GEOMETRIC OPTIMIZATION

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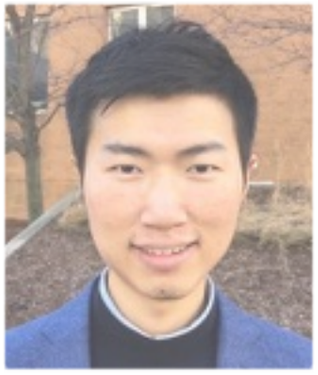
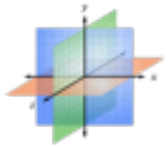
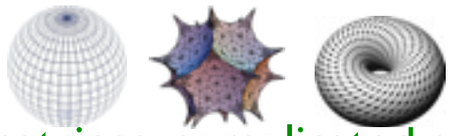


- **Vector spaces**



- **Manifolds**
(hypersphere, orthogonal matrices, complicated surfaces)



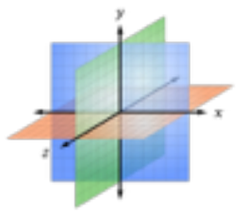
- **Convex sets**
(probability simplex, semidefinite cone, polyhedra)

Geometric Optimization

- **Metric spaces**
(tree space, Wasserstein spaces, CAT(0), space-of-spaces)

Machine Learning
Graphics
Robotics
Vision
BCI
NLP
Statistics

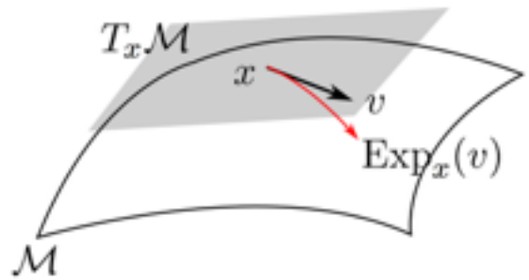
Example: Riemannian optimization



Vector space optimization

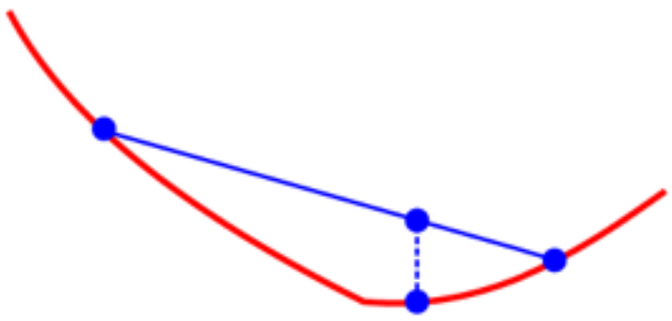
Orthogonality constraint	Stiefel manifold
Fixed-rank constraint	Grassmann manifold
Positive semi-definite constraint	PSD manifold
… …	… …

Riemannian optimization

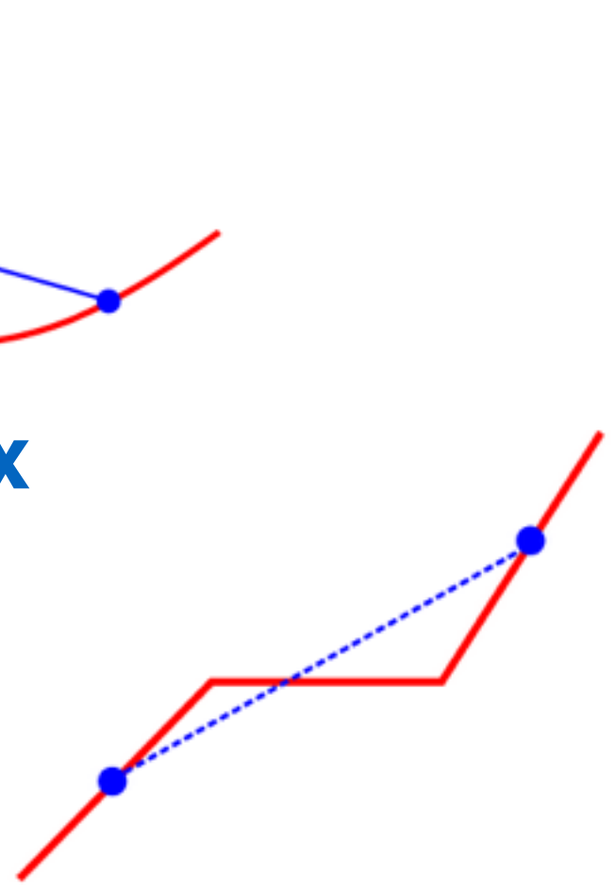


[Udriste, 1994; Absil et al., 2009]

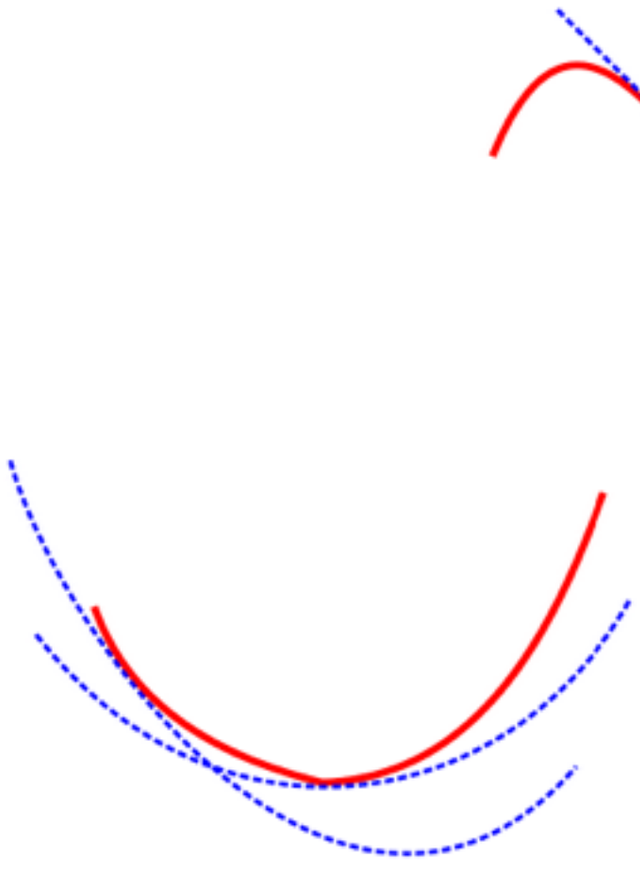
Classes of function in optimization



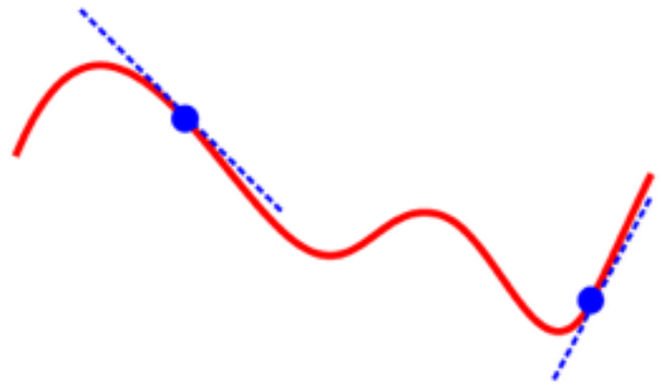
Convex



Lipschitz

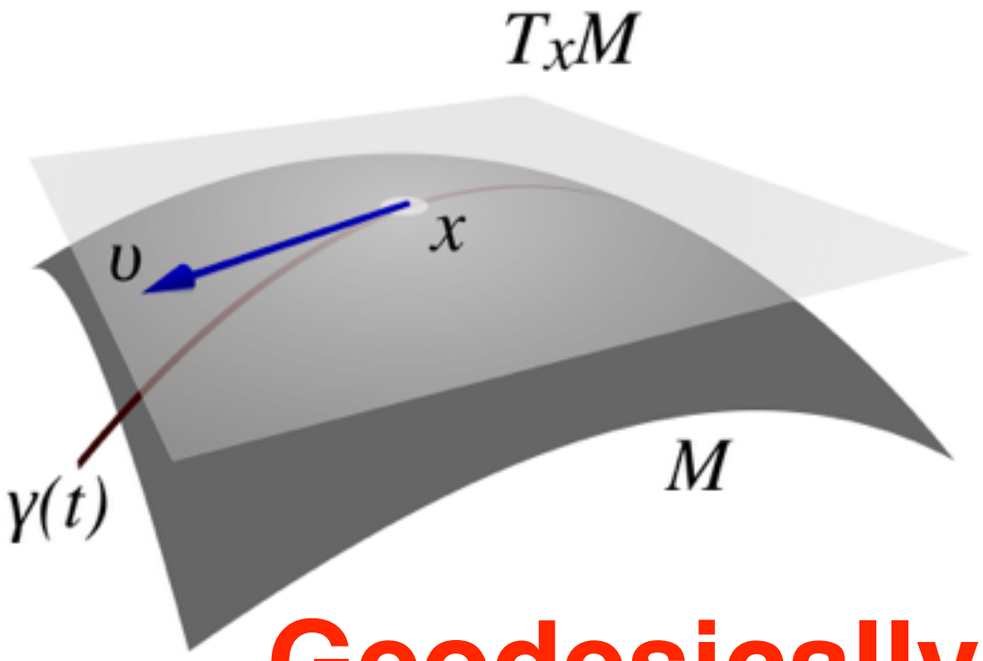


Strongly convex

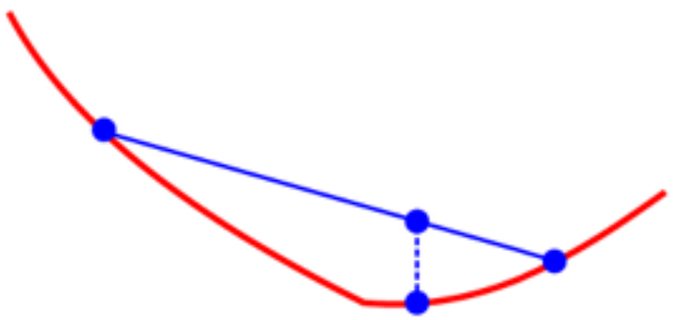


Smooth

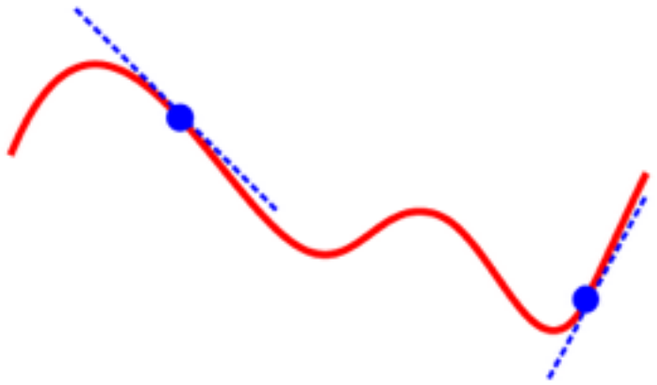
Classes of function in optimization



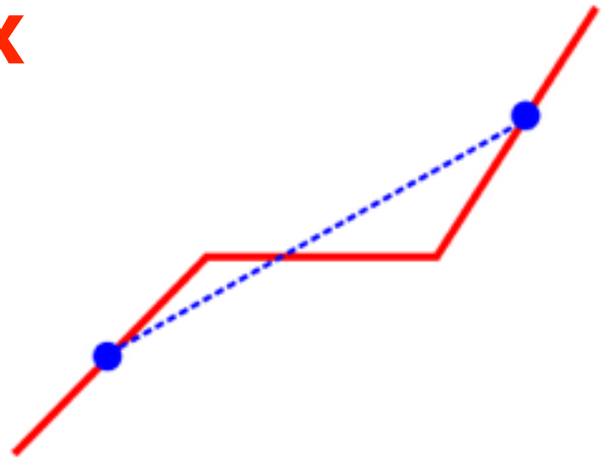
Geodesically



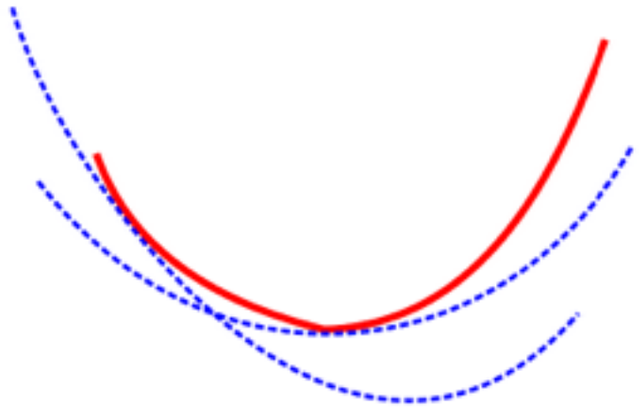
Convex



Smooth



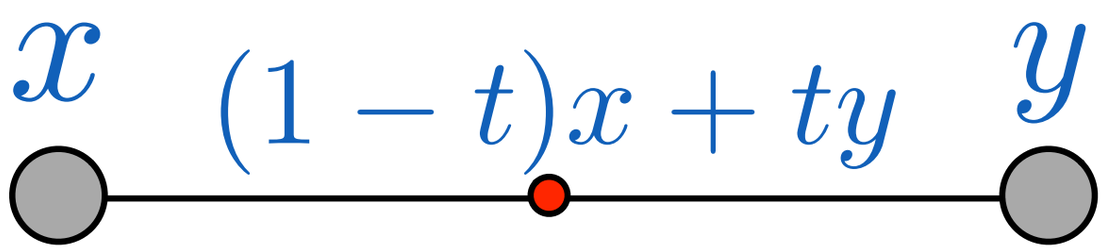
Lipschitz



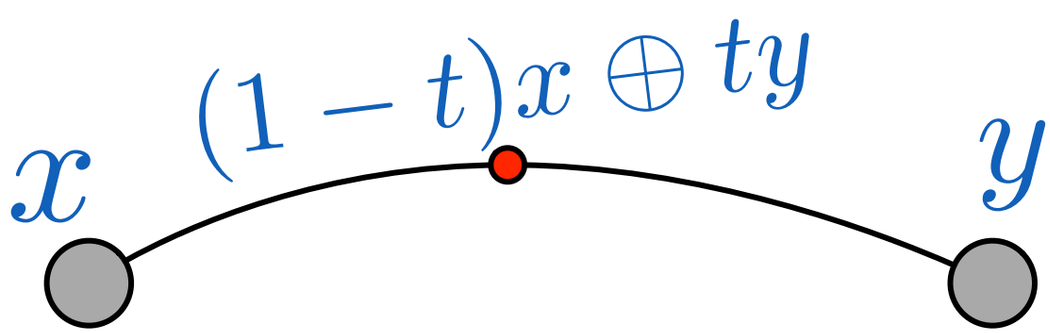
Strongly convex

What is geodesic convexity?

Convexity



Geodesic convexity



$$f((1-t)x \oplus ty) \leq (1-t)f(x) + tf(y)$$

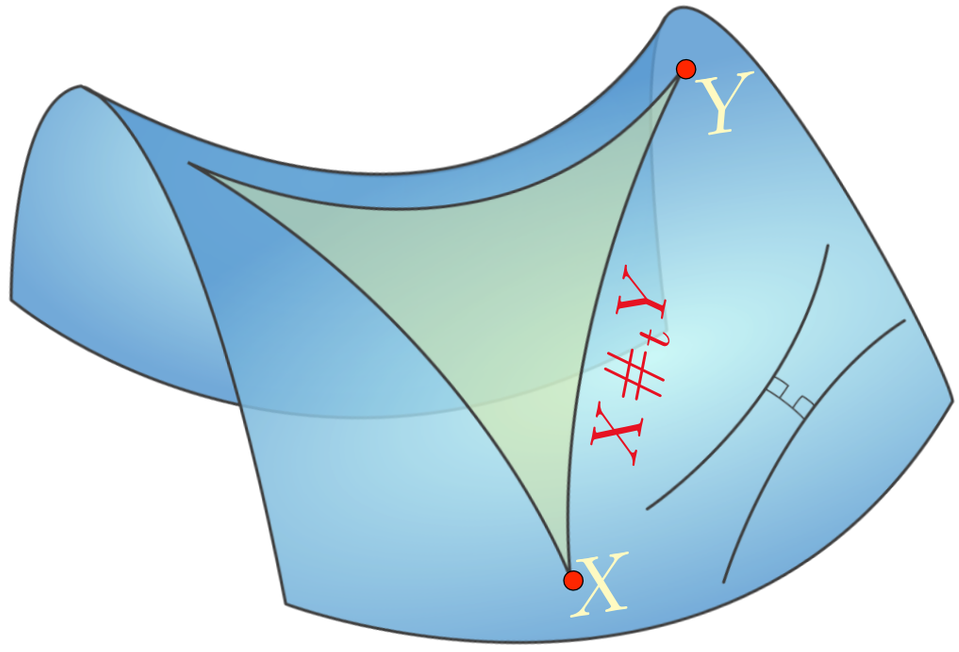
on a Riemannian manifold $f(y) \geq f(x) + \left\langle g_x, \mathrm{Exp}_x^{-1}(y) \right\rangle_x$

Metric spaces & curvature: [Menger; Alexandrov; Busemann; Bridson, Häflinger; Gromov; Perelman]

Example: Positive definite matrices

Geodesic

$$X \#_t Y := X^{\frac{1}{2}} (X^{-\frac{1}{2}} Y X^{-\frac{1}{2}})^t X^{\frac{1}{2}}$$
$$= (1-t)X \oplus tY$$



Examples

$$f(X) = \begin{cases} \log\det(X), & \log\mathrm{tr}(X), \\ \mathrm{tr}(X^\alpha), & \|X^\alpha\|. \quad (\alpha > 0) \end{cases}$$

Exercise: verify for above examples

$$f(X \#_t Y) \leq (1-t) f(X) + t f(Y)$$

PSD manifold and g-convexity

Recognizing, constructing, and optimizing g-convex functions

[Sra, Hosseini (2013,2015)]

- *[Wiesel 2012]*
- *[Rápcsák 1984]*
- *[Udriste 1994]*

Corollaries

$$X \mapsto \log\det(B + \sum\nolimits_i A_i^* X A_i)$$

$$X \mapsto \log\mathrm{per}(B + \sum\nolimits_i A_i^* X A_i)$$

$$\delta_R^2(X,Y), \quad \delta_S^2(X,Y)$$

(jointly g-convex)

Many more theorems and corollaries

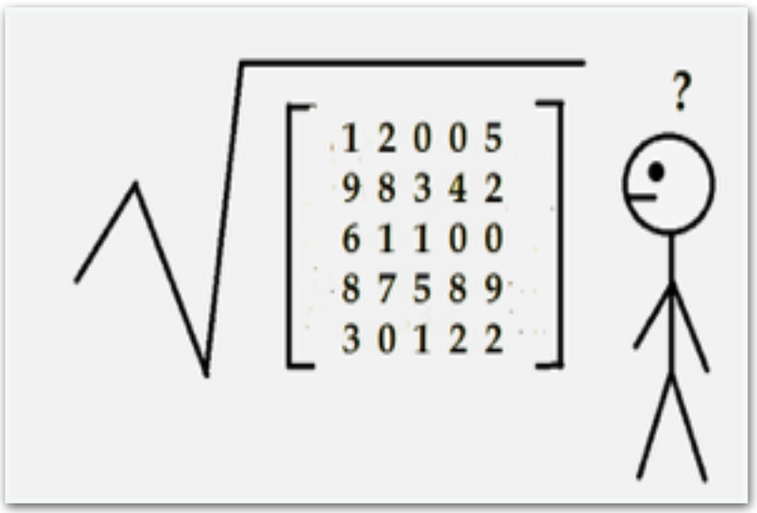
One-D version known as: **Geometric Programming**
www.stanford.edu/~boyd/papers/gp_tutorial.html

[Boyd, Kim, Vandenberghe, Hassibi (2007). 61pp.]

Examples

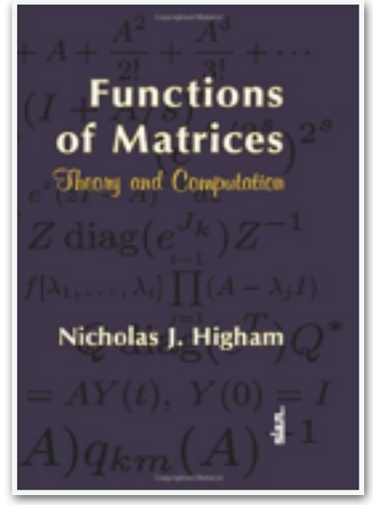
$$X \succ 0$$

Matrix square root



Broadly applicable

Key to '`logm`'



Matrix square root

Nonconvex optimization through the Euclidean lens

[Jain, Jin, Kakade, Netrapalli; Jul 2015]

$$\min_{X \in \mathbb{R}^{n \times n}} \|M - X^2\|_F^2$$

Gradient descent

$$X_{t+1} \leftarrow X_t - \eta(X_t^2 - M)X_t - \eta X_t(X_t^2 - M)$$

Simple algorithm; linear convergence; **nontrivial** analysis

Matrix square root

Geodesic

$$X \#_t Y := X^{\frac{1}{2}} \left(X^{-\frac{1}{2}} Y X^{-\frac{1}{2}} \right)^t X^{\frac{1}{2}}$$

Midpoint

$$A^{\frac{1}{2}} = A \#_{\frac{1}{2}} I$$

Matrix square root

Nonconvex optimization through **non-Euclidean** lens

[Sra; Jul 2015]

$$\min_{X \succ 0} \quad \delta_S^2(X, A) + \delta_S^2(X, I)$$

Fixed-point iteration

$$X_{k+1} \leftarrow [(X_k + A)^{-1} + (X_k + I)^{-1}]^{-1}$$

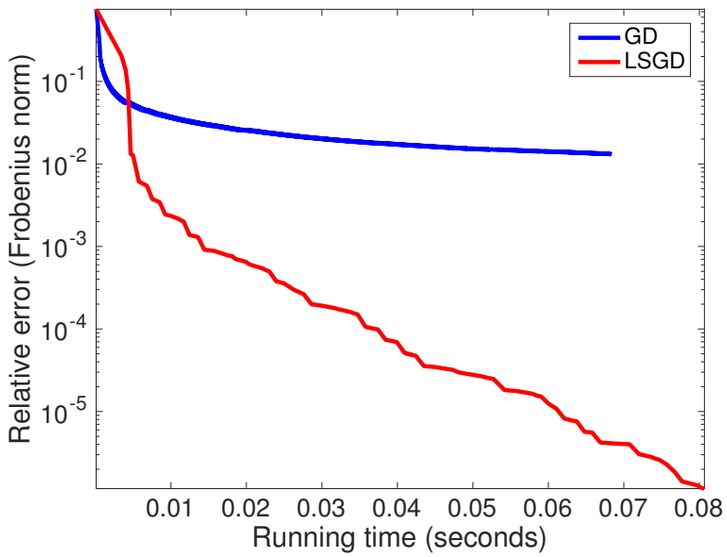
Simple method; linear convergence; 1/2 page analysis!

Global optimality thanks to geodesic convexity

$$\delta_S^2(X, Y) := \tfrac{1}{2} \log\det\left(\tfrac{X+Y}{2}\right) - \tfrac{1}{2} \log\det(XY)$$

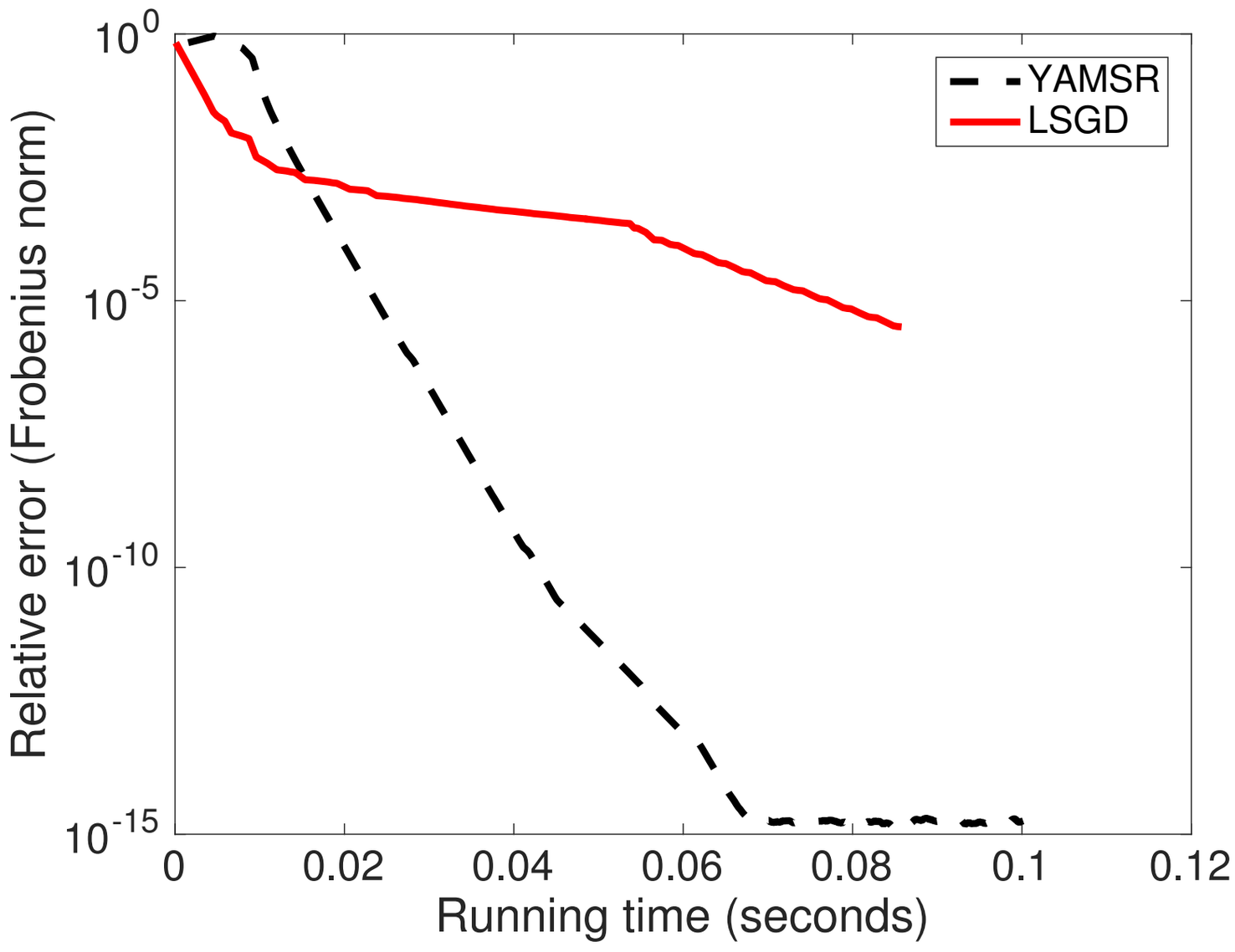
(Curiously, this is the Jensen-Shannon divergence between multivariate Gaussians!)

Matrix square root



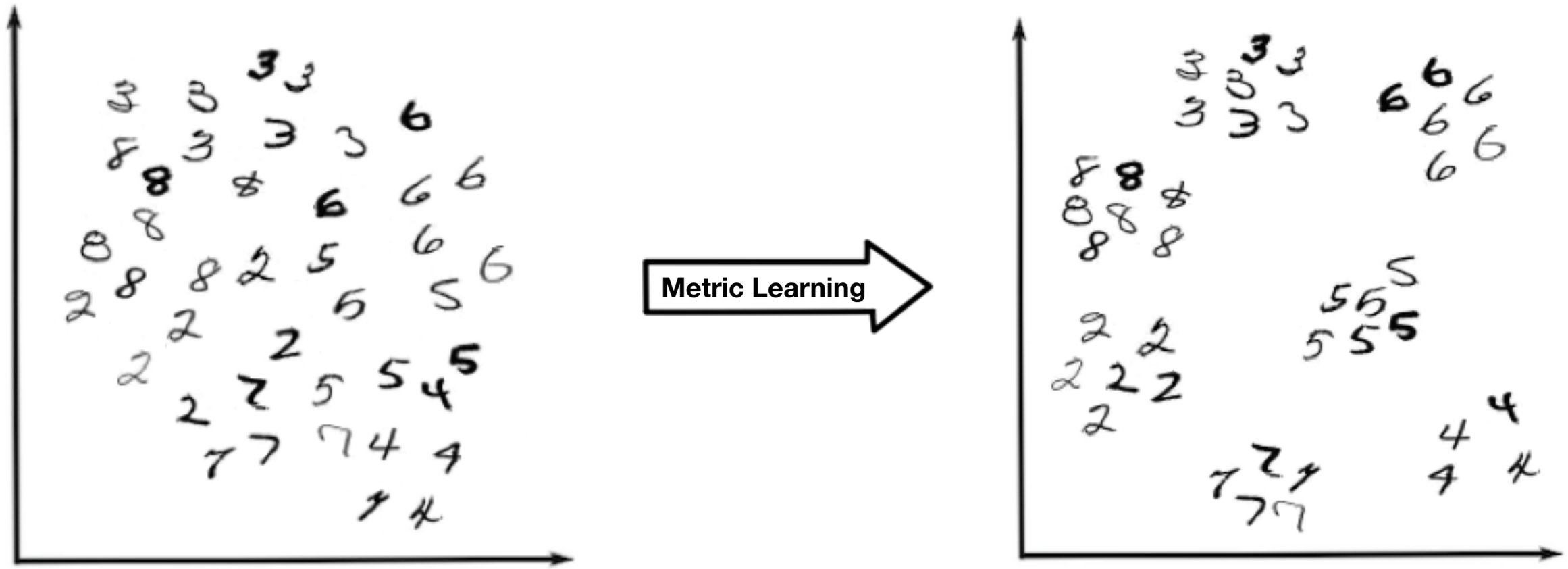
50×50 matrix $I + \beta UU^T$

$\kappa \approx 64$



Metric learning

What does a metric learning method do?



Euclidean metric learning

Pairwise constraints

$$\mathcal{S} := \{(\boldsymbol{x}_i, \boldsymbol{x}_j) \mid \boldsymbol{x}_i \text{ and } \boldsymbol{x}_j \text{ are in the same class}\}$$
$$\mathcal{D} := \{(\boldsymbol{x}_i, \boldsymbol{x}_j) \mid \boldsymbol{x}_i \text{ and } \boldsymbol{x}_j \text{ are in different classes}\}$$

Goal

given pairwise constraints learn Mahalanobis distance

$$d_{\boldsymbol{A}}(\boldsymbol{x}, \boldsymbol{y}) := (\boldsymbol{x} - \boldsymbol{y})^T \boldsymbol{A} (\boldsymbol{x} - \boldsymbol{y})$$

*Positive definite matrix **A***

Metric learning methods

MMC

[Xing, Jordan, Russell, Ng 2002]

$$\min_{\boldsymbol{A}\succeq 0} \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{S}} d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j)$$
$$\text{such that} \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{D}} \sqrt{d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j)} \geq 1$$

LMNN

[Weinberger, Saul 2005]

$$\min_{\boldsymbol{A}\succeq 0} \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{S}} \Big[(1-\mu)d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j) + \mu \sum\nolimits_l (1-y_{il})\xi_{ijl}\Big]$$
$$d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_l) - d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j) \geq 1-\xi_{ijl}$$
$$\xi_{ijl} \geq 0$$

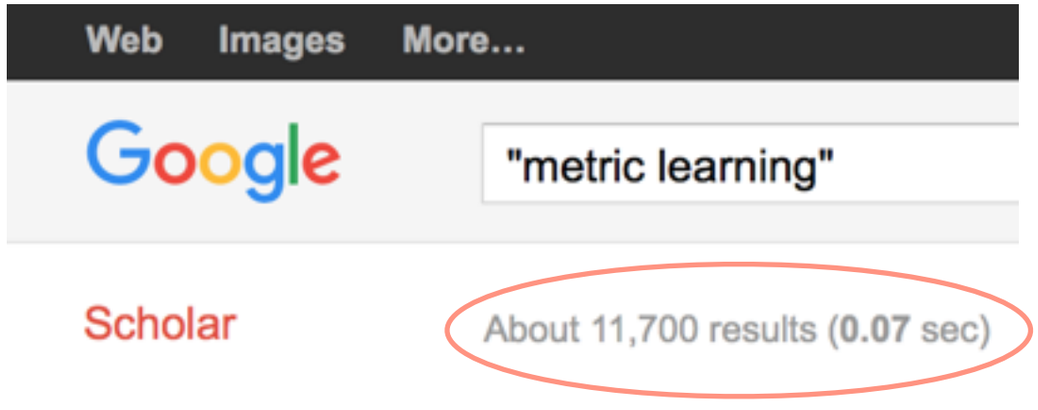
ITML

[Davis, Kulis, Jain, Sra, Dhillon 2007]

$$\min_{\boldsymbol{A}\succeq 0} \quad D_{\mathrm{ld}}(\boldsymbol{A},\boldsymbol{A}_0)$$
$$\text{such that} \quad d_{\boldsymbol{A}}(\boldsymbol{x},\boldsymbol{y}) \leq u, \quad (\boldsymbol{x},\boldsymbol{y})\in\mathcal{S},$$
$$d_{\boldsymbol{A}}(\boldsymbol{x},\boldsymbol{y}) \geq l, \quad (\boldsymbol{x},\boldsymbol{y})\in\mathcal{D}$$

$$D_{\mathrm{ld}}(\boldsymbol{A},\boldsymbol{A}_0) := \mathrm{tr}(\boldsymbol{A}\boldsymbol{A}_0^{-1}) - \log\det(\boldsymbol{A}\boldsymbol{A}_0^{-1}) - d$$

tons of other methods!



A simple new way for metric learning

Euclidean idea

$$\min_{\boldsymbol{A}\succeq 0} \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{S}} d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j) - \lambda \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{D}} d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j)$$

New idea

$$\min_{\boldsymbol{A}\succeq 0} \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{S}} d_{\boldsymbol{A}}(\boldsymbol{x}_i,\boldsymbol{x}_j) + \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{D}} d_{\boldsymbol{A}^{-1}}(\boldsymbol{x}_i,\boldsymbol{x}_j)$$

Equivalently solve

$$\min_{\boldsymbol{A}\succ 0} \quad h(\boldsymbol{A}) := \operatorname{tr}(\boldsymbol{A}\boldsymbol{S}) + \operatorname{tr}(\boldsymbol{A}^{-1}\boldsymbol{D})$$

$$\boldsymbol{S} := \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{S}} (\boldsymbol{x}_i-\boldsymbol{x}_j)(\boldsymbol{x}_i-\boldsymbol{x}_j)^T,$$

$$\boldsymbol{D} := \sum_{(\boldsymbol{x}_i,\boldsymbol{x}_j)\in\mathcal{D}} (\boldsymbol{x}_i-\boldsymbol{x}_j)(\boldsymbol{x}_i-\boldsymbol{x}_j)^T$$

[Habibzadeh, Hosseini, Sra, ICML 2016]

A simple new way for metric learning

$$X \#_t Y := X^{\frac{1}{2}} (X^{-\frac{1}{2}} Y X^{-\frac{1}{2}})^t X^{\frac{1}{2}}$$

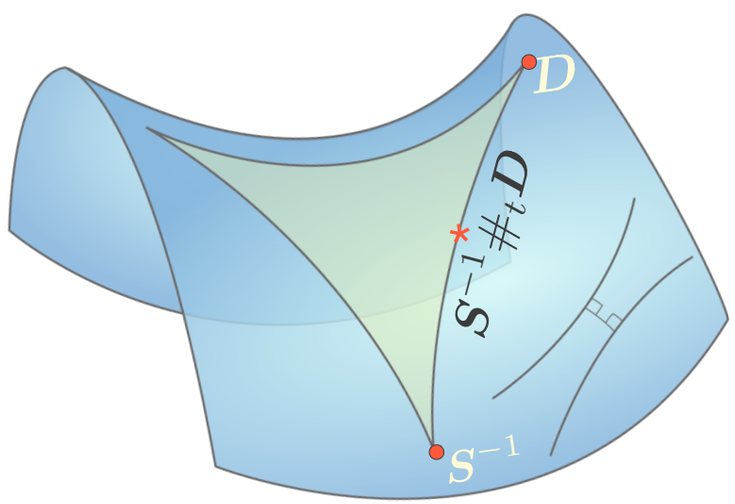
Closed form solution!

$$\nabla h(\boldsymbol{A}) = 0 \quad \Leftrightarrow \quad \boldsymbol{S} - \boldsymbol{A}^{-1} \boldsymbol{D} \boldsymbol{A}^{-1} = 0$$

$$\boldsymbol{A} = \boldsymbol{S}^{-1} \#_{\frac{1}{2}} \boldsymbol{D}$$

More generally

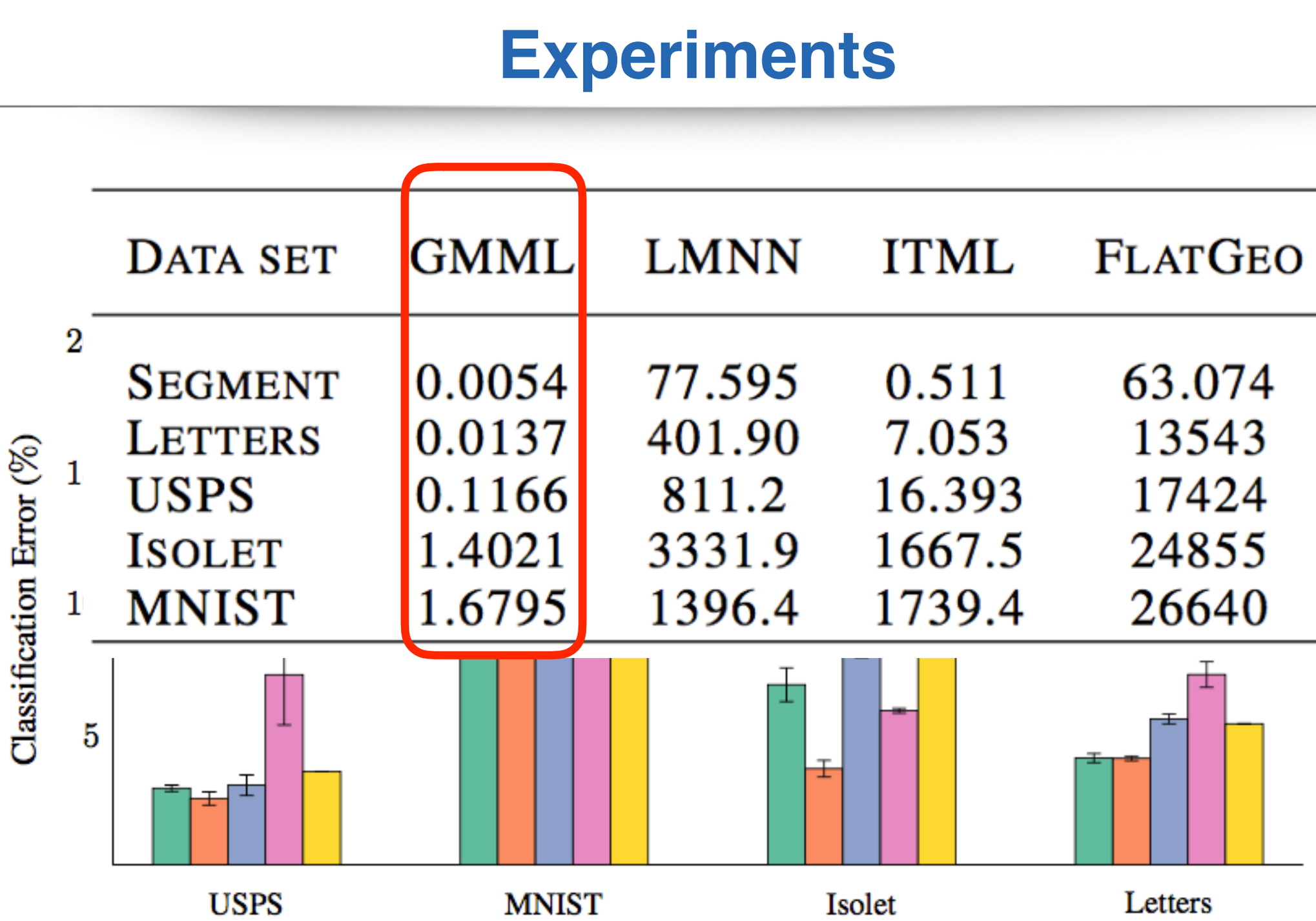
$$\min_{\boldsymbol{A} \succ 0} \quad (1-t)\delta_R^2(\boldsymbol{S}^{-1}, \boldsymbol{A}) + t\delta_R^2(\boldsymbol{D}, \boldsymbol{A})$$



$$\boldsymbol{S}^{-1} \#_t \boldsymbol{D}$$

Experiments

Data set	GMML	LMNN	ITML	FlatGeo
Segment	0.0054	77.595	0.511	63.074
Letters	0.0137	401.90	7.053	13543
USPS	0.1166	811.2	16.393	17424
Isolet	1.4021	3331.9	1667.5	24855
MNIST	1.6795	1396.4	1739.4	26640



[Habibzadeh, Hosseini, Sra ICML 2016]

Brascamp-Lieb Constant

$$\int_{\mathbb{R}^n} \prod_{i=1}^{m} f_i(B_i x)^{p_i}\, dx \leq D^{-1/2} \prod_{i=1}^{m} \left(\int_{\mathbb{R}^{n_i}} f_i(y)\, dy \right)^{p_i}$$

$$D := \inf \left\{ \frac{\det\left(\sum_i p_i B_i^* X_i B_i\right)}{\prod_i (\det X_i)^{p_i}} \,\middle|\, X_i \succ 0, n_i \times n_i, \right\}$$

$$p_i > 0, f_i \geq 0 \qquad \sum_{i=1}^{m} p_i n_i = n$$

powerful inequality; includes Hölder, Loomis-Whitney, Young's, many others!

Brascamp-Lieb constant

$$\min_{X_1,\ldots,X_m \succ 0} \log\det\left(\sum\nolimits_i p_i B_i^* X_i B_i\right) - \sum\nolimits_i p_i \log\det X_i$$

- Arises in geometric complexity theory:
  [Garg, Gurvits, Oliveira, Wigderson; Jul 2016]

Exercise

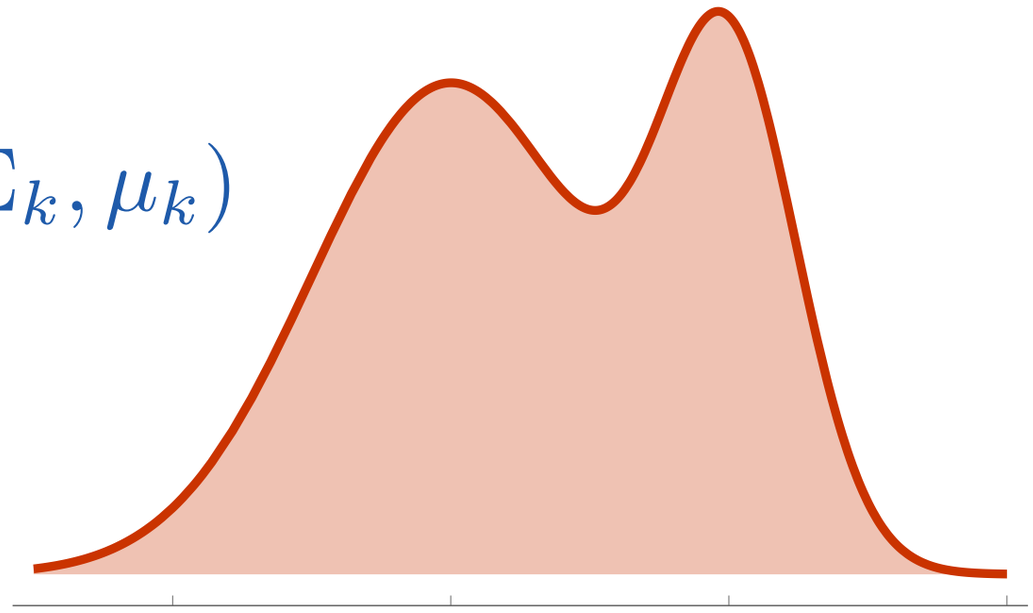
Prove this is a g-convex opt problem

- G-convexity yields transparent algorithms & complexity analysis for global optimum.

Gaussian mixture models

$$p_{\text{mix}}(x) := \sum_{k=1}^{K} \pi_k p_{\mathcal{N}}(x; \Sigma_k, \mu_k)$$

$$\max \prod\nolimits_i p_{\text{mix}}(x_i)$$



Expectation maximization (EM): default choice

$$p_{\mathcal{N}}(x; \Sigma, \mu) \propto \frac{1}{\sqrt{\det(\Sigma)}} \exp\left(-\tfrac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$

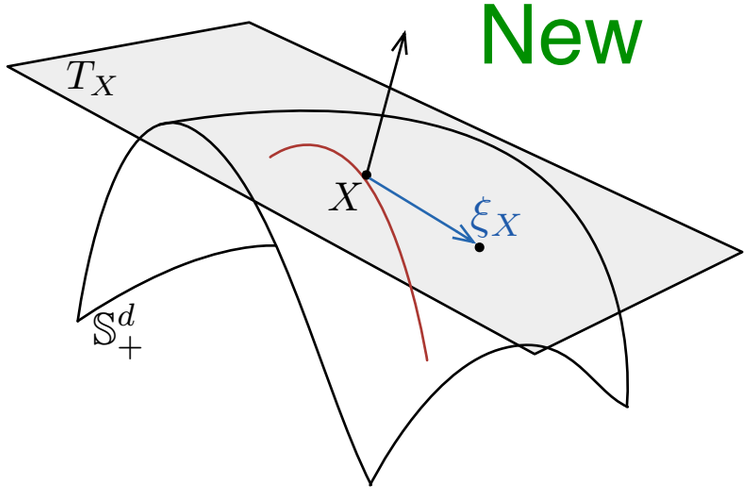
Gaussian mixture models

- **Nonconvex –** difficult, possibly several local optima
- **GMMs –** Recent surge of theoretical results
- **In Practice –** EM still default choice

Difficulty: Positive definiteness constraint on Σ_k

Geometric opt

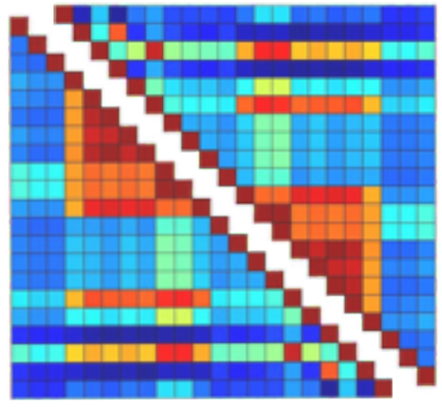
New



Unconstrained, Cholesky

Folklore

$$LL^T$$



[Hosseini, Sra NIPS 2015]

Failure of "obvious" LL^T

sep.	EM	CG-LL^T
0.2	52s // 12.7	614s // 12.7
1	160s // 13.4	435s // 13.5
5	72s // 12.8	426s // 12.8

$$\|\mu_i - \mu_j\| \geq \text{sep} \max_{ij}\{\text{tr}\Sigma_i, \text{tr}\Sigma_j\}$$

d=20
simulation

Failure of Riemannian optimization

K	EM	Riem-CG
2	17s // 29.28	947s // 29.28
5	202s // 32.07	5262s // 32.07
10	2159s // 33.05	17712s // 33.03

manopt.org

Riemannian opt. toolbox

d=35 images dataset

What's wrong?

log-likelihood for one component

$$-\frac{n}{2}\log\det\Sigma - \frac{1}{2}\sum_{i=1}^{n}(x_i-\mu)^T\Sigma^{-1}(x_i-\mu)$$

Euclidean convex problem
Not geodesically convex

Reformulate as g-convex

$$y_i = \begin{bmatrix} x_i \\ 1 \end{bmatrix} \quad S = \begin{bmatrix} \Sigma + \mu\mu^T & \mu \\ \mu^T & 1 \end{bmatrix}$$

$$\max_{S\succ 0} \ \widehat{\mathcal{L}}(S) := \sum_{i=1}^{n} \log q_{\mathcal{N}}(y_i; S),$$

Thm. The modified log-likelihood is g-convex. Local max of modified mixture LL is local max of original.

Success of geometric optimization

K	EM	Riem-CG	L-RBFGS
2	17s // 29.28	**18s** // 29.28	**14s** // 29.28
5	202s // 32.07	**140s** // 32.07	**117s** // 32.07
10	2159s // 33.05	**1048s** // 33.06	**658s** // 33.06

Riem-CG (manopt) savings:

947→**18**; 5262 →**140**; 17712→**1048**

d=35 images dataset

github.com/utvisionlab/mixest

First-order algorithms

[Zhang, Sra, COLT 2016]

first-order g-convex optimization

$$\min_{x \in \mathcal{X} \subset \mathcal{M}} \quad f(x)$$

$\mathcal{X}$ g-convex set; f g-convex func; $\mathcal{M}$ Riemannian manifold

oracle access to exact or stochastic (sub)gradients

$$x \leftarrow \operatorname{Exp}_x(-\eta \nabla f(x))$$

---

analog to: $x \leftarrow x - \eta \nabla f(x)$

In particular, we study the global complexity of first-order g-convex optimization

Global Complexity

Gradient Descent

Stochastic Gradient Descent

Coordinate Descent

Accelerated Gradient Descent

Fast Incremental Gradient

... ...

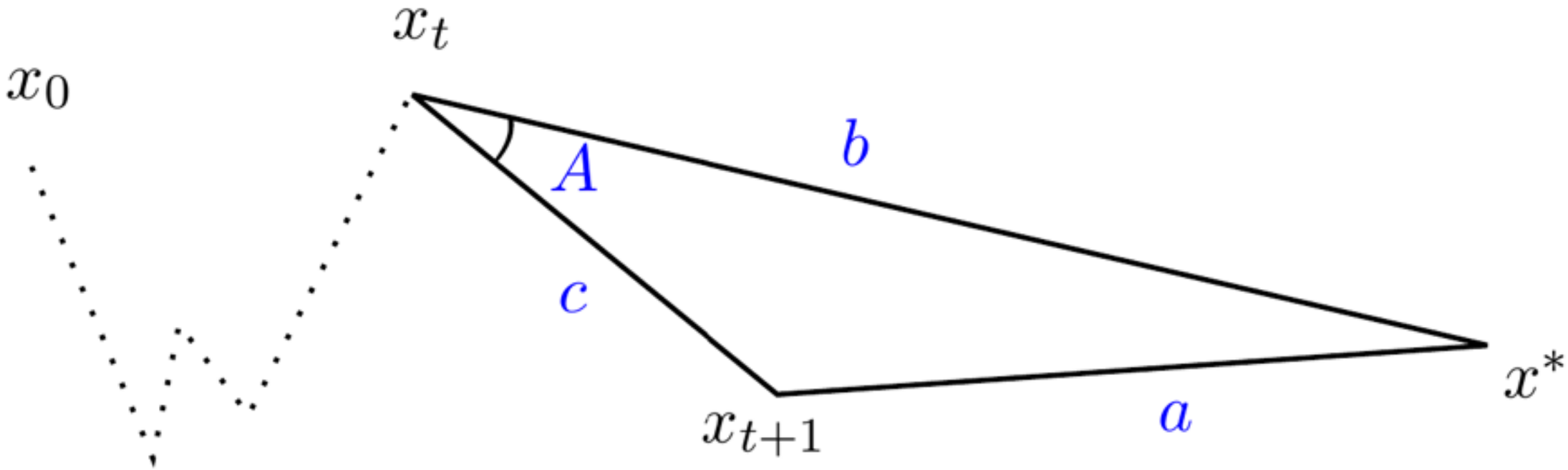
$$\mathbb{E}[f(x_a) - f(x^*)] \leq ?$$

Convex Optimization

G-Convex Optimization

The Euclidean law of cosines is essential to bound $d^2(x_{t+1},x^*)$ in analysis of usual convex opt. methods

$$x_{t+1} = x_t - \eta_t g_t$$



$$a^2 = b^2 + c^2 - 2bc\cos(A)$$

$$\Downarrow$$

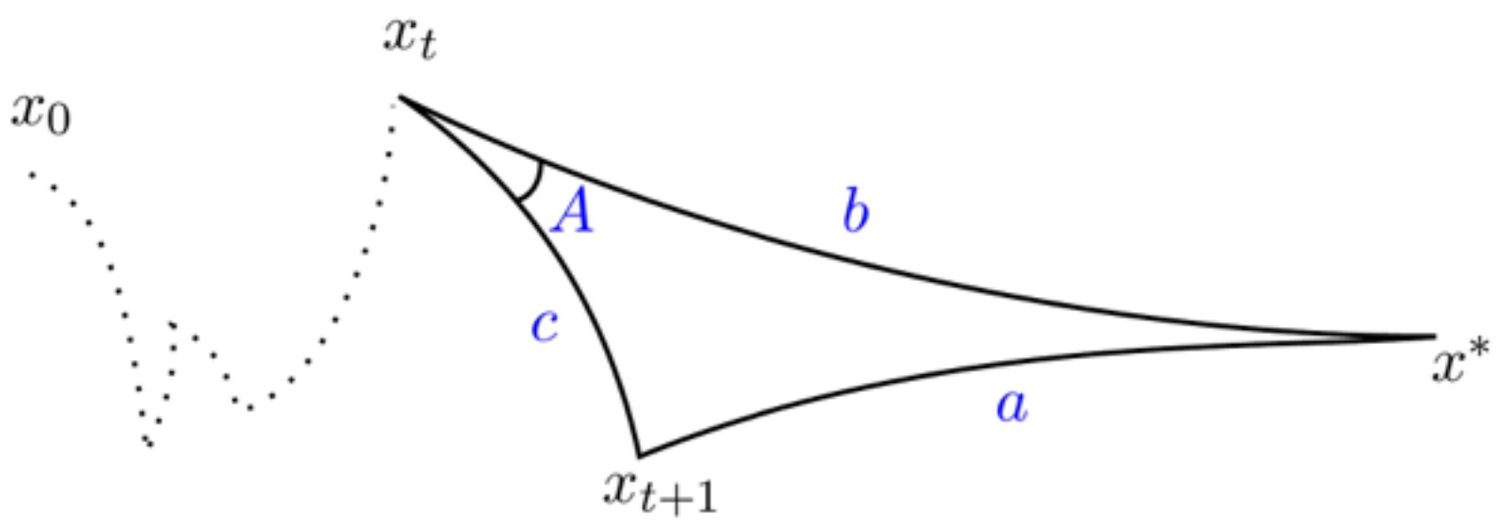
$$\|x_{t+1} - x^*\|^2 = \|x_t - x^*\|^2 + \eta_t^2\|g_t\|^2 - 2\eta_t \langle g_t, x_t - x^* \rangle$$

We develop a corresponding inequality to bound $d^2(x_{t+1}, x^*)$ on manifolds

$$\cosh(-\kappa a) = \cosh(-\kappa b)\cosh(-\kappa c) + \sinh(-\kappa b)\sinh(-\kappa c)\cos(A)$$

Toponogov's theorem

Grönwall's inequality



$$a^2 \leq b^2 + \zeta(\kappa_{\min}, b)c^2 - 2bc\cos(A)$$

$$\zeta(\kappa_{\min}, b) \triangleq \frac{\sqrt{|\kappa_{\min}|}b}{\tanh(\sqrt{|\kappa_{\min}|}b)}$$

Rediscovers and generalizes result of:
C.-Erausquin, McCann, Schmuckenschläger, *Invent. Math.* (2001).

Convergence rates depend on lower bounds on the sectional curvature

(Sub)gradient	convex	g-convex
Lipschitz	$O\left(\sqrt{\frac{1}{t}}\right)$	$O\left(\sqrt{\frac{\zeta_{\max}}{t}}\right)$
Strongly convex / smooth	$O\left(\frac{1}{t}\right)$	$O\left(\frac{\zeta_{\max}}{t}\right)$
Strongly convex & smooth	$O\left((1-\frac{\mu}{L_g})^t\right)$	$O\left((1-\min\{\frac{1}{\zeta_{\max}}, \frac{\mu}{L_g}\})^t\right)$
Stochastic (sub)gradient	... ...	

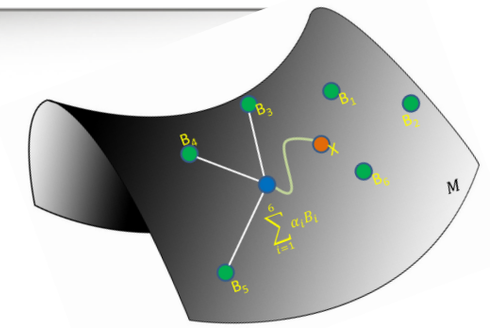
$$\zeta_{\max} \triangleq \frac{\sqrt{|\kappa_{\min}|}D}{\tanh\left(\sqrt{|\kappa_{\min}|}D\right)}$$

See paper for other interesting results *[Zhang, Sra, COLT 2016]*

Is that all?

Riemannian finite-sum problems

$$\min_{x \in \mathcal{M}} \quad f(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$



- $\mathcal{M}$ is a Riemannian manifold
- g-convex and g-nonconvex ‘f’ allowed
- First global complexity results for stochastic methods on Riemannian manifolds
- Riemannian SVRG

[Zhang, Reddi, Sra, NIPS 2016]

Stochastic eigenvector computation

$$\min_{x^T x = 1} \quad -x^T \left(\sum_{i=1}^{n} z_i z_i^T \right) x$$

compute dominant eigenvector

Online PCA, stochastic power method, SVRG accelerated, etc.

[Garber, Hazan 2015; Jin, Kakade, Musco, Netrapalli, Sidford 2015; Shamir 2015, 2016]

Key insight:

A non-convex problem on sphere; "satisfies" manifold version of Polyak-Łojasiewicz inequality; RSVRG analysis delivers simple proof of linear convergence

[Zhang, Reddi, Sra, NIPS 2016]

Invitation for more!

- Faster stochastic optimization
- Beyond Riemannian manifolds
- Faster gradient based algorithms
- Handling more complex constraints
- Lower bound theory
- …

Thanks!