and $(-\sqrt{2}/2, -\sqrt{2}/2)$ (the red points in the figure),

– two minimum at $(\sqrt{2}/2, -\sqrt{2}/2)$ and $(-\sqrt{2}/2, \sqrt{2}/2)$ (the blue points in the figure).





As stated in the introduction in (4) & (5) we consider the problem P

$$\min_{A\,x\,=\,b} \left|\left| \sum_{j=1}^{p} x_j\, v_j - y \right|\right|^2$$

which leads to find the stationary points of the following Lagrangian function

$$L(x,\lambda) = \frac{1}{2} \left|\left| \sum_{j=1}^{p} x_j\, v_j - y \right|\right|^2 + \sum_{i=1}^{m} \lambda_i \left(\sum_{j=1}^{p} a_{ij}\, x_j \; - \; b_i \right) \tag{12}$$

where matrix $A = \big(a_{ij}\big)_{1\le i\le m,\, 1\le j\le p}$ and vector $b = (b_1, \ldots, b_m)^T$ represent the constraints and where $y, v_1, \ldots, v_p$ are given vectors in $\mathbb{R}^n$ that characterize the objective function.

- We thus need to solve the following system

$$\left\{ \begin{array}{rcl} \dfrac{\partial L}{\partial x}(x,\lambda) & = & 0 \\[2ex] \dfrac{\partial L}{\partial \lambda}(x,\lambda) & = & 0 \end{array} \right. \quad \Leftrightarrow \quad \left\{ \begin{array}{rcll} \dfrac{\partial L}{\partial x_k}(x,\lambda) & = & 0, & k = 1,2,\ldots,p \\[2ex] \dfrac{\partial L}{\partial \lambda_i}(x,\lambda) & = & 0, & i = 1,2,\ldots,m \end{array} \right.$$

$$\Leftrightarrow \quad \left\{ \begin{array}{rcll} \left\langle \displaystyle\sum_{j=1}^{p} x_j\, v_j - y,\; v_k \right\rangle + \displaystyle\sum_{i=1}^{m} \lambda_i\, a_{ik} & = & 0, & k = 1,2,\ldots,p \\[3ex] \displaystyle\sum_{j=1}^{p} a_{ij}\, x_j \; - \; b_i & = & 0, & i = 1,2,\ldots,m \end{array} \right.$$

$$\Leftrightarrow \quad \left\{ \begin{array}{llll} \displaystyle\sum_{j=1}^{p} x_j \left\langle v_j,\, v_k \right\rangle + \sum_{i=1}^{m} \lambda_i\, a_{ik} & = & \left\langle y,\, v_k \right\rangle, & k = 1, 2, \ldots, p \\ \displaystyle\sum_{j=1}^{p} a_{ij}\, x_j & = & b_i, & i = 1, 2, \ldots, m \end{array} \right.$$

which leads to solve the $(p+m, p+m)$ linear system

$$\left(\begin{array}{ccc|ccc} \langle v_1,\, v_1 \rangle & \cdots & \langle v_1,\, v_p \rangle & a_{11} & \cdots & a_{m1} \\ \vdots & & \vdots & \vdots & & \vdots \\ \vdots & & \vdots & \vdots & & \vdots \\ \vdots & & \vdots & \vdots & & \vdots \\ \langle v_p,\, v_1 \rangle & \cdots & \langle v_p,\, v_p \rangle & a_{1p} & \cdots & a_{mp} \\ \hline a_{11} & \cdots & a_{1p} & & & \\ \vdots & & \vdots & & 0 & \\ a_{m1} & \cdots & a_{mp} & & & \end{array} \right) \begin{pmatrix} x_1 \\ \vdots \\ \vdots \\ \vdots \\ x_p \\ \lambda_1 \\ \vdots \\ \lambda_m \end{pmatrix} = \begin{pmatrix} \langle y,\, v_1 \rangle \\ \vdots \\ \vdots \\ \vdots \\ \langle y,\, v_p \rangle \\ b_1 \\ \vdots \\ b_m \end{pmatrix}$$

$$\Leftrightarrow \quad \begin{cases} \sum_{j=1}^{p} x_j \left\langle v_j,\, v_k \right\rangle + \sum_{i=1}^{m} \lambda_i \, a_{ik} & = \quad \left\langle y,\, v_k \right\rangle, \qquad k = 1, 2, \ldots, p \\ \sum_{j=1}^{p} a_{ij} \, x_j & = \quad b_i, \qquad i = 1, 2, \ldots, m \end{cases}$$

which leads to solve the $(p+m, p+m)$ linear system

$$\left(\begin{array}{c|c} \left\langle v_j,\, v_k \right\rangle & A^T \\ \hline A & 0 \end{array} \right) \begin{pmatrix} x_j \\ \lambda_i \end{pmatrix} = \begin{pmatrix} \left\langle y,\, v_k \right\rangle \\ b_i \end{pmatrix} \tag{13}$$

or, more simply

$$\left(\begin{array}{c|c} F^T F & A^T \\ \hline A & 0 \end{array} \right) \begin{pmatrix} x \\ \lambda \end{pmatrix} = \begin{pmatrix} F^T y \\ b \end{pmatrix} \tag{14}$$

Problem

Consider a strictly increasing sequence of n points

$$\alpha = t_1 < t_2 < \cdots < t_i < \cdots < t_n = \beta,$$

a given function $f \in C^0[\alpha, \beta]$, as well as a family of p linearly independant functions $v_j \in C^0[\alpha, \beta], j = 1, 2, \ldots, p$.

We consider the following problem.

Find a function $x(t) = \sum_{j=1}^{p} x_j \, v_j(t)$ which minimizes $\sum_{i=1}^{n} \Big[x(t_i) - f(t_i)\Big]^2$ subject to the integral constraint $\int_\alpha^\beta x(t)\, dt = b$, where b is a prescribed value.

Lagrangian modeling

The constraint can be written as follows

$$\int_{\alpha}^{\beta} x(t)\,dt = \int_{\alpha}^{\beta} \sum_{j=1}^{p} x_j\, v_j(t)\,dt = \sum_{j=1}^{p} x_j \underbrace{\int_{\alpha}^{\beta} v_j(t)\,dt}_{a_j} = \sum_{j=1}^{p} a_j\, x_j = b$$

So that our problem is as follows

$$\min_{\sum_{j=1}^{p} a_j\, x_j = b} \quad \sum_{i=1}^{n} \Big[\sum_{j=1}^{p} x_j\, v_j(t_i) - f(t_i) \Big]^2$$

and we introduce the Lagrangian as in the previous section

$$L(x,\lambda) = \frac{1}{2} \sum_{i=1}^{n} \Big[\sum_{j=1}^{p} x_j\, v_j(t_i) - f(t_i) \Big]^2 + \lambda \Big(\sum_{j=1}^{p} a_j\, x_j - b \Big)$$

Lagrangian equations

Then, with the notations

$$y = \big(f(t_1), f(t_2), \ldots, f(t_n)\big)^T \qquad \& \qquad V_j = \big(v_j(t_1), v_j(t_2), \ldots, v_j(t_n)\big)^T, \quad j = 1, \ldots, p$$

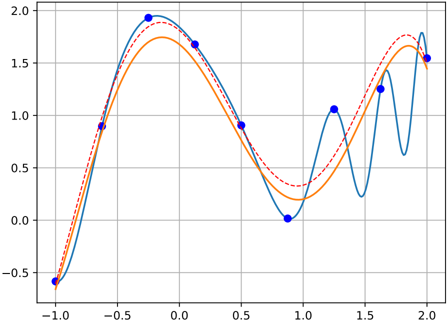
stationary points of the Lagrangian are obtained by solving the linear equations

$$\begin{cases} \displaystyle\sum_{j=1}^{p} x_j \, \langle V_k, V_j \rangle \; + \; \lambda \, a_k \; = \; \langle y, V_k \rangle, \qquad k = 1, 2, \ldots, p \\ \displaystyle\sum_{j=1}^{p} a_j \, x_j \; = \; b \end{cases}$$

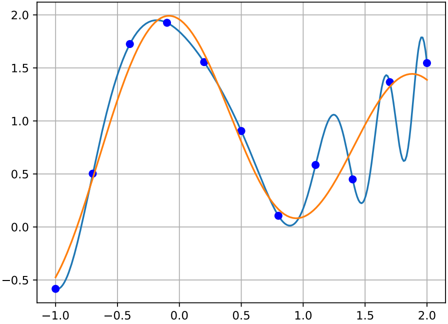
which leads to solve the $(p+1, p+1)$ linear system

$$\left(\begin{array}{ccc|c} \langle V_1, V_1 \rangle & \cdots & \langle V_1, V_p \rangle & a_1 \\ \vdots & & \vdots & \vdots \\ \vdots & & \vdots & \vdots \\ \vdots & & \vdots & \vdots \\ \langle V_p, V_1 \rangle & \cdots & \langle V_p, V_p \rangle & a_p \\ \hline a_1 & \cdots & a_p & 0 \end{array}\right) \begin{pmatrix} x_1 \\ \vdots \\ \vdots \\ \vdots \\ x_p \\ \lambda \end{pmatrix} = \begin{pmatrix} \langle y, V_1 \rangle \\ \vdots \\ \vdots \\ \vdots \\ \langle y, V_p \rangle \\ b \end{pmatrix}$$

Example — Approximation under integral constraint



<u>Polynomial</u> least squares approximation of the function $f(t) = \sin(t^2 - 2t + 1) + \cos^2(t + t^3)$ *(the blue curve) at 9 evenly spaced points.*
— Dotted curves : least squares approximation by polynomials of degree 5.
— Solid curves : least squares approximation by polynomials of degree 5 subject to satisfy the integral of the initial function f.



<u>Trigonometric</u> least squares approximation of the function $f(t) = \sin(t^2 - 2t + 1) + \cos^2(t + t^3)$ *(the blue curve) at 11 evenly spaced points, by a function of the space* $\{1, \cos(2t), \sin(2t), \cos(3t), \sin(3t)\}$ *subject to satisfy the integral of the initial function* f.