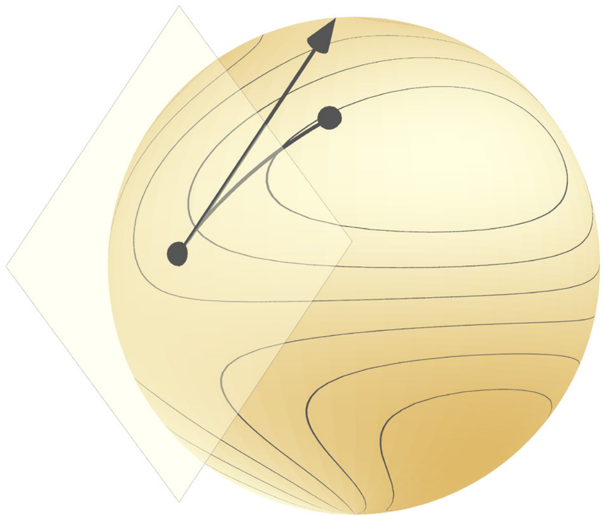
001

Context and applications



Spring 2023

Optimization on manifolds, MATH 512 @ EPFL

Instructor: Nicolas Boumal

Step 0 in optimization

It starts with a set S and a function $f\colon S \to \mathbf{R}$. We want to compute:

$$\min_{x \in S} f(x)$$

These bare objects fully specify the problem.

Any additional structure on S and f may (and should) be exploited for algorithmic purposes but is not part of the problem.

Classical unconstrained optimization

The search space *is* a linear space, e.g., $S = \mathbf{R}^n$:

$$\min_{x \in \mathbf{R}^n} f(x)$$

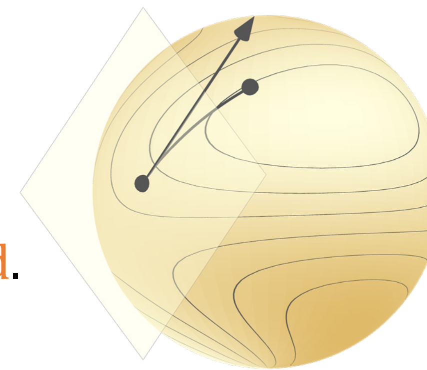
We can *choose* to turn $\mathbf{R}^n$ into a Euclidean space: $\langle u, v \rangle = u^\top v$.

If f is differentiable, we have a gradient $\mathrm{grad} f$ and Hessian $\mathrm{Hess} f$.
We can build algorithms with them: gradient descent, Newton's...

This course: optimization on manifolds

We target applications where $S = \mathcal{M}$ *is* a smooth manifold:

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



We can *choose* to turn $\mathcal{M}$ into a Riemannian manifold.

If f is differentiable, we have a Riemannian gradient and Hessian.

We can build algorithms with them: gradient descent, Newton's...

Proposed by Luenberger in 1972

MANAGEMENT SCIENCE
Vol. 18, No. 11, July, 1972
Printed in U.S.A.

THE GRADIENT PROJECTION METHOD ALONG GEODESICS*†

DAVID G. LUENBERGER
Stanford University

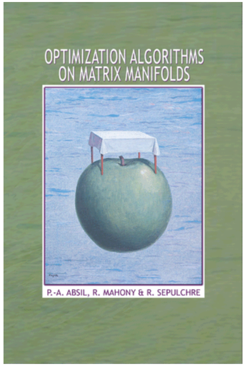
Practical since 1990s with numerical linear algebra

SIAM J. MATRIX ANAL. APPL.
Vol. 20, No. 2, pp. 303–353

THE GEOMETRY OF ALGORITHMS WITH ORTHOGONALITY CONSTRAINTS*

ALAN EDELMAN†, TOMÁS A. ARIAS‡, AND STEVEN T. SMITH§

Popularized in the 2010s by Absil et al.'s book



Becoming mainstream now.

How do manifolds come up in optimization?

Example 1: $A \in \mathbf{R}^{n\times n}$, $A = A^\top$; want: the largest eigenvalue of A.

$$A = \sum_{i=1}^{n} \lambda_i v_i v_i^T, \qquad \lambda_1 \geq \cdots \geq \lambda_n ; \quad v_1 \cdots v_n \in \mathbb{R}^n \text{ orthonormal.}$$

$$f(x) = x^T A x \; ; \quad f(v_1) = v_1^T \underbrace{A v_1}_{\lambda_1 v_1} = \lambda_1 \underbrace{v_1^T v_1}_{1} = \lambda_1 .$$

Claim: $\left[\max_{x \in \mathbb{R}^n} f(x) \text{ s.t. } \underbrace{x^T x = 1}_{} \right] = \lambda_1 .$

$$S^{n-1} = \{ x \in \mathbb{R}^n : x^T x = 1 \} \text{ is a manifold.}$$

Example 2: $M \in \mathbf{R}^{m\times n}$; want: the largest singular value of M.

SVD: $M = \sum_{i=1}^{r} \sigma_i u_i v_i^T$, $\sigma_1 \geq \cdots \geq \sigma_r$

$u_1, \ldots, u_r$ are orthonormal in $\mathbb{R}^m$

$v_1, \ldots, v_r$ are orthonormal in $\mathbb{R}^n$.

$f(x,y) = x^T M y$; $f(u_1, v_1) = u_1^T M v_1 = \sigma_1$.

Claim: $\left[\max_{\substack{x \in \mathbb{R}^m \\ y \in \mathbb{R}^n}} f(x,y) \text{ s.t. } \begin{array}{l} x^T x = 1 \\ y^T y = 1 \end{array} \right] = \sigma_1$.

$S^{m-1} \times S^{n-1}$ is a manifold.

Example 3: $A \in \mathbf{R}^{n\times n}$, $A = A^\top$; want: top-k eigenspace of A.

$$St(n,k) = \{X \in \mathbb{R}^{n\times k} : X^T X = I_k\}$$

Stiefel

$$f(X) = \mathrm{Tr}[X^T A X].$$

Claim: $$\left[\max_{X\in\mathbb{R}^{n\times k}} f(X) \quad \text{s.t. } X^T X = I_k\right] = \lambda_1 + \dots + \lambda_k$$

(Courant-Fischer, Ky-Fan)

$$Q \in O(k) = \{ Q \in \mathbb{R}^{k\times k} : Q^T Q = Q Q^T = I_k \}$$

$$X \in St(n,k),\ Q \in O(k) \implies f(XQ) = Tr[(XQ)^T A XQ]$$

$$= Tr[Q^T X^T A X Q]$$

$$= Tr[X^T A X Q Q^T]$$

$$= f(X).$$

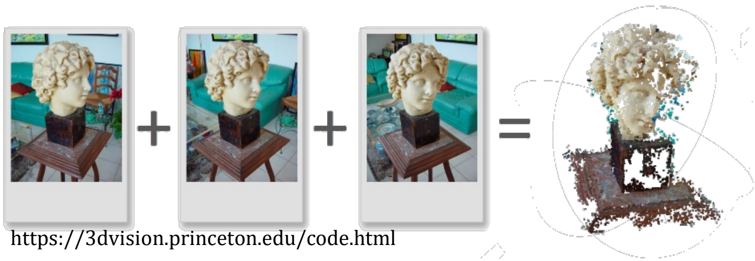
<u>define</u>: $X_1 \sim X_2 \iff X_1 = X_2 Q$ for some $Q \in O(k)$.

$$[X] = \{ XQ : Q \in O(k) \}$$

$$St(n,k) / \sim$$

More examples from applications

Structure from motion (SfM)



https://3dvision.princeton.edu/code.html

Simultaneous localization and mapping (SLAM)

https://www.popsci.com/new-roomba-knows-location

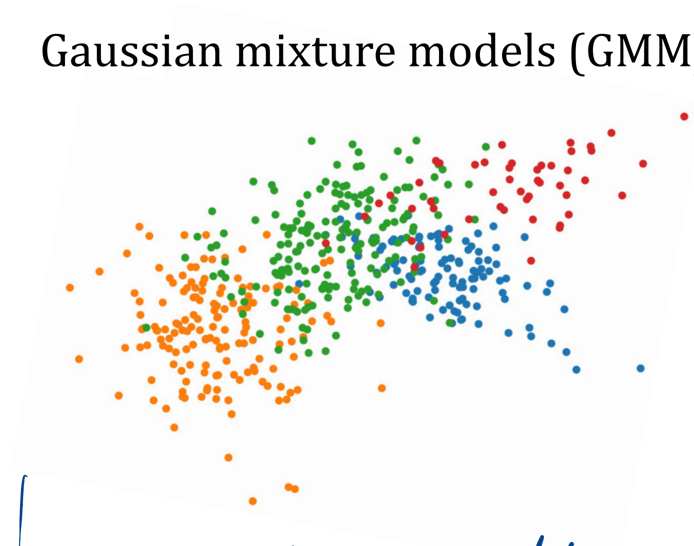
$\mathbb{R}^3 \times SO(3)$

$SO(d) = \{ R \in \mathbb{R}^{d \times d} : R^T R = I_d, \det(R) = +1 \}$

Recommender systems

$$\mathbb{R}_r^{m\times n} = \{ X \in \mathbb{R}^{m\times n} : \operatorname{rank}(X) = r \}$$

Gaussian mixture models (GMM)



$$\mathbb{R}^d \times \{ \Sigma \in \mathbb{R}^{d\times d} : \Sigma \succ 0 \}$$

Image credit: Netflix, https://i.stack.imgur.com/bWcIo.png