Optimization On Manifolds

Pierre-Antoine Absil
Robert Mahony
Rodolphe Sepulchre

Based on ''Optimization Algorithms on Matrix Manifolds'', Princeton University Press, January 2008

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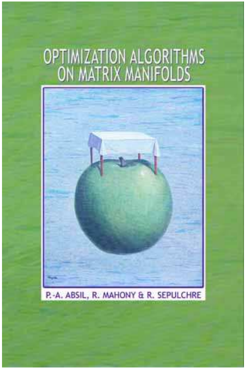
Collaboration

Chris Baker
(Florida State University and Sandia National Laboratories)
Kyle Gallivan
(Florida State University)
Paul Van Dooren
(Université catholique de Louvain)

Reference



Optimization Algorithms on Matrix Manifolds
P.-A. Absil, R. Mahony, R. Sepulchre
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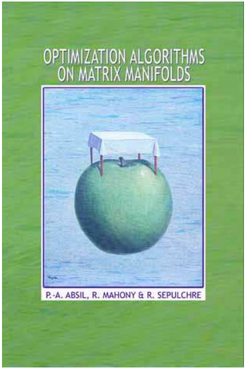
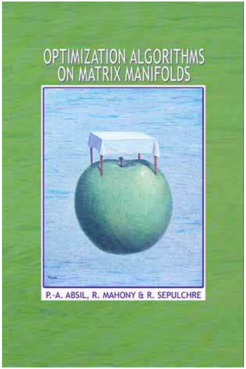
About the reference



- The publisher, Princeton University Press, has been a non-profit company since 1910.
- Official publication date is January 2008.
- Copies are already shipping.

Reference: contents



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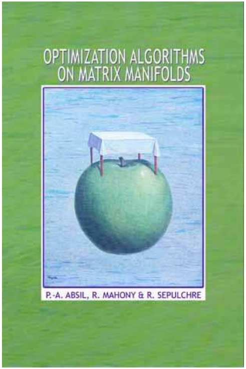
2. Motivation and applications
3. Matrix manifolds: first-order geometry
4. Line-search algorithms
5. Matrix manifolds: second-order geometry
6. Newton's method
7. Trust-region methods
8. A constellation of superlinear algorithms



Chap 3: Matrix Manifolds: first-order geometry

1. Charts, atlases, manifolds
2. Differentiable functions
3. Embedded submanifolds
4. Quotient manifolds
5. Tangent vectors and differential maps
6. Riemannian metric, distance, gradient

Smooth optimization in $\mathbb{R}^n$

General unconstrained optimization problem in $\mathbb{R}^n$:
Let

$$f : \mathbb{R}^n \to \mathbb{R},$$

The real-valued function f is termed the *cost function* or *objective function*.
Problem: find $x_* \in \mathbb{R}^n$ such that there exists $\epsilon > 0$ for which

$$f(x) \geq f(x_*) \text{ whenever } \|x - x_*\| < \epsilon.$$

Such a point x_* is called a *local minimizer* of f.

Smooth optimization in $\mathbb{R}^n$

General unconstrained optimization problem in $\mathbb{R}^n$:
Let

$$f : \mathbb{R}^n \to \mathbb{R},$$

The real-valued function f is termed the *cost function* or *objective function*.
Problem: find $x_* \in \mathbb{R}^n$ such that there exists a neighborhood $\mathcal{N}$ of x_* such that

$$f(x) \geq f(x_*) \text{ whenever } x \in \mathcal{N}.$$

Such a point x_* is called a *local minimizer* of f.

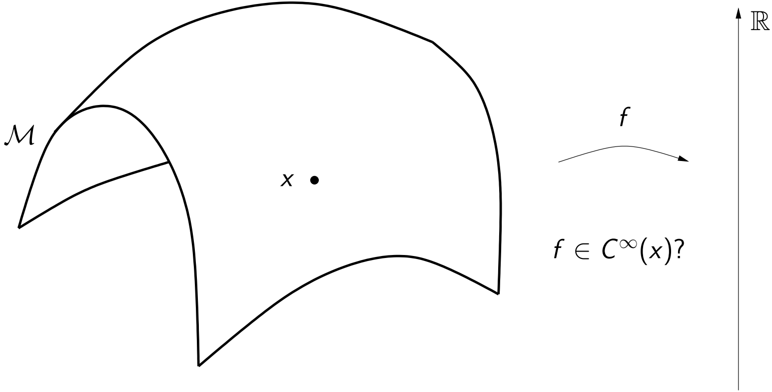
Smooth optimization *beyond* $\mathbb{R}^n$

$$? \ \arg\min_{x \in \mathbb{R}^n} f(x)$$

- Several optimization techniques require the cost function to be differentiable to some degree:
  - Steepest-descent at x requires $\mathrm{D}f(x)$.
  - Newton's method at x requires $\mathrm{D}^2 f(x)$.
- Can we go beyond $\mathbb{R}^n$ without losing the concept of differentiability?

$$\arg\min_{x \in \mathbb{R}^n} f(x) \qquad \rightsquigarrow \qquad \arg\min_{x \in \mathcal{M}} f(x)$$

Smooth optimization on a manifold: what "smooth" means



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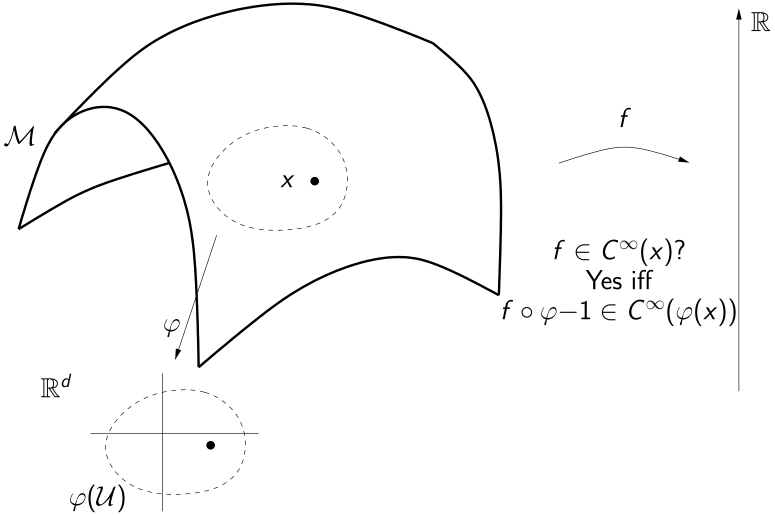

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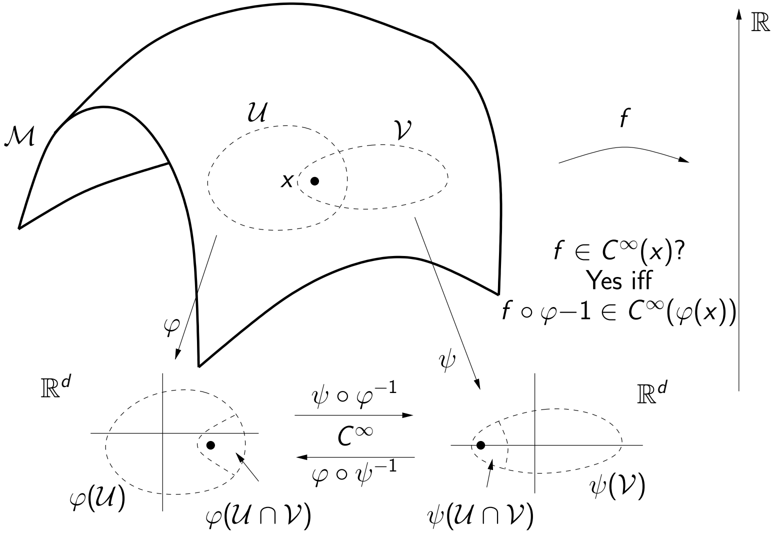

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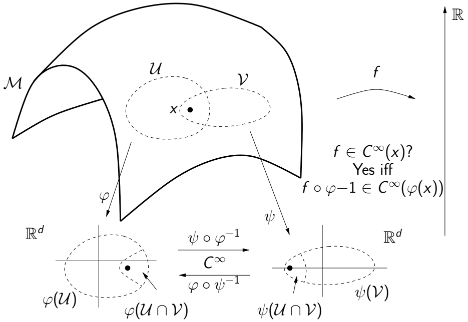
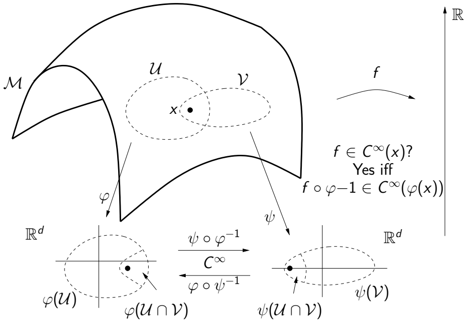


Chart: $\mathcal{U} \xrightarrow[\text{bij.}]{\varphi} \varphi(\mathcal{U})$

Atlas: Collection of "compatible chars" that cover $\mathcal{M}$

Manifold: Set with an atlas

Optimization on manifolds in its most abstract formulation

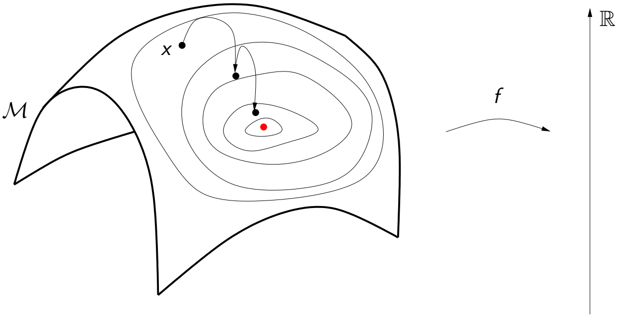


Given:

- A set $\mathcal{M}$ endowed (explicitly or implicitly) with a manifold structure (i.e., a collection of compatible charts).
- A function $f : \mathcal{M} \to \mathbb{R}$, smooth in the sense of the manifold structure.

Task: Compute a local minimizer of f.

Optimization on manifolds: algorithms

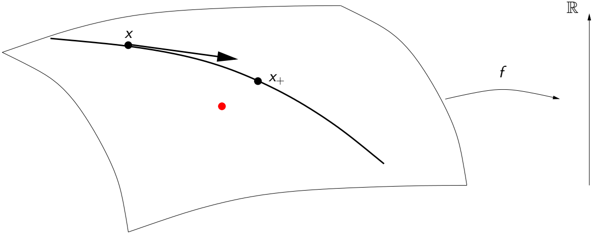


Given:

- A set $\mathcal{M}$ endowed (explicitly or implicitly) with a manifold structure (i.e., a collection of compatible charts).
- A function $f : \mathcal{M} \to \mathbb{R}$, smooth in the sense of the manifold structure.

Task: Compute a local minimizer of f.

Previous work on Optimization On Manifolds



Luenberger (1973), *Introduction to linear and nonlinear programming*.
Luenberger mentions the idea of performing line search along geodesics, "which we would use if it were computationally feasible (which it definitely is not)".

The purely Riemannian era

Gabay (1982), *Minimizing a differentiable function over a differential manifold*. Stepest descent along geodesics; Newton's method along geodesics; Quasi-Newton methods along geodesics.

Smith (1994), *Optimization techniques on Riemannian manifolds*. Levi-Civita connection ∇; Riemannian exponential; parallel translation. But Remark 4.9: If Algorithm 4.7 (Newton's iteration on the sphere for the Rayleigh quotient) is simplified by replacing the exponential update with the update

$$x_{k+1} = \frac{x_k + \eta_k}{\|x_k + \eta_k\|}$$

then we obtain the Rayleigh quotient iteration.

The pragmatic era

Manton (2002), *Optimization algorithms exploiting unitary constraints* "The present paper breaks with tradition by not moving along geodesics". The geodesic update $\mathrm{Exp}_x \eta$ is replaced by a projective update $\pi(x + \eta)$, the *projection* of the point $x + \eta$ onto the manifold.

Adler, Dedieu, Shub, et al. (2002), *Newton's method on Riemannian manifolds and a geometric model for the human spine*. The exponential update is relaxed to the general notion of *retraction*. The geodesic can be replaced by any (smoothly prescribed) curve tangent to the search direction.

Looking ahead: Newton on abstract manifolds

Required: Riemannian manifold $\mathcal{M}$; retraction R on $\mathcal{M}$; affine connection ∇ on $\mathcal{M}$; real-valued function f on $\mathcal{M}$.
Iteration $x_k \in \mathcal{M} \mapsto x_{k+1} \in \mathcal{M}$ defined by

1. Solve the Newton equation

   $$\operatorname{Hess} f(x_k)\eta_k = -\operatorname{grad} f(x_k)$$

   for the unknown $\eta_k \in T_{x_k}\mathcal{M}$, where

   $$\operatorname{Hess} f(x_k)\eta_k := \nabla_{\eta_k}\operatorname{grad} f.$$

2. Set

   $$x_{k+1} := R_{x_k}(\eta_k).$$

Looking ahead: Newton on submanifolds of $\mathbb{R}^n$

Required: Riemannian submanifold $\mathcal{M}$ of $\mathbb{R}^n$; retraction R on $\mathcal{M}$; real-valued function f on $\mathcal{M}$.

Iteration $x_k \in \mathcal{M} \mapsto x_{k+1} \in \mathcal{M}$ defined by

1. Solve the Newton equation

$$\mathrm{Hess}\, f(x_k)\eta_k = -\mathrm{grad}\, f(x_k)$$

for the unknown $\eta_k \in T_{x_k}\mathcal{M}$, where

$$\mathrm{Hess}\, f(x_k)\eta_k := \mathrm{P}_{T_{x_k}\mathcal{M}} \mathrm{grad}\, f(x_k).$$

2. Set

$$x_{k+1} := R_{x_k}(\eta_k).$$

Looking ahead: Newton on the unit sphere S^{n-1}

Required: real-valued function f on S^{n-1}.
Iteration $x_k \in \mathcal{M} \mapsto x_{k+1} \in S^{n-1}$ defined by

1. Solve the Newton equation

$$\begin{cases} \mathrm{P}_{x_k}\mathrm{D}(\mathrm{grad}\, f)(x_k)[\eta_k] = -\mathrm{grad}\, f(x_k) \\ x^T\eta_k = 0, \end{cases}$$

   for the unknown $\eta_k \in \mathbb{R}^n$, where

$$\mathrm{P}_{x_k} = (I - x_k x_k^T).$$

2. Set

$$x_{k+1} := \frac{x_k + \eta_k}{\|x_k + \eta_k\|}.$$

Looking ahead: Newton for Rayleigh quotient optimization on unit sphere

Iteration $x_k \in S^{n-1} \mapsto x_{k+1} \in S^{n-1}$ defined by

1. Solve the Newton equation

$$\begin{cases} \mathrm{P}_{x_k} A \mathrm{P}_{x_k} \eta_k - \eta_k x_k^T A x_k = -\mathrm{P}_{x_k} A x_k, \\ x_k^T \eta_k = 0, \end{cases}$$

   for the unknown $\eta_k \in \mathbb{R}^n$, where

$$\mathrm{P}_{x_k} = (I - x_k x_k^T).$$

2. Set

$$x_{k+1} := \frac{x_k + \eta_k}{\|x_k + \eta_k\|}.$$

Programme

- Provide background in differential geometry instrumental for algorithmic development
- Present manifold versions of some classical optimization algorithms: steepest-descent, Newton, conjugate gradients, trust-region methods
- Show how to turn these abstract geometric algorithms into practical implementations
- Illustrate several problems that can be rephrased as optimization problems on manifolds.

Some important manifolds

- Stiefel manifold $\mathrm{St}(p, n)$: set of all orthonormal $n \times p$ matrices.
- Grassmann manifold $\mathrm{Grass}(p, n)$: set of all p-dimensional subspaces of $\mathbb{R}^n$
- Euclidean group $SE(3)$: set of all rotations-translations
- Flag manifold, shape manifold, oblique manifold...
- Several unnamed manifolds

A manifold-based approach to the symmetric eigenvalue problem

OPT

EVP

OPT

EVP

Opt algorithms

for $f : \mathbb{R}^n \to \mathbb{R}$

Algorithms

for EVP

OPT | EVP

$$\begin{array}{c} \text{Opt algorithms} \\ \text{for } f : \mathbb{R}^n \to \mathbb{R} \end{array} \xrightarrow{f \,\equiv\, \text{Rayleigh quotient}} \begin{array}{c} \text{Algorithms} \\ \text{for EVP} \end{array}$$

Rayleigh quotient

Rayleigh quotient of (A, B):

$$f : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y}$$

Let A, B in $\mathbb{R}^{n \times n}$, $A = A^T$, $B = B^T \succ 0$,

$$A v_i = \lambda_i B v_i$$

with $\lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$.
Stationary points of f: αv_i, for all $\alpha \neq 0$.
Local (and global) minimizers of f: αv_1, for all $\alpha \neq 0$.

OPT		EVP
Opt algorithms for $f : \mathbb{R}^n \to \mathbb{R}$	$\xrightarrow{f \equiv \text{Rayleigh quotient}}$	Algorithms for EVP

“Block” Rayleigh quotient

Let $\mathbb{R}_*^{n \times p}$ denote the set of all full-column-rank $n \times p$ matrices.
Generalized (“block”) Rayleigh quotient:

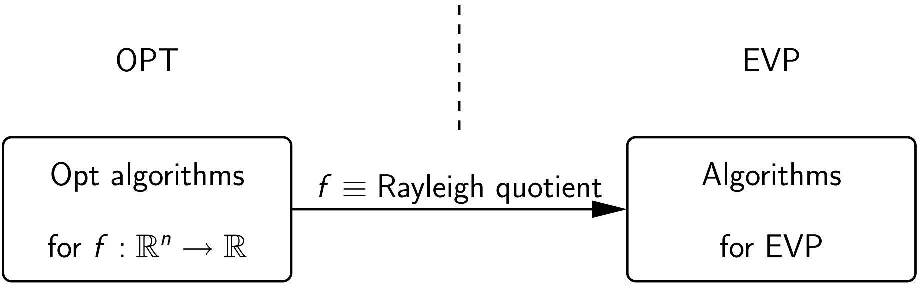
$$f : \mathbb{R}_*^{n \times p} \to \mathbb{R} : f(Y) = \operatorname{trace}\left((Y^T B Y)^{-1} Y^T A Y\right)$$

Stationary points of f:

$$\begin{bmatrix} v_{i_1} & \dots & v_{i_p} \end{bmatrix} M, \quad \text{for all } M \in \mathbb{R}_*^{p \times p}.$$

Minimizers of f:

$$\begin{bmatrix} v_1 & \dots v_p \end{bmatrix} M, \quad \text{for all } M \in \mathbb{R}_*^{p \times p}.$$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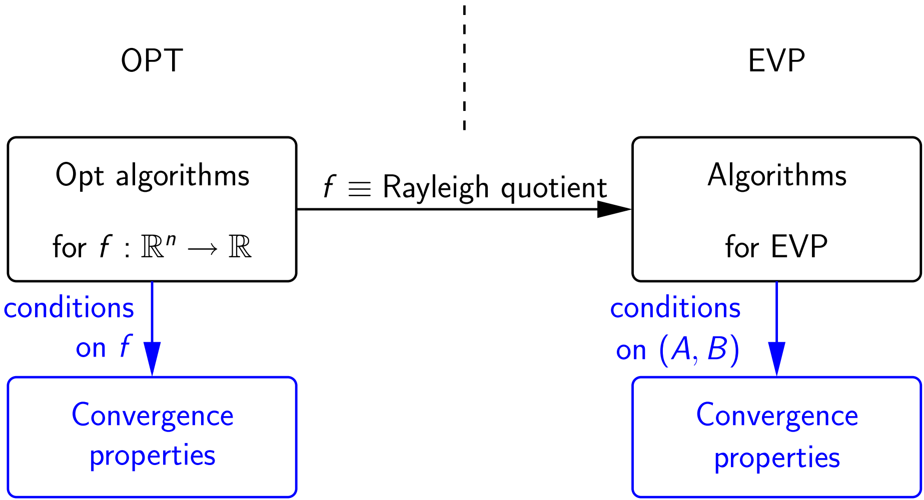
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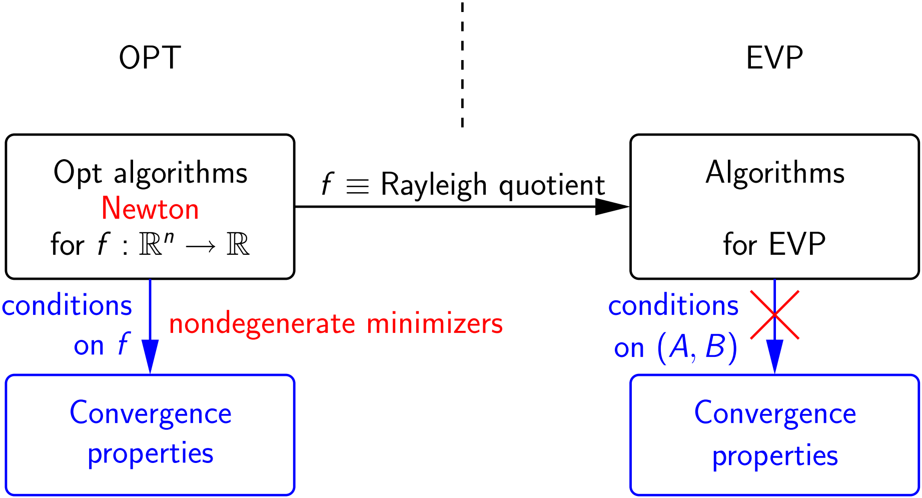
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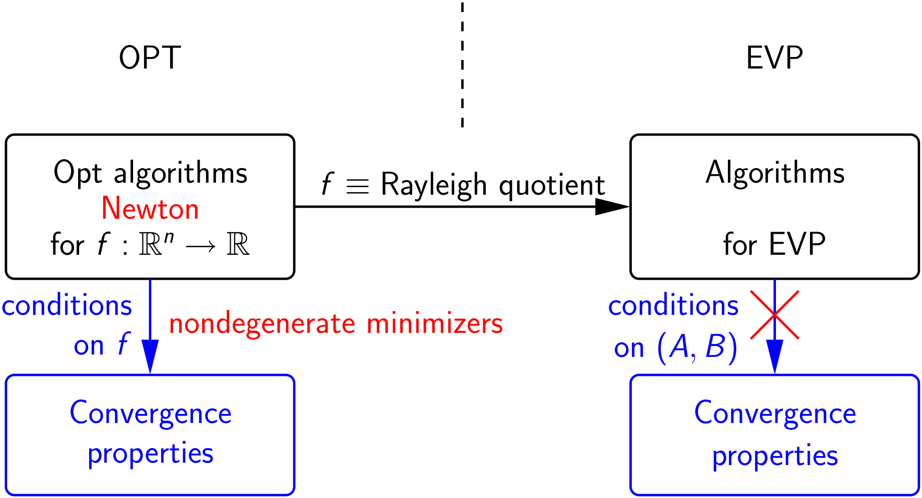
Newton for Rayleigh quotient in $\mathbb{R}_0^n$

Let f denote the Rayleigh quotient of (A, B).
Let $x \in \mathbb{R}_0^n$ be any point such that $f(x) \notin \mathrm{spec}(B^{-1}A)$.
Then the Newton iteration

$$x \mapsto x - \left(\mathrm{D}^2 f(x)\right)^{-1} \cdot \mathrm{grad}\, f(x)$$

reduces to the iteration

$$x \mapsto 2x.$$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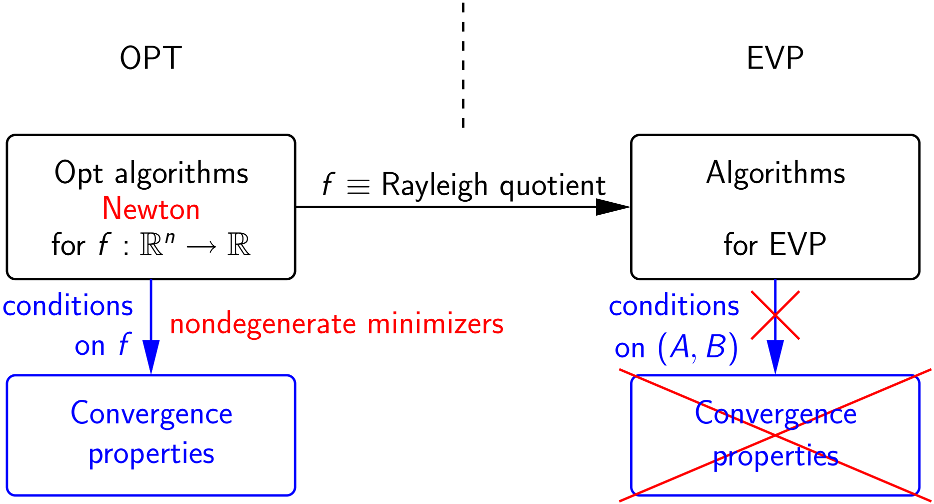
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Invariance properties of the Rayleigh quotient

Rayleigh quotient of (A, B):

$$f : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y}$$

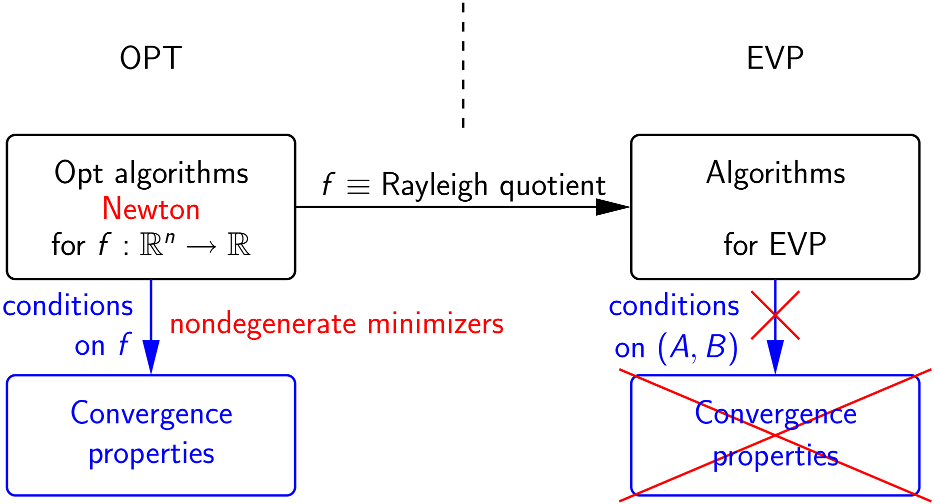
Invariance: $f(\alpha y) = f(y)$ for all $\alpha \in \mathbb{R}_0$.

Invariance properties of the Rayleigh quotient

Generalized ("block") Rayleigh quotient:

$$f : \mathbb{R}_*^{n \times p} \to \mathbb{R} : f(Y) = \operatorname{trace}\left((Y^T B Y)^{-1} Y^T A Y\right)$$

Invariance: $f(YM) = f(Y)$ for all $M \in \mathbb{R}_*^{p \times p}$.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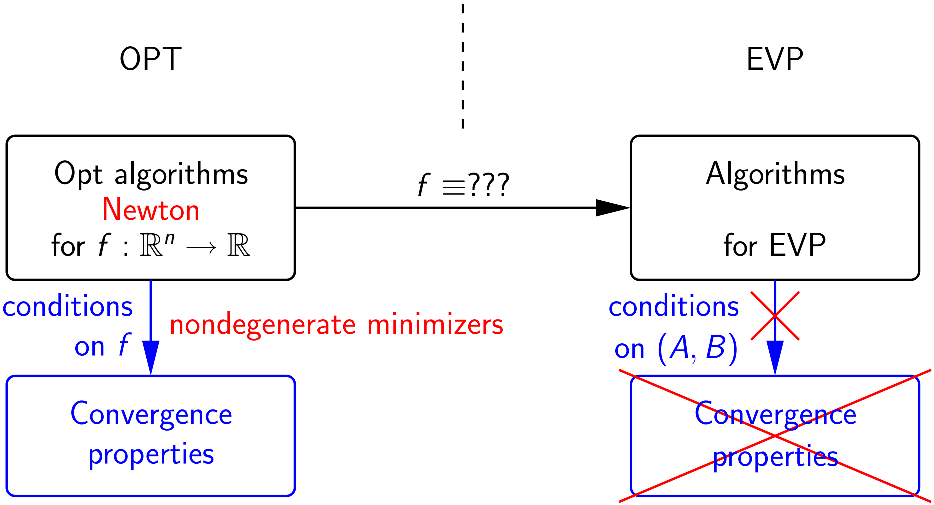
~~Convergence properties~~

Remedy 1: modify f



Remedy 1: modify f

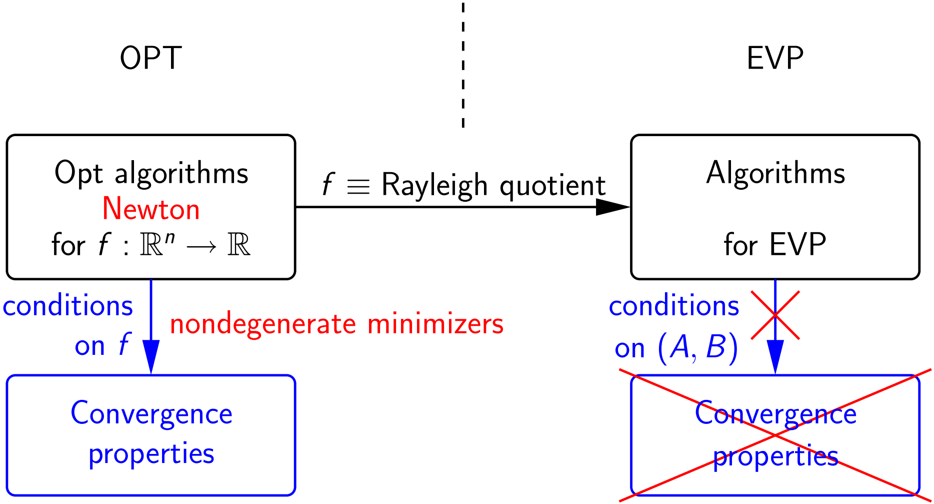
Consider

$$P_A : \mathbb{R}^n \to \mathbb{R} : x \mapsto P_A(x) := (x^T x)^2 - 2x^T Ax.$$

Theorem
(i)

$$\min_{x \in \mathbb{R}^n} P_A(x) = -\lambda_n^2$$

The minimum is attained at any $\sqrt{\lambda_n} v_n$, where v_n is a unitary eigenvector related to λ_n.
(ii) The set of critical points of P_A is $\{0\} \cup \{\sqrt{\lambda_k} v_k\}$.
References: Auchmuty (1989), Mongeau and Torki (2004).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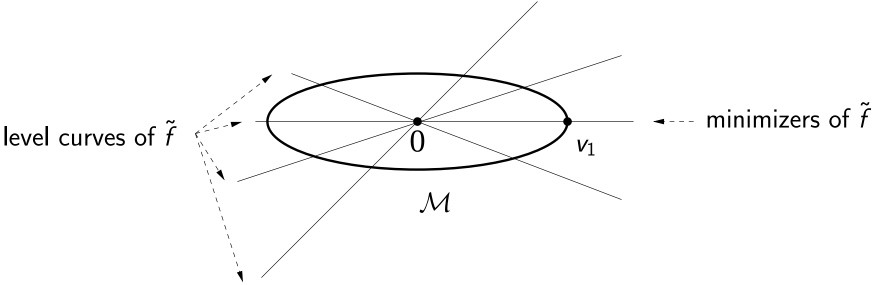
EVP: optimization on ellipsoid

$f(\alpha y) = f(y)$



Remedy 2: modify the search space

Instead of

$$f : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y},$$

minimize

$$f : \mathcal{M} \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y},$$

where

$$\mathcal{M} = \{y \in \mathbb{R}^n : y^T B y = 1\}.$$

Stationary points of f: $\pm v_i$.
Local (and global) minimizers of f: $\pm v_1$.

Remedy 2: modify search space: block case

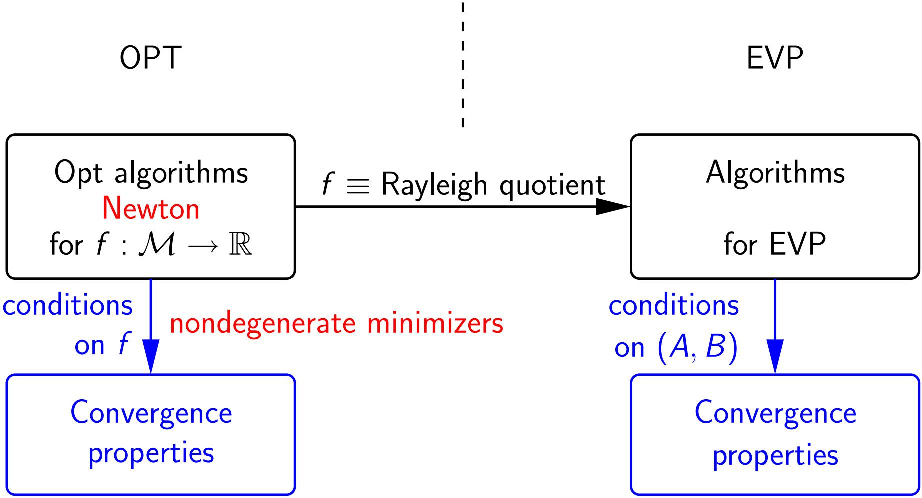
Instead of generalized ("block") Rayleigh quotient:

$$f : \mathbb{R}_*^{n\times p} \to \mathbb{R} : f(Y) = \mathrm{trace}\left((Y^T BY)^{-1} Y^T AY\right),$$

minimize

$$f : \mathrm{Grass}(p, n) \to \mathbb{R} : f(\mathrm{col}(Y)) = \mathrm{trace}\left((Y^T BY)^{-1} Y^T AY\right),$$

where $\mathrm{Grass}(p, n)$ denotes the set of all p-dimensional subspaces of $\mathbb{R}^n$, called the *Grassmann manifold*.
Stationary points of f: $\mathrm{col}(\begin{bmatrix} v_{i_1} & \dots & v_{i_p} \end{bmatrix})$.
Minimizer of f: $\mathrm{col}(\begin{bmatrix} v_1 & \dots v_p \end{bmatrix})$.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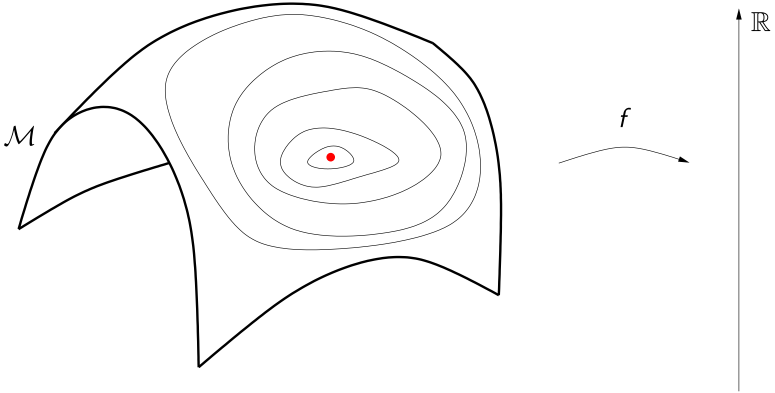
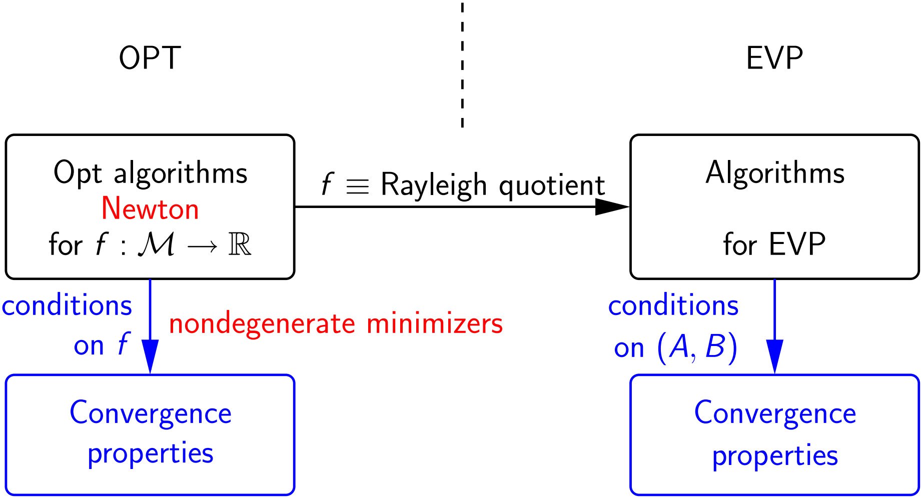
Smooth optimization on a manifold: big picture



Smooth optimization on a manifold: tools

	Purely Riemannian way	Pragmatic way
Search direction	Tangent vector	Tangent vector
Steepest descent dir.	$-\mathrm{grad}\, f(x)$	$-\mathrm{grad}\, f(x)$
Derivative of vector field	Levi-Civita connection $\overset{g}{\nabla}$	Any connection ∇
Update	Search along the geodesic tangent to the search direction	Search along any curve ta to the search direction scribed by a *retraction*)
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	Vector Transport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Newton's method on abstract manifolds

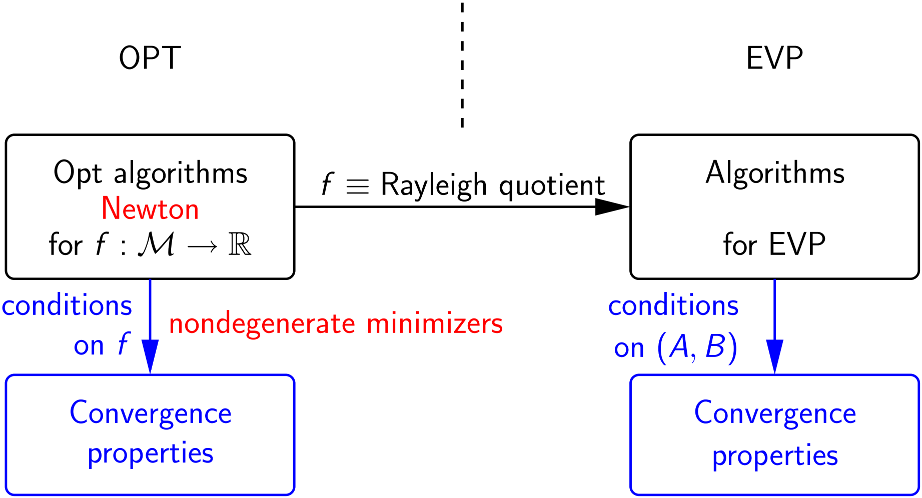
Required: Riemannian manifold $\mathcal{M}$; retraction R on $\mathcal{M}$; affine connection ∇ on $\mathcal{M}$; real-valued function f on $\mathcal{M}$.
Iteration $x_k \in \mathcal{M} \mapsto x_{k+1} \in \mathcal{M}$ defined by

1. Solve the Newton equation

$$\operatorname{Hess} f(x_k)\eta_k = -\operatorname{grad} f(x_k)$$

   for the unknown $\eta_k \in T_{x_k}\mathcal{M}$, where $\operatorname{Hess} f(x_k)\eta_k := \nabla_{\eta_k} \operatorname{grad} f$.
2. Set

$$x_{k+1} := R_{x_k}(\eta_k).$$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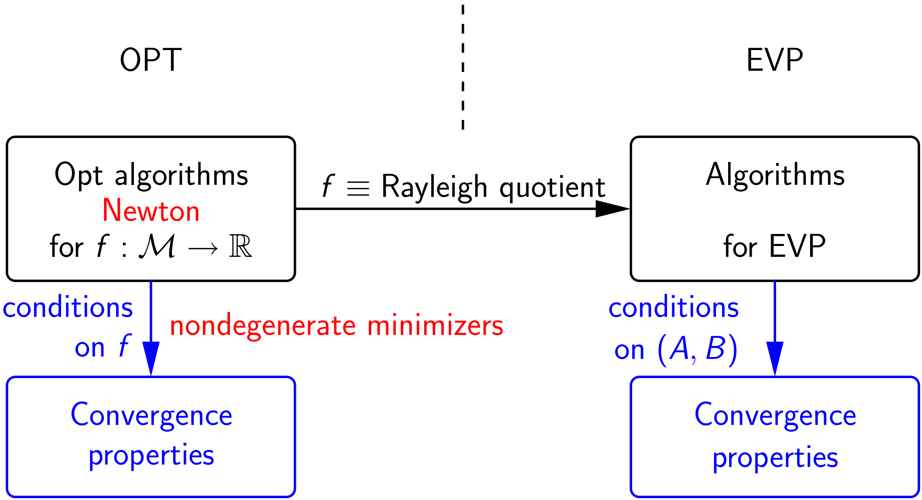
Convergence of Newton's method on abstract manifolds

Theorem

Let $x_* \in \mathcal{M}$ be a nondegenerate critical point of f, i.e., $\operatorname{grad} f(x_*) = 0$ and $\operatorname{Hess} f(x_*)$ invertible.

Then there exists a neighborhood $\mathcal{U}$ of x_* in $\mathcal{M}$ such that, for all $x_0 \in \mathcal{U}$, Newton's method generates an infinite sequence $(x_k)_{k=0,1,\dots}$ converging superlinearly (at least quadratically) to x_*.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Geometric Newton for Rayleigh quotient optimization

Iteration $x_k \in S^{n-1} \mapsto x_{k+1} \in S^{n-1}$ defined by

1. Solve the Newton equation

$$\begin{cases} \mathrm{P}_{x_k} A \mathrm{P}_{x_k} \eta_k - \eta_k x_k^T A x_k = -\mathrm{P}_{x_k} A x_k, \\ x_k^T \eta_k = 0, \end{cases}$$

   for the unknown $\eta_k \in \mathbb{R}^n$, where

$$P_{x_k} = (I - x_k x_k^T).$$

2. Set

$$x_{k+1} := \frac{x_k + \eta_k}{\|x_k + \eta_k\|}.$$

Geometric Newton for Rayleigh quotient optimization: block case

Iteration $\mathrm{col}(Y_k) \in \mathrm{Grass}(p,n) \mapsto \mathrm{col}(Y_{k+1}) \in \mathrm{Grass}(p,n)$ defined by

1. Solve the linear system

$$\begin{cases} \mathrm{P}^h_{Y_k}\left(AZ_k - Z_k(Y_k^T Y_k)^{-1} Y_k^T A Y_k\right) = -\mathrm{P}^h_{Y_k}(AY_k) \\ Y_k^T Z_k = 0 \end{cases}$$

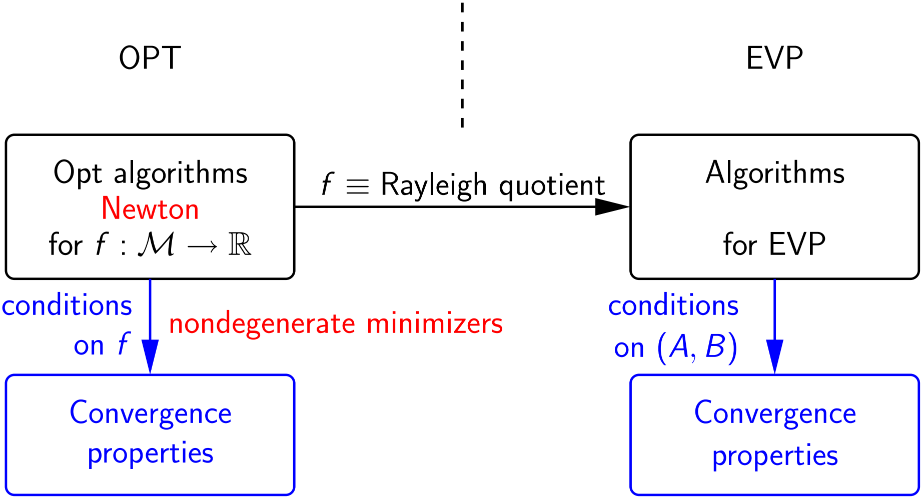
   for the unknown $Z_k \in \mathbb{R}^{n\times p}$, where

$$\mathrm{P}^h_{Y_k} = (I - Y_k(Y_k^T Y_k)^{-1} Y_k^T).$$

2. Set

$$Y_{k+1} = (Y_k + Z_k)N_k$$

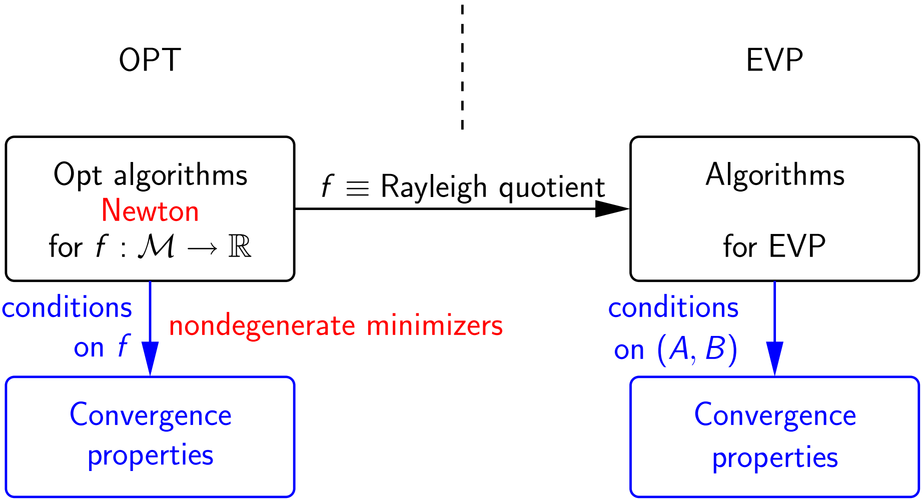
   where N_k is a nonsingular $p \times p$ matrix chosen for normalization.


OPT
EVP
Opt algorithms
Newton
for $f : \mathcal{M} \to \mathbb{R}$
$f \equiv$ Rayleigh quotient
Algorithms
for EVP
conditions
on f
nondegenerate minimizers
conditions
on (A, B)
Convergence
properties
Convergence
properties

Convergence of the EVP algorithm

Theorem

Let $Y_* \in \mathbb{R}^{n \times p}$ be such that $\mathrm{col}(Y_*)$ is a spectral invariant subspace of $B^{-1}A$. Then there exists a neighborhood $\mathcal{U}$ of $\mathrm{col}(Y_*)$ in $\mathrm{Grass}(p, n)$ such that, for all $Y_0 \in \mathbb{R}^{n \times p}$ with $\mathrm{col}(Y_0) \in \mathcal{U}$, Newton's method generates an infinite sequence $(Y_k)_{k=0,1,\ldots}$ such that $(\mathrm{col}(Y_k))_{k=0,1,\ldots}$ converges superlinearly (at least quadratically) to $\mathrm{col}(Y_*)$ on $\mathrm{Grass}(p, n)$.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$f \equiv$ Rayleigh quotient
Algorithms
for EVP
conditions
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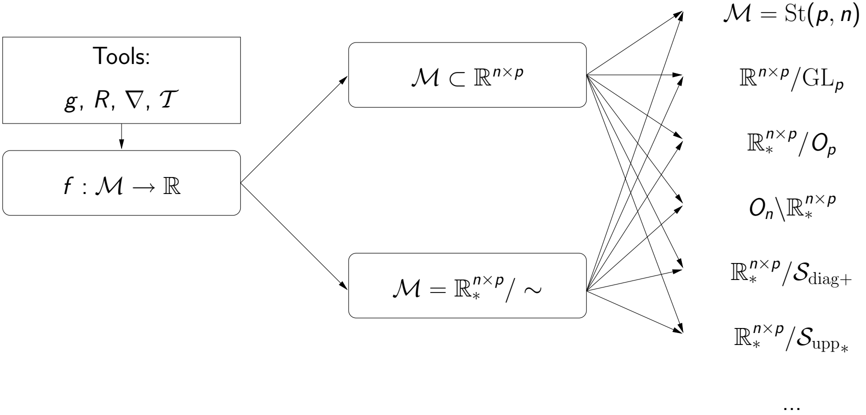
nondegenerate minimizers
conditions
on (A, B)
Convergence
properties
Convergence
properties

Other optimization methods

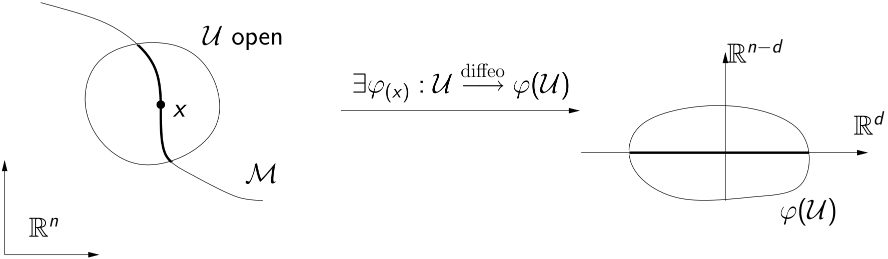
- Trust-region methods: PAA, C. G. Baker, K. A. Gallivan, *Trust-region methods on Riemannian manifolds*, Foundations of Computational Mathematics, 2007.
- "Implicit" trust-region methods: PAA, C. G. Baker, K. A. Gallivan, submitted.

Manifolds

Manifolds, submanifolds, quotient manifolds

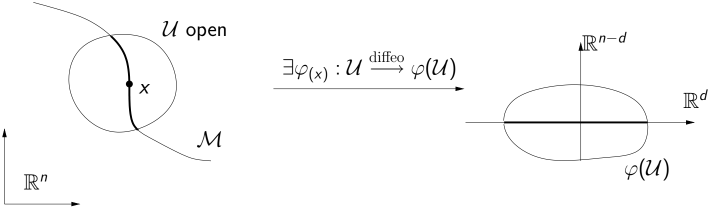


Submanifolds of $\mathbb{R}^n$



The *set* $\mathcal{M} \subset \mathbb{R}^n$ is termed a *submanifold* of $\mathbb{R}^n$ if the situation described above holds for all $x \in \mathcal{M}$.

Submanifolds of $\mathbb{R}^n$



The manifold structure on $\mathcal{M}$ is defined in a unique way as the manifold structure generated by the atlas $\left\{ \begin{bmatrix} e_1^T \\ \vdots \\ e_d^T \end{bmatrix} \varphi_{(x)}\big|_{\mathcal{M}} : x \in \mathcal{M} \right\}$.

Back to the basics: partial derivatives in $\mathbb{R}^n$

Let $F : \mathbb{R}^n \to \mathbb{R}^q$.
Define $\partial_i F : \mathbb{R}^n \to \mathbb{R}^q$ by

$$\partial_i F(x) = \lim_{t \to 0} \frac{F(x + te_i) - F(x)}{t}.$$

If $\partial_i F$ is defined and continuous on $\mathbb{R}^n$, then F is termed *continuously differentiable*, denoted by $F \in C^1$.

Back to the basics: (Fréchet) derivative in $\mathbb{R}^n$

If $F \in C^1$, then

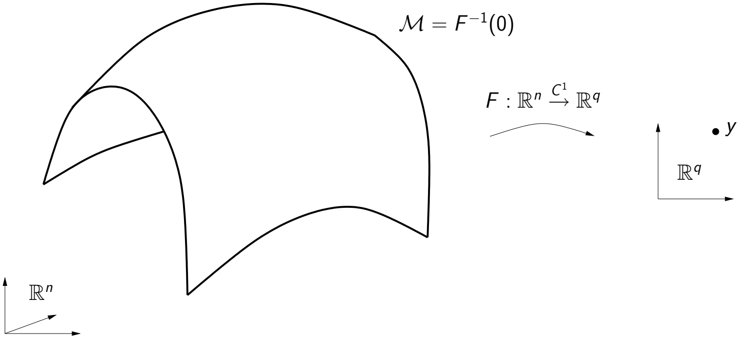
$$\mathrm{D}F(x) : \mathbb{R}^n \xrightarrow{\text{lin}} \mathbb{R}^q : z \mapsto \mathrm{D}F(x)[z] := \lim_{t \to 0} \frac{F(x + tz) - F(x)}{t}$$

is the *derivative* (or *differential*) of F at x.
We have $\mathrm{D}F(x)[z] = \mathrm{J}_F(x)z$, where the matrix

$$\mathrm{J}_F(x) = \begin{bmatrix} \partial_1(e_1^T F)(x) & \cdots & \partial_n(e_1^T F)(x) \\ \vdots & \ddots & \vdots \\ \partial_1(e_q^T F)(x) & \cdots & \partial_n(e_q^T F)(x) \end{bmatrix}$$

is the *Jacobian matrix* of F at x.

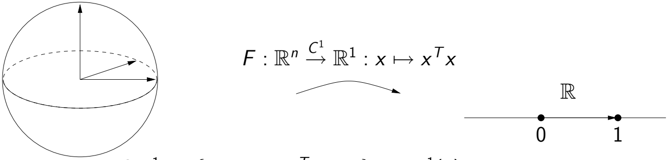
Submanifolds of $\mathbb{R}^n$: sufficient condition



$y \in \mathbb{R}^q$ is a *regular value* of F if, for all $x \in F^{-1}(y)$, $\mathrm{D}F(x)$ is an onto function (*surjection*).

Theorem (submersion theorem): If $y \in \mathbb{R}^q$ is a regular value of F, then $F^{-1}(y)$ is a submanifold of $\mathbb{R}^n$.

Submanifolds of $\mathbb{R}^n$: sufficient condition: application



$S^{n-1} := \{x \in \mathbb{R}^n : x^T x = 1\} = F^{-1}(1)$

The unit sphere

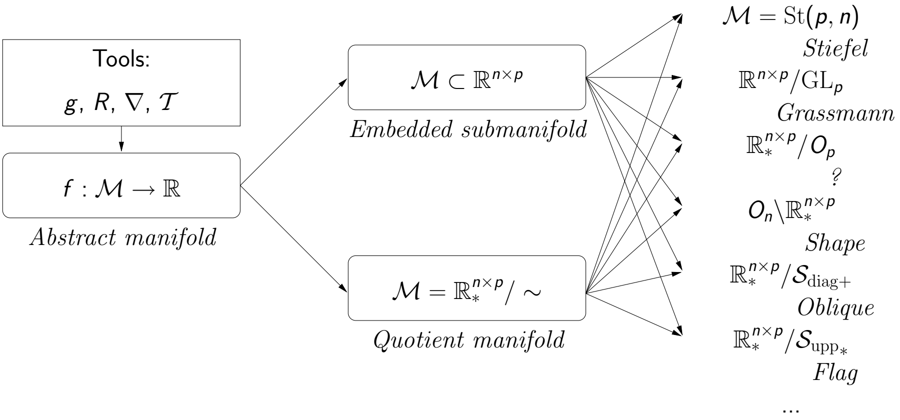
$$S^{n-1} := \{x \in \mathbb{R}^n : x^T x = 1\}$$

is a submanifold of $\mathbb{R}^n$.
Indeed, for all $x \in S^{n-1}$, we have that

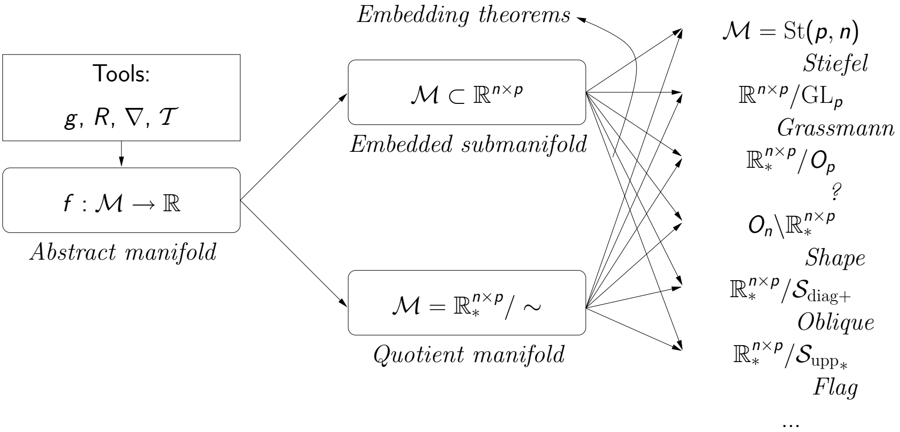
$$\mathrm{D}F(x) : \mathbb{R}^n \to \mathbb{R} : z \mapsto \mathrm{D}F(x)[z] = x^T z + z^T x$$

is an onto function.

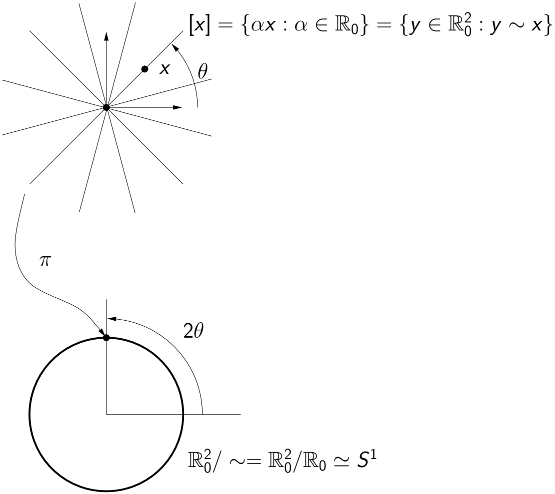
Manifolds, submanifolds, quotient manifolds



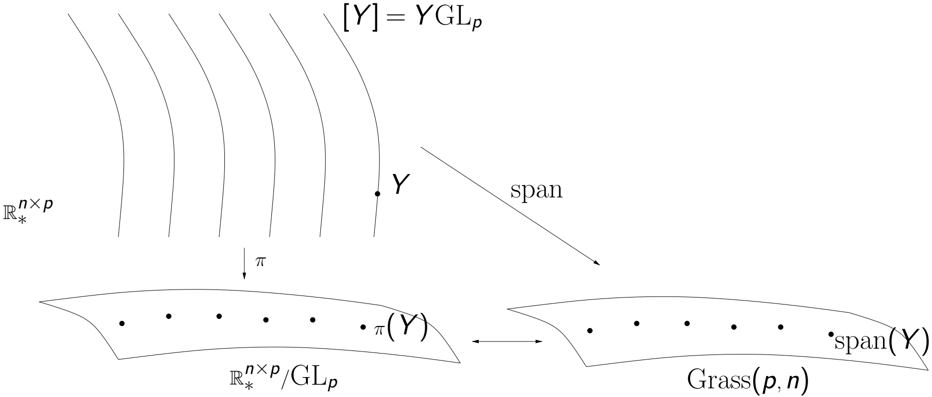
Manifolds, submanifolds, quotient manifolds



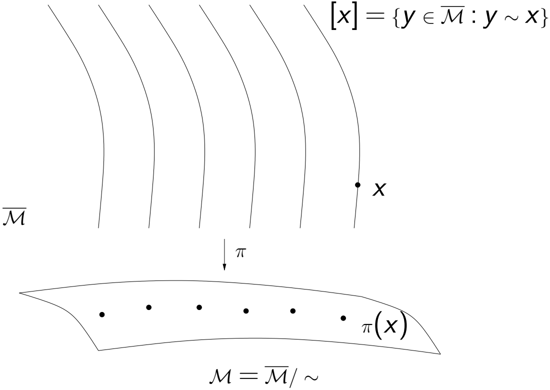
A simple quotient set: the projective space



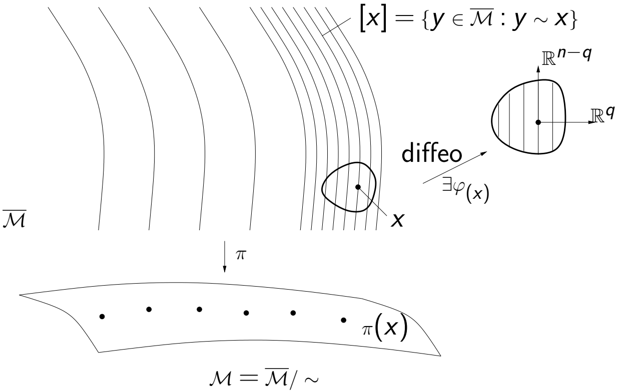
A slightly less simple quotient set: $\mathbb{R}_*^{n\times p}/\mathrm{GL}_p$



Abstract quotient set $\overline{\mathcal{M}}/\sim$

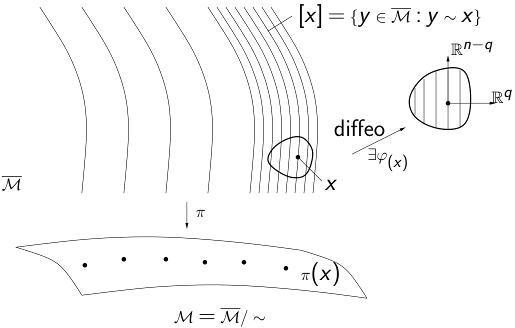


Abstract quotient manifold $\overline{\mathcal{M}}/\sim$



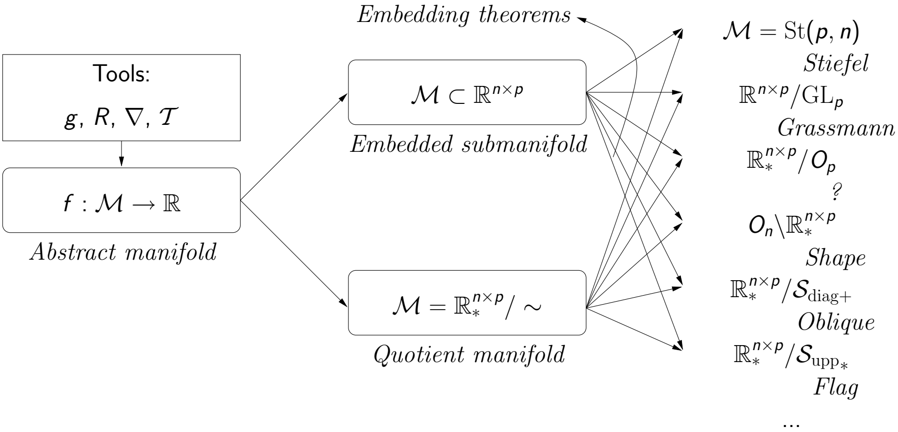
The set $\overline{\mathcal{M}}/\sim$ is termed a *quotient manifold* if the situation described above holds for all $x \in \overline{\mathcal{M}}$.

Abstract quotient manifold $\overline{\mathcal{M}}/\sim$



The manifold structure on $\overline{\mathcal{M}}/\sim$ is defined in a unique way as the manifold structure generated by the atlas $\left\{ \begin{bmatrix} e_1^T \\ \vdots \\ e_q^T \end{bmatrix} \varphi_{(x)} \circ \pi^{-1} : x \in \overline{\mathcal{M}} \right\}$.

Manifolds, submanifolds, quotient manifolds



Manifolds, and where they appear

- Stiefel manifold $\mathrm{St}(p, n)$ and orthogonal group $O_p = \mathrm{St}(n, n)$

$$\mathrm{St}(p, n) = \{X \in \mathbb{R}^{n \times p} : X^T X = I_p\}$$

  Applications: computer vision; principal component analysis; independent component analysis...
- Grassmann manifold $\mathrm{Grass}(p, n)$

  Set of all p-dimensional subspaces of $\mathbb{R}^n$

  Applications: various dimension reduction problems...
- $\mathbb{R}_*^{n \times p} / O_p$

$$X \sim Y \Leftrightarrow \exists Q \in O_p : Y = XQ$$

  Applications: Low-rank approximation of symmetric matrices; low-rank approximation of tensors...

Manifolds, and where they appear

- Shape manifold $O_n/\mathbb{R}_*^{n\times p}$

$$Y \sim Y \Leftrightarrow \exists U \in O_n : Y = UX$$

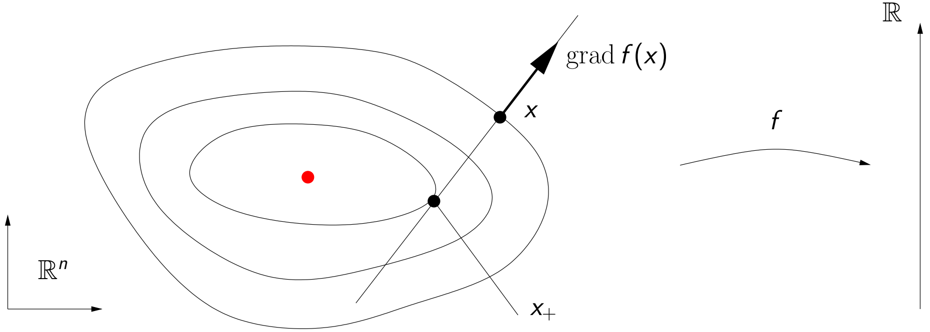
  Applications: shape analysis
- Oblique manifold $\mathbb{R}_*^{n\times p}/\mathcal{S}_{\mathrm{diag}+}$

$$\mathbb{R}_*^{n\times p}/\mathcal{S}_{\mathrm{diag}+} \simeq \{Y \in \mathbb{R}_*^{n\times p} : \mathrm{diag}(Y^T Y) = I_p\}$$

  Applications: independent component analysis; factor analysis (oblique Procrustes problem)...
- Flag manifold $\mathbb{R}_*^{n\times p}/\mathcal{S}_{\mathrm{upp}_*}$
  Elements of the flag manifold can be viewed as a p-tuble of linear subspaces $(\mathcal{V}_1, \ldots, \mathcal{V}_p)$ such that $\dim(\mathcal{V}_i) = i$ and $\mathcal{V}_i \subset \mathcal{V}_{i+1}$.
  Applications: analysis of QR algorithm...

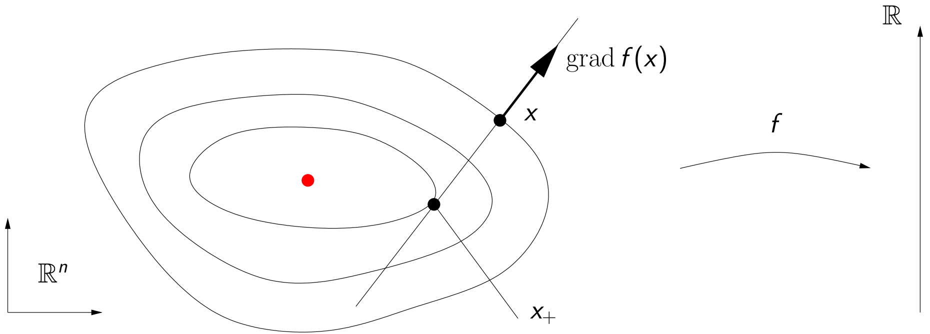
Steepest-descent methods on manifolds

Steepest-descent in $\mathbb{R}^n$



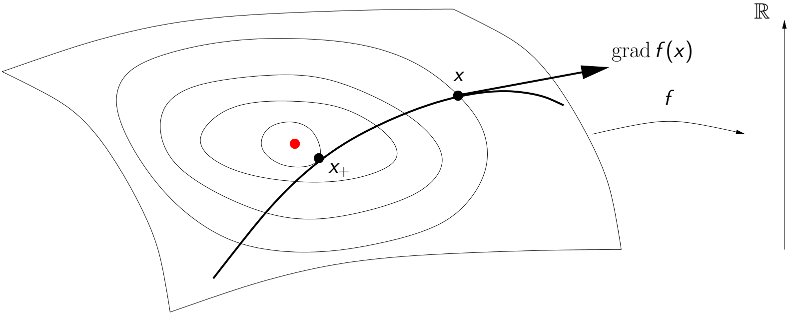
$$\operatorname{grad} f(x) = \begin{bmatrix} \partial_1 f(x) & \cdots & \partial_n f(x) \end{bmatrix}^T$$

Steepest-descent: from $\mathbb{R}^n$ to manifolds



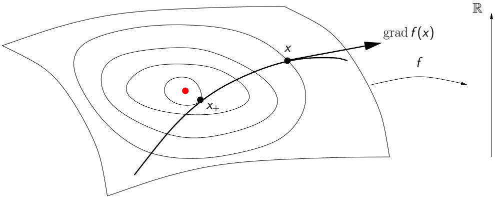
	$\mathbb{R}^n$	Manifold
Search direction	Vector at x	Tangent vector at x
Steepest-desc. dir.	$-\mathrm{grad}\, f(x)$	$-\mathrm{grad}\, f(x)$
Curve	$\gamma : t \mapsto x - t\, \mathrm{grad}\, f(x)$	γ s.t. $\gamma(0) = x$ and $\dot\gamma(0) = -\mathrm{grad}\, f(x)$

Steepest-descent: from $\mathbb{R}^n$ to manifolds



	$\mathbb{R}^n$	Manifold
Search direction	Vector at x	Tangent vector at x
Steepest-desc. dir.	$-\operatorname{grad} f(x)$	$-\operatorname{grad} f(x)$
Curve	$\gamma : t \mapsto x - t \operatorname{grad} f(x)$	γ s.t. $\gamma(0) = x$ and $\dot\gamma(0) = -\operatorname{grad} f(x)$

Update directions: tangent vectors



Let γ be a curve in the manifold $\mathcal{M}$ with $\gamma(0) = x$.

For an abstract manifold, the definition $\dot{\gamma}(0) = \frac{\mathrm{d}\gamma}{\mathrm{d}t}(0) = \lim_{t \to 0} \frac{\gamma(t) - \gamma(0)}{t}$ is meaningless.

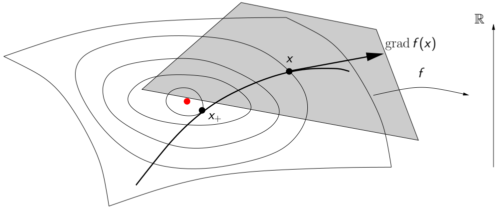
Instead, define: $\mathrm{D}f(x)[\dot{\gamma}(0)] := \frac{\mathrm{d}}{\mathrm{d}t} f(\gamma(t))\big|_{t=0}$

If $\mathcal{M} \subset \mathbb{R}^n$ and $f = \overline{f}|_{\mathcal{M}}$, then

$$\mathrm{D}f(x)[\dot{\gamma}(0)] = \mathrm{D}\overline{f}(x)\left[\frac{\mathrm{d}\gamma}{\mathrm{d}t}(0)\right].$$

The application $\dot{\gamma}(0) : f \mapsto \mathrm{D}f(x)[\dot{\gamma}(0)]$ is a *tangent vector* at x.

Update directions: tangent spaces



The set

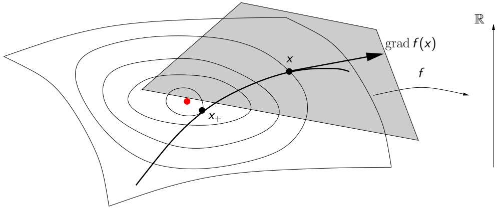
$$T_x\mathcal{M} = \{\dot{\gamma}(0) : \gamma \text{ curve in } \mathcal{M} \text{ through } x \text{ at } t = 0\}$$

is the *tangent space* to $\mathcal{M}$ at x.
With the definition

$$\alpha\dot{\gamma}_1(0) + \beta\dot{\gamma}_2(0) : f \mapsto \alpha \mathrm{D}f(x)[\dot{\gamma}_1(0)] + \beta \mathrm{D}f(x)[\dot{\gamma}_2(0)],$$

the tangent space $T_x\mathcal{M}$ becomes a linear space.
The *tangent bundle* $T\mathcal{M}$ is the set of all tangent vectors to $\mathcal{M}$.

Tangent vectors: submanifolds of Euclidean spaces

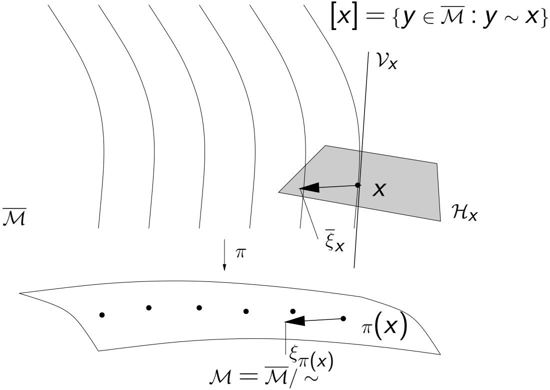


If $\mathcal{M}$ is a submanifold of $\mathbb{R}^n$ and $f = \overline{f}|_{\mathcal{M}}$, then

$$\mathrm{D}f(x)[\dot{\gamma}(0)] = \mathrm{D}\overline{f}(x)\left[\frac{\mathrm{d}\gamma}{\mathrm{d}t}(0)\right].$$

Proof: The left-hand side is equal to $\frac{\mathrm{d}}{\mathrm{d}t}f(\gamma(t))\big|_{t=0}$. This is equal to $\frac{\mathrm{d}}{\mathrm{d}t}\overline{f}(\gamma(t))\big|_{t=0}$ because $\gamma(t) \in \mathcal{M}$ for all t. The classical chain rule yields the right-hand side.

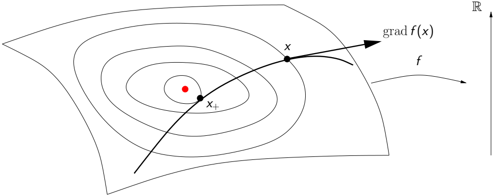
Tangent vectors: quotient manifolds



Let $\overline{\mathcal{M}}/\sim$ be a quotient manifold. Then $[x]$ is a submanifold of $\overline{\mathcal{M}}$. The tangent space $T_x[x]$ is the *vertical space* $\mathcal{V}_x$. A *horizontal space* is a subspace of $T_x\overline{\mathcal{M}}$ complementary to $\mathcal{V}_x$.
Let $\xi_{\pi(x)}$ be a tangent vector to $\overline{\mathcal{M}}/\sim$ at $\pi(x)$.
Theorem: In $\mathcal{H}_x$ there is one and only one $\bar{\xi}_x$ such that

$$\mathrm{D}\pi(x)[\bar{\xi}_x] = \xi_{\pi(x)}.$$

Steepest-descent: norm of tangent vectors



The steepest ascent direction is along

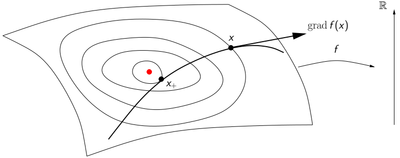
$$\mathop{\arg\max}_{\substack{\xi \in T_x\mathcal{M} \\ \|\xi\|=1}} \mathrm{D}f(x)[\xi].$$

To this end, we need a norm on $T_x\mathcal{M}$.
For all $x \in \mathcal{M}$, let g_x denote an inner product in $T_x\mathcal{M}$, and define

$$\|\xi_x\| := \sqrt{g_x(\xi_x, \xi_x)}.$$

When g_x "smoothly" depends on x, we say that $(\mathcal{M}, g)$ is a *Riemannian manifold*.

Steepest-descent: gradient



There is a unique $\operatorname{grad} f(x)$, called the *gradient* of f at x, such that

$$\begin{cases} \operatorname{grad} f(x) \in T_x\mathcal{M} \\ g_x(\operatorname{grad} f(x), \xi_x) = \mathrm{D}f(x)[\xi_x], \quad \forall \xi_x \in T_x\mathcal{M}. \end{cases}$$

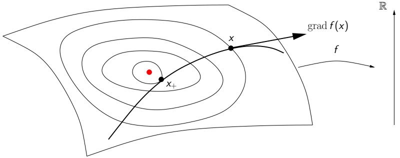
We have

$$\frac{\operatorname{grad} f(x)}{\|\operatorname{grad} f(x)\|} = \underset{\substack{\xi \in T_x\mathcal{M} \\ \|\xi\|=1}}{\arg\max}\, \mathrm{D}f(x)[\xi]$$

and

$$\|\operatorname{grad} f(x)\| = \mathrm{D}f(x)\left[\frac{\operatorname{grad} f(x)}{\|\operatorname{grad} f(x)\|}\right].$$

Steepest-descent: Riemannian submanifolds



Let $(\overline{\mathcal{M}}, \overline{g})$ be a Riemannian manifold and $\mathcal{M}$ be a submanifold of $\overline{\mathcal{M}}$. Then

$$g_x(\xi_x, \zeta_x) := \overline{g}_x(\xi_x, \eta_x), \ \forall \xi_x, \zeta_x \in T_x\mathcal{M}$$

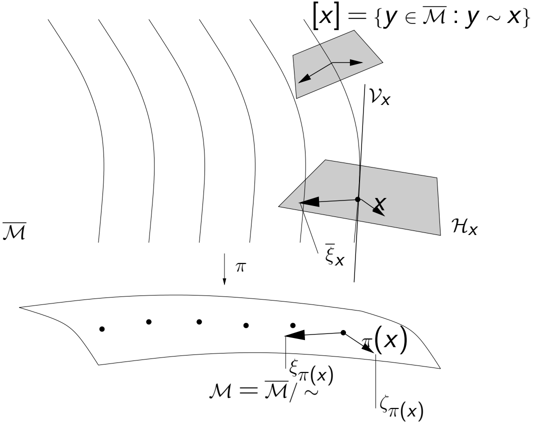
defines a Riemannian metric g on $\mathcal{M}$. With this Riemannian metric, $\mathcal{M}$ is a *Riemannian submanifold* of $\overline{\mathcal{M}}$.

Every $z \in T_x\overline{\mathcal{M}}$ admits a decomposition $z = \underbrace{\mathrm{P}_x z}_{\in T_x\mathcal{M}} + \underbrace{\mathrm{P}_x^{\perp} z}_{\in T_x^{\perp}\mathcal{M}}$.

If $\overline{f} : \overline{\mathcal{M}} \to \mathbb{R}$ and $f = \overline{f}|_{\mathcal{M}}$, then

$$\operatorname{grad} f(x) = \mathrm{P}_x \operatorname{grad} \overline{f}(x).$$

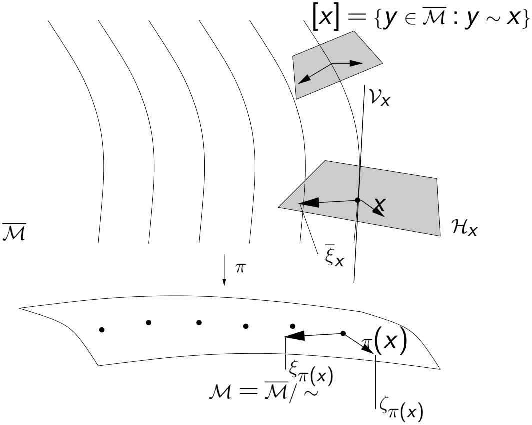
Steepest-descent: Riemannian quotient manifolds



Let $\tilde{g}$ be a Riemannian metric on $\overline{\mathcal{M}}$.
Suppose that, for all $\xi_{\pi(x)}$ and $\zeta_{\pi(x)}$ in $T_{\pi(x)}\overline{\mathcal{M}}/\sim$, and all $\tilde{x} \in \pi^{-1}(\pi(x))$, we have

$$\overline{g}_{\tilde{x}}(\overline{\xi}_{\tilde{x}}, \overline{\zeta}_{\tilde{x}}) = \overline{g}_x(\overline{\xi}_x, \overline{\zeta}_x).$$

Steepest-descent: Riemannian quotient manifolds

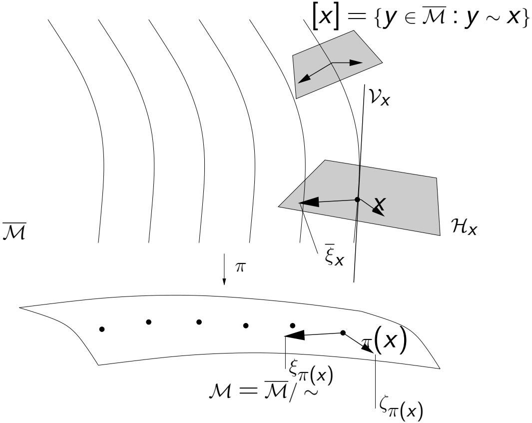


Then

$$g_{\pi(x)}(\xi_{\pi(x)}, \zeta_{\pi(x)}) := \overline{g}_x(\overline{\xi}_x, \overline{\zeta}_x).$$

defines a Riemannian metric on $\overline{\mathcal{M}}/\sim$. This turns $\overline{\mathcal{M}}/\sim$ into a Riemannian quotient manifold.

Steepest-descent: Riemannian quotient manifolds



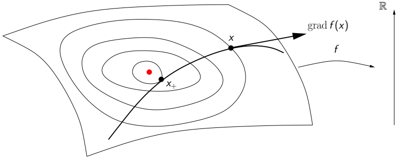
Let $f : \overline{\mathcal{M}}/\sim \to \mathbb{R}$. Let $\mathrm{P}_x^{h,\overline{g}}$ denote the orthogonal projection onto $\mathcal{H}_x$.

$$\overline{\operatorname{grad} f}_x = \mathrm{P}_x^{h,\overline{g}} \operatorname{grad}(f \circ \pi)(x).$$

If $\mathcal{H}_x$ is the orthogonal complement of $\mathcal{V}_x$ in the sense of $\overline{g}$ (π is a *Riemannian submersion*), then $\operatorname{grad}(f \circ \pi)(x)$ is already in $\mathcal{H}_x$, and thus

$$\overline{\operatorname{grad} f}_x = \operatorname{grad}(f \circ \pi)(x).$$

Steepest-descent: choosing the search curve



It remains to choose a curve γ through x at $t = 0$ such that

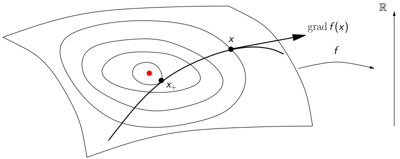
$$\dot{\gamma}(0) = -\mathrm{grad}\, f(x).$$

Let $R : T\mathcal{M} \to \mathcal{M}$ be a *retraction* on $\mathcal{M}$, that is

1. $R(0_x) = x$, where 0_x denotes the origin of $T_x\mathcal{M}$;
2. $\frac{\mathrm{d}}{\mathrm{d}t} R(t\xi_x) = \xi_x$.

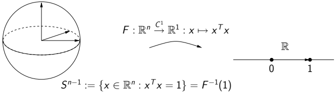
Then choose $\gamma : t \mapsto R(-t\mathrm{grad}\, f(x))$.

Steepest-descent: line-search procedure



Find t such that $f(\gamma(t))$ is "sifficiently smaller" than $f(\gamma(0))$. Since $t \mapsto f(\gamma(t))$ is just a function from $\mathbb{R}$ to $\mathbb{R}$, we can use the step selection techniques that are available for classical line-search methods.
For example: exact minimization, Armijo backtracking,...

Steepest-descent: Rayleigh quotient on unit sphere



Let the manifold be the unit sphere

$$S^{n-1} = \{x \in \mathbb{R}^n : x^T x = 1\} = F^{-1}(1),$$

where $F : \mathbb{R}^n \to \mathbb{R} : x \mapsto x^T x$.
Let $A = A^T \in \mathbb{R}^{n \times n}$ and let the cost function be the Rayleigh quotient

$$f : S^{n-1} \to \mathbb{R} : x \mapsto x^T A x.$$

The tangent space to S^{n-1} at x is

$$T_x S^{n-1} = \ker(\mathrm{D}F(x)) = \{z \in \mathbb{R}^n : x^T z = 0\}.$$

Derivation formulas

If F is linear, then

$$\mathrm{D}F(x)[z] = F(z).$$

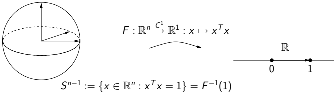
Chain rule: If $\mathrm{range}(F) \subseteq \mathrm{dom}(G)$, then

$$\mathrm{D}(G \circ F)(x)[z] = \mathrm{D}G(F(x))[\mathrm{D}F(x)[z]].$$

Product rule: If the ranges of F and G are in matrix spaces of compatible dimension, then

$$\mathrm{D}(FG)(x)[z] = \mathrm{D}F(x)[z]G(x) + F(x)\mathrm{D}G(x)[z].$$

Steepest-descent: Rayleigh quotient on unit sphere



Rayleigh quotient:

$$f : S^{n-1} \to \mathbb{R} : x \mapsto x^T A x.$$

The tangent space to S^{n-1} at x is

$$T_x S^{n-1} = \ker(\mathrm{D}F(x)) = \{z \in \mathbb{R}^n : x^T z = 0\}.$$

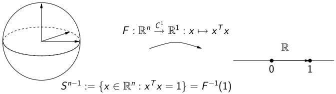
Product rule:

$$\mathrm{D}(FG)(x)[z] = \mathrm{D}F(x)[z]G(x) + F(x)\mathrm{D}G(x)[z].$$

Differential of f at $x \in S^{n-1}$:

$$\mathrm{D}f(x)[z] = x^T A z + z^T A x = 2z^T A x, \quad z \in T_x S^{n-1}.$$

Steepest-descent: Rayleigh quotient on unit sphere



"Natural" Riemannian metric on S^{n-1}:

$$g_x(z_1, z_2) = z_1^T z_2, \quad z_1, z_2 \in T_x S^{n-1}.$$

Differential of f at $x \in S^{n-1}$:

$$\mathrm{D}f(x)[z] = 2z^T A x = 2g_x(z, Ax), \quad z \in T_x S^{n-1}.$$

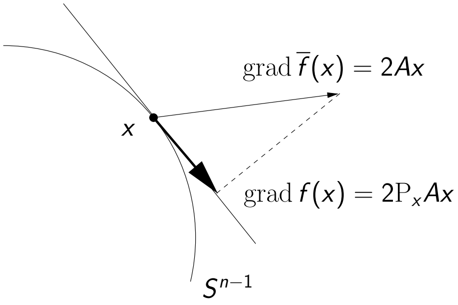
Gradient:

$$\operatorname{grad} f(x) = 2\mathrm{P}_x A x = 2(I - xx^T)Ax.$$

Check:

$$\begin{cases} \operatorname{grad} f(x) \in T_x S^{n-1} \\ \mathrm{D}f(x)[z] = g_x(\operatorname{grad} f(x), z), \ \forall z \in T_x S^{n-1}. \end{cases}$$

Steepest-descent: Rayleigh quotient on unit sphere



$$f : S^{n-1} \to \mathbb{R} : x \mapsto x^T Ax$$

$$\bar{f} : \mathbb{R}^n \to \mathbb{R} : x \mapsto x^T Ax$$

$$\operatorname{grad} \bar{f}(x) = 2Ax$$

$$\operatorname{grad} f(x) = 2\mathrm{P}_x Ax = 2(I - xx^T)Ax.$$

Newton's method on manifolds

Newton in $\mathbb{R}^n$

Let $f : \mathbb{R}^n \to \mathbb{R}$.
Recall $\operatorname{grad} f(x) = \begin{bmatrix} \partial_1 f(x) & \cdots & \partial_n f(x) \end{bmatrix}^T$.
Newton's iteration:

1. Solve, for the unknown $z \in \mathbb{R}^n$,

$$\mathrm{D}(\operatorname{grad} f)(x)[z] = -\operatorname{grad} f(x).$$

2. Set

$$x_+ = x + z.$$

Newton in $\mathbb{R}^n$: how it may fail

Let $f : \mathbb{R}^n_0 \to \mathbb{R} : x \mapsto \frac{x^T A x}{x^T x}$.
Newton's iteration:

1. Solve, for the unknown $z \in \mathbb{R}^n$,

$$\mathrm{D}(\operatorname{grad} f)(x)[z] = -\operatorname{grad} f(x).$$

2. Set

$$x_+ = x + z.$$

Proposition: For all x such that $f(x)$ is not an eigenvalue of A, we have

$$x_+ = 2x.$$

Newton: how to make it work for RQ

Let $f : S^{n-1} \to \mathbb{R} : x \mapsto \frac{x^T A x}{x^T x}$.
Newton's iteration:

1. Solve, for the unknown $z \in \mathbb{R}^n \rightsquigarrow \eta_x \in T_x S^{n-1}$

$$\mathrm{D}(\mathrm{grad}\, f)(x)[z] = -\mathrm{grad}\, f(x) \quad \rightsquigarrow \boxed{?}(\mathrm{grad}\, f)(x)[\eta_x] = -\mathrm{grad}\, f(x)$$

2. Set

$$x_+ = x + z \quad \rightsquigarrow x_+ = R(\eta_x)$$

Newton's equation on an abstract manifold

Let $\mathcal{M}$ be a manifold and let $f : \mathcal{M} \to \mathbb{R}$ be a cost function.
The mapping $x \in \mathcal{M} \mapsto \operatorname{grad} f(x) \in T_x\mathcal{M}$ is a *vector field*.

$$\mathrm{D}(\operatorname{grad} f)(x)[z] = -\operatorname{grad} f(x) \quad \rightsquigarrow \boxed{?}(\operatorname{grad} f)(x)[\eta_x] = -\operatorname{grad} f(x)$$

The new object has to be such that

- In $\mathbb{R}^n$, $\boxed{?}$ reduces to the classical derivative
- $\boxed{?}(\operatorname{grad} f)(x)[\eta_x]$ belongs to $T_x\mathcal{M}$
- $\boxed{?}$ has the same linearity properties and multiplication rule as the classical derivative.

Differential geometry offers a concept that matches these conditions: the concept of an *affine connection*.

Newton: affine connections

Let $\mathfrak{X}(\mathcal{M})$ denote the set of smooth vector fields on $\mathcal{M}$ and $\mathfrak{F}(\mathcal{M})$ the set of real-valued functions on $\mathcal{M}$.
An *affine connection* ∇ on a manifold $\mathcal{M}$ is a mapping

$$\nabla : \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \to \mathfrak{X}(\mathcal{M}),$$

which is denoted by $(\eta, \xi) \xrightarrow{\nabla} \nabla_\eta \xi$ and satisfies the following properties:

i) $\mathfrak{F}(\mathcal{M})$-linearity in η: $\quad \nabla_{f\eta+g\chi}\xi = f\nabla_\eta\xi + g\nabla_\chi\xi$,
ii) $\mathbb{R}$-linearity in ξ: $\quad \nabla_\eta(a\xi + b\zeta) = a\nabla_\eta\xi + b\nabla_\eta\zeta$,
iii) Product rule (Leibniz' law): $\quad \nabla_\eta(f\xi) = (\eta f)\xi + f\nabla_\eta\xi$,

in which $\eta, \chi, \xi, \zeta \in \mathfrak{X}(\mathcal{M})$, $f, g \in \mathfrak{F}(\mathcal{M})$, and $a, b \in \mathbb{R}$.

Newton's method on abstract manifolds

Cost function: $f : \mathbb{R}^n \to \mathbb{R} \rightsquigarrow f : \mathcal{M} \to \mathbb{R}$.
Newton's iteration:

1. Solve, for the unknown $z \in \mathbb{R}^n \rightsquigarrow \eta_x \in T_x\mathcal{M}$

$$\mathrm{D}(\mathrm{grad}\, f)(x)[z] = -\mathrm{grad}\, f(x) \quad \rightsquigarrow \nabla(\mathrm{grad}\, f)(x)[\eta_x] = -\mathrm{grad}\, f(x)$$

2. Set

$$x_+ = x + z \quad \rightsquigarrow x_+ = R(\eta_x)$$

In the algorithm above, ∇ is an affine connection on $\mathcal{M}$ and R is a retraction on $\mathcal{M}$.

Newton's method on S^{n-1}

If $\mathcal{M}$ is a Riemannian submanifold of $\mathbb{R}^n$, then ∇ defined by

$$\nabla_{\eta_x}\xi = \mathrm{P}_x \mathrm{D}\xi(x)[\eta_x], \quad \eta_x \in T_x\mathcal{M},\ \xi \in \mathfrak{X}(\mathcal{M})$$

is a particular affine connection, called *Riemannian connection*.
For the unit sphere S^{n-1}, this yields

$$\nabla_{\eta_x}\xi = (I - xx^T)\mathrm{D}\xi(x)[\eta_x], \quad x^T\eta_x = 0.$$

Newton's method for Rayleigh quotient on S^{n-1}

Let $f : \begin{cases} \mathbb{R}^n \\ \mathcal{M} \\ S^{n-1} \end{cases} \to \mathbb{R} : x \mapsto \begin{cases} f(x) \\ f(x) \\ \frac{x^T A x}{x^T x} \end{cases}$.

Newton's iteration:

1. Solve, for the unknown $z \in \mathbb{R}^n \rightsquigarrow \eta_x \in T_x\mathcal{M} \rightsquigarrow x^T \eta_x = 0$

$$\mathrm{D}(\operatorname{grad} f)(x)[z] = -\operatorname{grad} f(x)$$
$$\rightsquigarrow \nabla(\operatorname{grad} f)(x)[\eta_x] = -\operatorname{grad} f(x)$$
$$\rightsquigarrow (I - xx^T)(A - f(x)I)\eta_x = -(I - xx^T)Ax$$

2. Set

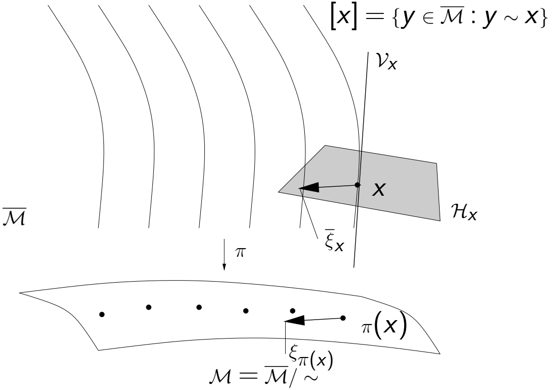
$$x_+ = x + z \quad \rightsquigarrow x_+ = R(\eta_x) \quad \rightsquigarrow x_+ = \frac{x + \eta_x}{\|x + \eta_x\|}$$

Newton for RQ on S^{n-1}: a closer look

$$
\begin{aligned}
(I - xx^T)(A - f(x)I)\eta_x &= -(I - xx^T)Ax \\
\Rightarrow (I - xx^T)(A - f(x)I)(x + \eta_x) &= 0 \\
\Rightarrow (A - f(x)I)(x + \eta_x) &= \alpha x
\end{aligned}
$$

Therefore, x_+ is collinear with $(A - f(x)I)^{-1}x$, which is the vector computed by the Rayleigh quotient iteration.

Newton method on quotient manifolds

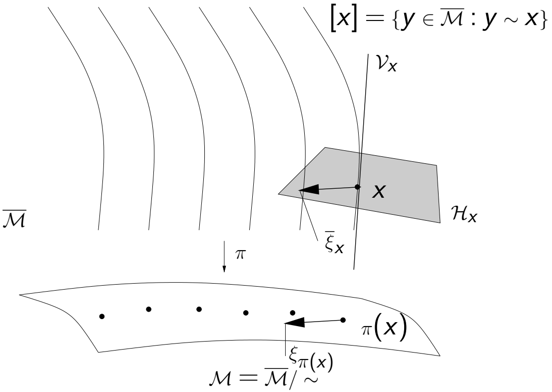


Affine connection: choose ∇ defined by

$$\overline{\nabla_\eta \xi}_x = \mathrm{P}_x^h \overline{\nabla}_{\overline{\eta}_x} \overline{\xi},$$

provided that this really defines a horizontal lift. This requires special choices of $\overline{\nabla}$.

Newton method on quotient manifolds



If $\pi : \overline{\mathcal{M}} \to \overline{\mathcal{M}}/\sim$ is a Riemannian submersion, then the Riemannian connection on $\overline{\mathcal{M}}/\sim$ is given by

$$\overline{\nabla_\eta \xi}_x = \mathrm{P}_x^h \overline{\nabla}_{\overline{\eta}_x} \overline{\xi},$$

where $\overline{\nabla}$ denotes the Riemannian connection on $\overline{\mathcal{M}}$.

A detailed exercise

Newton's method for the Rayleigh quotient on the Grassmann manifold

Manifold: Grassmann

The manifold is the Grassmann manifold of p-planes in $\mathbb{R}^n$:

$$\mathrm{Grass}(p, n) \simeq \mathrm{ST}(p, n)/\mathrm{GL}_p.$$

The one-to-one correspondence is

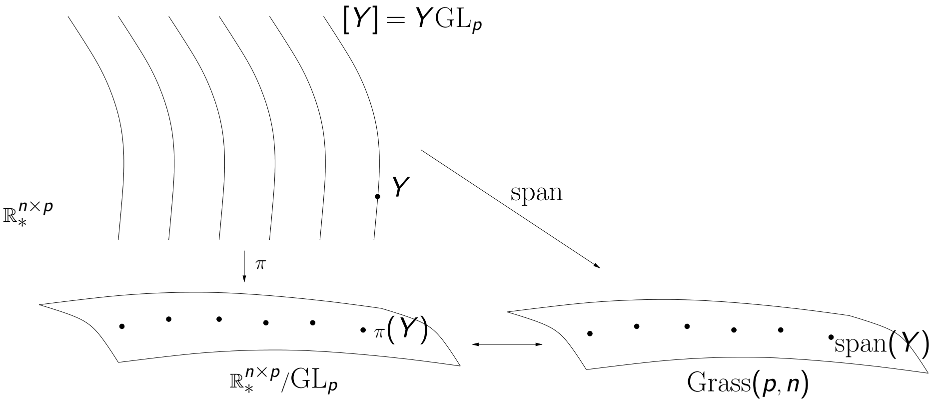
$$\mathrm{Grass}(p, n) \ni \mathcal{Y} \;\leftrightarrow\; Y\,\mathrm{GL}_p \in \mathrm{ST}(p, n)/\mathrm{GL}_p$$

such that $\mathcal{Y}$ is the column space of Y.
The quotient map

$$\pi : \mathrm{ST}(p, n) \to \mathrm{Grass}(p, n)$$

is the “column space” or “span” operation.

Grassmann and its quotient representation



Total space: the noncompact Stiefel manifold

The total space of the quotient is

$$\mathrm{ST}(p, n) = \{Y \in \mathbb{R}^{n \times p} : \mathrm{rank}(Y) = p\}.$$

This is an open submanifold of the Euclidean space $\mathbb{R}^{n \times p}$.
Tangent spaces: $T_Y \mathrm{ST}(p, n) \simeq \mathbb{R}^{n \times p}$.

Riemannian metric on the total space

Define a Riemannian metric $\overline{g}$ on $\mathrm{ST}(p, n)$ by

$$\overline{g}_Y(Z_1, Z_2) = \operatorname{trace}\left((Y^T Y)^{-1} Z_1^T Z_2\right).$$

This is not the canonical Riemannian metric, but it will allow us to turn the quotient map $\pi : \mathrm{ST}(p, n) \to \mathrm{Grass}(p, n)$ into a Riemannian submersion.

Vertical and horizontal spaces

The vertical spaces are the tangent spaces to the equivalence classes:

$$\mathcal{V}_Y := T_Y(Y\mathrm{GL}_p) = Y\ T_Y\mathrm{GL}_p = Y\mathbb{R}^{p\times p}.$$

Choice of horizontal space:

$$\begin{aligned}\mathcal{H}_Y &:= (\mathcal{V}_Y)^{\perp}\\ &= \{Z \in T_Y\mathrm{ST}(p,n) : \bar{g}_Y(Z,V) = 0, \forall V \in \mathcal{V}_Y\}\\ &= \{Z \in \mathbb{R}^{n\times p} : Y^T Z = 0\}.\end{aligned}$$

Horizontal projection:

$$\mathrm{P}_Y^h = (I - Y(Y^TY)^{-1}Y^T).$$

Compatibility equation for horizontal lifts

Given $\xi \in T_{\pi}(Y)\mathrm{Grass}(p, n)$, we have

$$\overline{\xi}_{YM} = \overline{\xi}_Y M.$$

To see this, observe that $\overline{\xi}_Y M$ is in $\mathcal{H}_{YM}$; moreover, since $YM + t\overline{\xi}_Y M$ and $Y + t\overline{\xi}_Y$ have the same column space for all t, one has

$$\mathrm{D}\pi(YM)[\overline{\xi}_Y M] = \mathrm{D}\pi(Y)[\overline{\xi}_Y] = \xi_{\pi(Y)}.$$

Thus $\overline{\xi}_Y M$ satisfies the conditions to be $\overline{\xi}_{YM}$.

Riemannian metric on the quotient

On $\mathrm{Grass}(p,n) \simeq \mathrm{ST}(p,n)/\mathrm{GL}_p$, define the Riemannian metric g by

$$g_{\pi(Y)}(\xi_{\pi(Y)}, \zeta_{\pi(Y)}) = \overline{g}_Y(\overline{\xi}_Y, \overline{\zeta}_Y).$$

This is well defined, because for all $\tilde{Y} \in \pi^{-1}(\pi(Y)) = Y\mathrm{GL}_p$, we have $\tilde{Y} = YM$ for some invertible M, and

$$\overline{g}_{YM}(\overline{\xi}_{YM}, \overline{\zeta}_{YM}) = \overline{g}_Y(\overline{\xi}_Y, \overline{\zeta}_Y).$$

This definition of g turns

$$\pi : (\mathrm{ST}(p,n), \overline{g}) \to (\mathrm{Grass}(p,n), g)$$

into a Riemannian submersion.

Cost function: Rayleigh quotient

Consider the cost function

$$f : \mathrm{Grass}(p, n) \to \mathbb{R} : \mathrm{span}(Y) \mapsto \mathrm{trace}\left((Y^T Y)^{-1} Y^T A Y\right).$$

This is the *projection* of

$$\overline{f} : \mathrm{ST}(p, n) \to \mathbb{R} : Y \mapsto \mathrm{trace}\left((Y^T Y)^{-1} Y^T A Y\right).$$

That is, $\overline{f} = f \circ \pi$.

Gradient of the cost function

For all $Z \in \mathbb{R}^{n\times p}$,

$$\mathrm{D}\overline{f}(Y)[Z] = 2\,\mathrm{trace}\left((Y^TY)^{-1}Z^T(AY - Y(Y^TY)^{-1}Y^TAY)\right).$$

Hence

$$\mathrm{grad}\,\overline{f}(Y) = 2\left(AY - Y(Y^TY)^{-1}Y^TAY\right),$$

and

$$\overline{\mathrm{grad}\,f}_Y = 2\left(AY - Y(Y^TY)^{-1}Y^TAY\right).$$

Riemannian connection

The quotient map is a Riemannian submersion. Therefore

$$\overline{\nabla_\eta \xi} = \mathrm{P}^h_Y \left(\overline{\nabla}_{\overline{\eta}_Y} \overline{\xi}\right)$$

It turns out that

$$\overline{\nabla_\eta \xi} = \mathrm{P}^h_Y \left(\mathrm{D}\overline{\xi}\,(Y)\,[\overline{\eta}_Y]\right).$$

(This is because the Riemanian metric $\overline{g}$ is "horizontally invariant".)
For the Rayleigh quotient f, this yields

$$\begin{aligned}\overline{\nabla_\eta \mathrm{grad}\, f} &= \mathrm{P}^h_Y \left(\mathrm{D}\overline{\mathrm{grad}\, f}\,(Y)\,[\overline{\eta}_Y]\right)\\ &= 2\,\mathrm{P}^h_Y \left(A\overline{\eta}_Y - \overline{\eta}_Y (Y^T Y)^{-1} Y^T A Y\right).\end{aligned}$$

Newton's equation

Newton's equation at $\pi(Y)$ is

$$\nabla_{\eta_{\pi(Y)}} \mathrm{grad}\, f = -\mathrm{grad}\, f(\pi(Y))$$

for the unknown $\eta_{\pi(Y)} \in T_{\pi(Y)}\mathrm{Grass}(p,n)$.
To turn this equation into a matrix equation, we take its horizontal lift. This yields

$$\mathrm{P}^h_Y \left(A\overline{\eta}_Y - \overline{\eta}_Y (Y^T Y)^{-1} Y^T A Y \right) = -\mathrm{P}^h_Y AY, \qquad \overline{\eta}_Y \in \mathcal{H}_Y,$$

whose solution $\overline{\eta}_Y$ in the horizontal space $\mathcal{H}_Y$ is the horizontal lift of the solution η of the Newton equation.

Retraction

Newton's method sends $\pi(Y)$ to $\mathcal{Y}_+$ according to

$$\nabla_{\eta_{\pi(Y)}} \mathrm{grad}\, f = -\mathrm{grad}\, f(\pi(Y))$$
$$\mathcal{Y}_+ = R_{\pi(Y)}(\eta_{\pi(Y)}).$$

It remains to pick the retraction R.
Choice: R defined by

$$R_{\pi(Y)}\xi_{\pi(Y)} = \pi(Y + \overline{\xi}_Y).$$

(This is a well-defined retraction.)

Newton's iteration for RQ on Grassmann

Require: Symmetric matrix A.
Input: Initial iterate $Y_0 \in \mathrm{ST}(p, n)$.
Output: Sequence of iterates $\{Y_k\}$ in $\mathrm{ST}(p, n)$.

for $k = 0, 1, 2, \dots$ **do**

Solve the linear system

$$\begin{cases} \mathrm{P}^h_{Y_k}\left(AZ_k - Z_k(Y_k^T Y_k)^{-1} Y_k^T A Y_k\right) = -\mathrm{P}^h_{Y_k}(AY_k) \\ Y_k^T Z_k = 0 \end{cases}$$

for the unknown Z_k, where P^h_Y is the orthogonal projector onto $\mathcal{H}_Y$. (The condition $Y_k^T Z_k$ expresses that Z_k belongs to the horizontal space $\mathcal{H}_{Y_k}$.)

Set

$$Y_{k+1} = (Y_k + Z_k) N_k$$

where N_k is a nonsingular $p \times p$ matrix chosen for normalization purposes.

end for

A new tool for Optimization On Manifolds:

Vector Transport

Filling a gap

	Purely Riemannian way	Pragmatic way
Update	Search along the geodesic tangent to the search direction	Search along any curve ta to the search direction scribed by a *retraction*)
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	??

Where do we use parallel translation?

In CG. Quoting (approximately) Smith (1994):

1. Select $x_0 \in \mathcal{M}$, compute $H_0 = -\mathrm{grad}\, f(x_0)$, and set $k = 0$
2. Compute t_k such that $f(\mathrm{Exp}_{x_k}(t_k H_k)) \leq f(\mathrm{Exp}_{x_k}(tH_k))$ for all $t \geq 0$.
3. Set $x_{k+1} = \mathrm{Exp}_{x_k}(t_k H_k)$.
4. Set $H_{k+1} = -\mathrm{grad}\, f(x_{k+1}) + \beta_k \tau H_k$, where τ is the parallel translation along the geodesic from x_k to x_{k+1}.

Where do we use parallel translation?

In BFGS. Quoting (approximately) Gabay (1982):
$x_{k+1} = \mathrm{Exp}_{x_k}(t_k \xi_k)$ (update along geodesic)
$\mathrm{grad}\, f(x_{k+1}) - \tau_0^{t_k} \mathrm{grad}\, f(x_k) = B_{k+1} \tau_0^{t_k}(t_k \xi_k)$ (requirement on approximate Jacobian B)
This leads to the a *generalized BFGS update formula* involving parallel translation.

Where else could we use parallel translation?

In finite-difference quasi-Newton.

Let ξ be a vector field on a Riemannian manifold $\mathcal{M}$. Exact Jacobian of ξ at $x \in \mathcal{M}$: $J_\xi(x)[\eta] = \nabla_\eta \xi$.

Finite difference approximation to J_ξ: choose a basis $(E_1, \cdots, E_d)$ of $T_x\mathcal{M}$ and define $\tilde{J}(x)$ as the linear operator that satisfies

$$\tilde{J}(x)[E_i] = \frac{\tau_h^0 \xi_{\mathrm{Exp}_x(hE_i)} - \xi_x}{h}.$$

Filling a gap

	Purely Riemannian way	Pragmatic way
Update	Search along the geodesic tangent to the search direction	Search along **any** pres curve tangent to the sear rection
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	??

Parallel translation can be tough

Edelman et al (1998): We are unaware of any closed form expression for the parallel translation on the Stiefel manifold (defined with respect to the Riemannian connection induced by the embedding in $\mathbb{R}^{n\times p}$).
Parallel transport along geodesics on Grassmannians:

$$\overline{\xi(t)}_{Y(t)} = -Y_0 V \sin(\Sigma t) U^T \overline{\xi(0)}_{Y_0} + U \cos(\Sigma t) U^T \overline{\xi(0)}_{Y_0} + (I - UU^T) \overline{\xi(0)}_{Y_0}.$$

where $\overline{\dot{\mathcal{Y}}(0)}_{Y_0} = U \Sigma V^T$ is a thin SVD.

Alternatives found in the literature

Edelman et al (1998): "extrinsic" CG algorithm. "Tangency of the search direction at the new point is imposed via the projection $I - YY^T$" (instead of via parallel translation).

Brace & Manton (2006), *An improved BFGS-on-manifold algorithm for computing weighted low rank approximation*. "The second change is that parallel translation is not defined with respect to the Levi-Civita connection, but rather is all but ignored."

Filling a gap

	Purely Riemannian way	Pragmatic way
Update	Search along the geodesic tangent to the search direction	Search along any curve ta to the search direction scribed by a *retraction*)
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	??

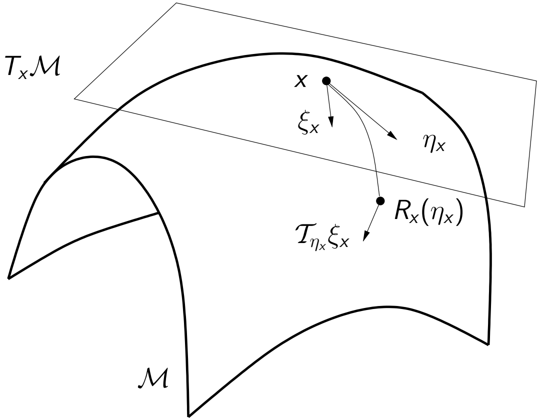
Filling a gap: Vector Transport

	Purely Riemannian way	Pragmatic way
Update	Search along the geodesic tangent to the search direction	Search along **any** curve ta to the search direction scribed by a *retraction*)
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	Vector Transport

Still to come

- Vector transport in one picture
- Formal definition
- Particular vector transports
- Applications: finite-difference Newton, BFGS, CG.

The concept of vector transport



Retraction

A *retraction* on a manifold $\mathcal{M}$ is a smooth mapping

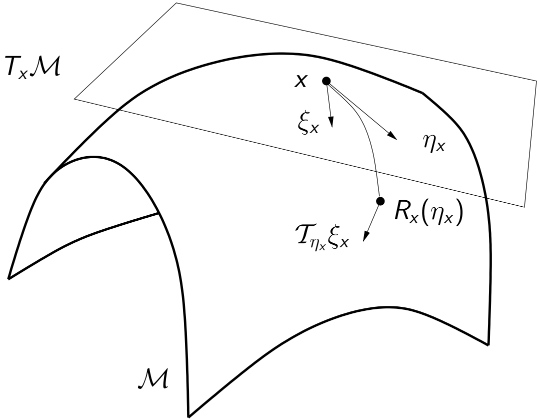
$$R : T\mathcal{M} \to \mathcal{M}$$

such that

1. $R(0_x) = x$ for all $x \in \mathcal{M}$, where 0_x denotes the origin of $T_x\mathcal{M}$;
2. $\frac{d}{dt}R(t\xi_x)\big|_{t=0} = \xi_x$ for all $\xi_x \in T_x\mathcal{M}$.

Consequently, the curve $t \mapsto R(t\xi_x)$ is a curve on $\mathcal{M}$ tangent to ξ_x.

The concept of vector transport – Whitney sum



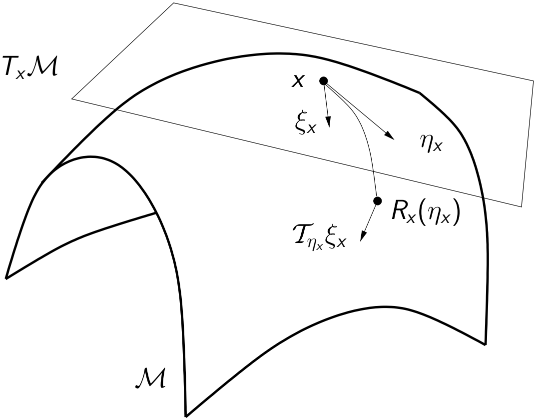
Whitney sum

Let $T\mathcal{M} \oplus T\mathcal{M}$ denote the set

$$T\mathcal{M} \oplus T\mathcal{M} = \{(\eta_x, \xi_x) : \eta_x, \xi_x \in T_x\mathcal{M},\ x \in \mathcal{M}\}.$$

This set admits a natural manifold structure.

The concept of vector transport – definition



Vector transport: definition

A *vector transport* on a manifold $\mathcal{M}$ on top of a retraction R is a smooth map

$$T\mathcal{M} \oplus T\mathcal{M} \to T\mathcal{M} : (\eta_x, \xi_x) \mapsto \mathcal{T}_{\eta_x}(\xi_x) \in T\mathcal{M}$$

satisfying the following properties for all $x \in \mathcal{M}$:

1. (Underlying retraction) $\mathcal{T}_{\eta_x}\xi_x$ belongs to $T_{R_x(\eta_x)}\mathcal{M}$.
2. (Consistency) $\mathcal{T}_{0_x}\xi_x = \xi_x$ for all $\xi_x \in T_x\mathcal{M}$;
3. (Linearity) $\mathcal{T}_{\eta_x}(a\xi_x + b\zeta_x) = a\mathcal{T}_{\eta_x}(\xi_x) + b\mathcal{T}_{\eta_x}(\zeta_x)$.

Inverse vector transport

When it exists, $(\mathcal{T}_{\eta_x})^{-1}(\xi_{R_x(\eta_x)})$ belongs to $T_x\mathcal{M}$. If η and ξ are two vector fields on $\mathcal{M}$, then $(\mathcal{T}_\eta)^{-1}\xi$ is naturally defined as the vector field satisfying

$$\left((\mathcal{T}_\eta)^{-1}\xi\right)_x = (\mathcal{T}_{\eta_x})^{-1}\left(\xi_{R_x(\eta_x)}\right).$$

Still to come

- Vector transport in one picture
- Formal definition
- Particular vector transports
- Applications: finite-difference Newton, BFGS, CG.

Parallel translation is a vector transport

Proposition

If ∇ is an affine connection and R is a retraction on a manifold $\mathcal{M}$, then

$$\mathcal{T}_{\eta_x}(\xi_x) := P_{\gamma}^{1 \leftarrow 0} \xi_x \tag{1}$$

is a vector transport with associated retraction R, where P_γ denotes the parallel translation induced by ∇ along the curve $t \mapsto \gamma(t) = R_x(t\eta_x)$.

Vector transport on Riemannian submanifolds

If $\mathcal{M}$ is an embedded submanifold of a Euclidean space $\mathcal{E}$ and $\mathcal{M}$ is endowed with a retraction R, then we can rely on the natural inclusion $T_y\mathcal{M} \subset \mathcal{E}$ for all $y \in \mathcal{N}$ to simply define the vector transport by

$$\mathcal{T}_{\eta_x}\xi_x := \mathrm{P}_{R_x(\eta_x)}\xi_x, \tag{2}$$

where P_x denotes the orthogonal projector onto $T_x\mathcal{N}$.

Still to come

- Vector transport in one picture
- Formal definition
- Particular vector transports
- Applications: finite-difference Newton, BFGS, CG.

Vector transport in finite differences

Let $\mathcal{M}$ be a manifold endowed with a vector transport $\mathcal{T}$ on top of a retraction R. Let $x \in \mathcal{M}$ and let $(E_1, \ldots, E_d)$ be a basis of $T_x\mathcal{M}$. Given a smooth vector field ξ and a real constant $h > 0$, let $\tilde{J}_\xi(x) : T_x\mathcal{M} \to T_x\mathcal{M}$ be the linear operator that satisfies, for $i = 1, \ldots, d$,

$$\tilde{J}_\xi(x)[E_i] = \frac{(\mathcal{T}_{hE_i})^{-1}\xi_{R(hE_i)} - \xi_x}{h}. \tag{3}$$

Lemma (finite differences)

Let x_* be a nondegenerate zero of ξ. Then there is $c > 0$ such that, for all x sufficiently close to x_* and all h sufficiently small, it holds that

$$\|\tilde{J}_\xi(x)[E_i] - J(x)[E_i]\| \leq c(h + \|\xi_x\|). \tag{4}$$

Convergence of Newton's method with finite differences

Proposition

Consider the geometric Newton method where the exact Jacobian $J(x_k)$ is replaced by the operator $\tilde{J}_\xi(x_k)$ with $h := h_k$. If

$$\lim_{k \to \infty} h_k = 0,$$

then the convergence to nondegenerate zeros of ξ is superlinear. If, moreover, there exists some constant c such that

$$h_k \leq c \|\xi_{x_k}\|$$

for all k, then the convergence is (at least) quadratic.

Vector transport in BFGS

With the notation

$$
\begin{aligned}
s_k &:= \mathcal{T}_{\eta_k}\eta_k \in T_{x_{k+1}}\mathcal{M},\\
y_k &:= \operatorname{grad} f(x_{k+1}) - \mathcal{T}_{\eta_k}(\operatorname{grad} f(x_k)) \in T_{x_{k+1}}\mathcal{M},
\end{aligned}
$$

we define the operator $A_{k+1} : T_{x_{k+1}}\mathcal{M} \mapsto T_{x_{k+1}}\mathcal{M}$ by

$$
A_{k+1}\eta = \tilde{A}_k\eta - \frac{\langle s_k, \tilde{A}_k\eta\rangle}{\langle s_k, \tilde{A}_k s_k\rangle}\tilde{A}_k s_k + \frac{\langle y_k, \eta\rangle}{\langle y_k, s_k\rangle} y_k \quad \text{for all } \eta \in T_{x_{k+1}}\mathcal{M},
$$

with

$$
\tilde{A}_k = \mathcal{T}_{\eta_k} \circ A_k \circ (\mathcal{T}_{\eta_k})^{-1}.
$$

Vector transport in CG

Compute a step size α_k and set

$$x_{k+1} = R_{x_k}(\alpha_k \eta_k). \tag{5}$$

Compute β_{k+1} and set

$$\eta_{k+1} = -\operatorname{grad} f(x_{k+1}) + \beta_{k+1} \mathcal{T}_{\alpha_k \eta_k}(\eta_k). \tag{6}$$

Filling a gap: Vector Transport

	Purely Riemannian way	Pragmatic way
Update	Search along the geodesic tangent to the search direction	Search along any curve ta to the search direction scribed by a *retraction*)
Displacement of tgt vectors	Parallel translation induced by $\overset{g}{\nabla}$	Vector Transport

Ongoing work

- Use vector transport wherever we can.
- Extend convergence analyses.
- Develop recipies for building efficient vector transports.

Trust-region methods on Riemannian manifolds

Motivating application: Mechanical vibrations

Mass matrix M, stiffness matrix K.
Equation of vibrations (for undamped discretized linear structures):

$$Kx = \omega^2 Mx$$

were

- ω is an angular frequency of vibration
- x is the corresponding mode of vibration

Task: find lowest modes of vibration.

Generalized eigenvalue problem

Given $n \times n$ matrices $A = A^T$ and $B = B^T \succ 0$, there exist $v_1, \ldots, v_n$ in $\mathbb{R}^n$ and $\lambda_1 \leq \ldots \leq \lambda_n$ in $\mathbb{R}$ such that

$$Av_i = \lambda_i B v_i$$
$$v_i^T B v_j = \delta_{ij}.$$

Task: find $\lambda_1, \ldots, \lambda_p$ and $v_1, \ldots, v_p$.
We assume throughout that $\lambda_p < \lambda_{p+1}$.

Case $p = 1$: optimization in $\mathbb{R}^n$

$$Av_i = \lambda_i B v_i$$

Consider the Rayleigh quotient

$$\tilde{f} : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y}$$

Invariance: $\tilde{f}(\alpha y) = \tilde{f}(y)$.
Stationary points of $\tilde{f}$: αv_i, for all $\alpha \neq 0$.
Minimizers of $\tilde{f}$: αv_1, for all $\alpha \neq 0$.
Difficulty: the minimizers are not isolated.
Remedy: optimization on manifold.

Case $p = 1$: optimization on ellipsoid

$$\tilde{f} : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y}$$

Invariance: $\tilde{f}(\alpha y) = \tilde{f}(y)$.
Remedy 1:

- $\mathcal{M} := \{y \in \mathbb{R}^n : y^T B y = 1\}$, *submanifold* of $\mathbb{R}^n$.
- $f : \mathcal{M} \to \mathbb{R} : f(y) = y^T A y$.

Stationary points of f: $\pm v_1, \ldots, \pm v_n$.
Minimizers of f: $\pm v_1$.

Case $p = 1$: optimization on projective space

$$\tilde{f} : \mathbb{R}^n_* \to \mathbb{R} : f(y) = \frac{y^T A y}{y^T B y}$$

Invariance: $\tilde{f}(\alpha y) = \tilde{f}(y)$.
Remedy 2:

- $[y] := y\mathbb{R} := \{y\alpha : \alpha \in \mathbb{R}\}$
- $\mathcal{M} := \mathbb{R}^n_*/\mathbb{R} = \{[y]\}$
- $f : \mathcal{M} \to \mathbb{R} : f([y]) := \tilde{f}(y)$

Stationary points of f: $[v_1], \ldots, [v_n]$.
Minimizer of f: $[v_1]$.

Case $p \geq 1$: optimization on the Grassmann manifold

$$\tilde{f} : \mathbb{R}_*^{n\times p} \to \mathbb{R} : \tilde{f}(Y) = \operatorname{trace}\left((Y^T BY)^{-1} Y^T AY\right)$$

Invariance: $\tilde{f}(YR) = \tilde{f}(Y)$.
Define:

- $[Y] := \{YR : R \in \mathbb{R}_*^{p\times p}\}, \quad Y \in \mathbb{R}_*^{n\times p}$
- $\mathcal{M} := \mathrm{Grass}(p, n) := \{[Y]\}$
- $f : \mathcal{M} \to \mathbb{R} : f([Y]) := \tilde{f}(Y)$

Stationary points of f: $\mathrm{span}\{v_{i_1}, \ldots, v_{i_p}\}$.
Minimizer of f: $[Y] = \mathrm{span}\{v_1, \ldots, v_p\}$.

Optimization on Manifolds

- Luenberger [Lue73], Gabay [Gab82]: optimization on submanifolds of $\mathbb{R}^n$.
- Smith [Smi93, Smi94] and Udriște [Udr94]: optimization on general Riemannian manifolds (steepest descent, Newton, CG).
- ...
- PAA, Baker and Gallivan [ABG07]: trust-region methods on Riemannian manifolds.
- PAA, Mahony, Sepulchre [AMS08]:*Optimization Algorithms on Matrix Manifolds*, textbook.

The Problem : Leftmost Eigenpairs of Matrix Pencil

Given $n \times n$ matrix pencil (A, B), $A = A^T$, $B = B^T \succ 0$ with (unknown) eigen-decomposition

$$A\,[v_1|\ldots|v_n] = B\,[v_1|\ldots|v_n]\,\mathrm{diag}(\lambda_1, \ldots, \lambda_n)$$

$[v_1|\ldots|v_n]^T\,B\,[v_1|\ldots|v_n] = I, \quad \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n.$
The problem is to compute the minor eigenvector $\pm v_1$.

The ideal algorithm

Given (A, B), $A = A^T$, $B = B^T \succ 0$ with (unknown) eigenvalues $0 < \lambda_1 \leq \ldots \lambda_n$ and associated eigenvectors $v_1, \ldots, v_n$.

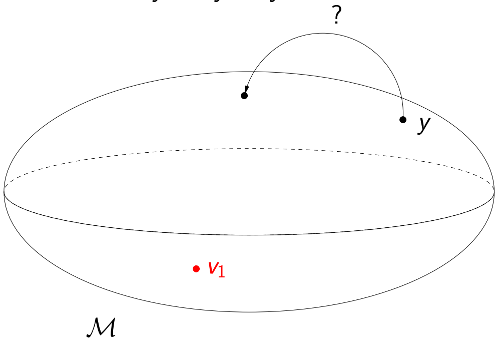
1. Global convergence:
   - Convergence to some eigenvector for all initial conditions.
   - Stable convergence to the "leftmost" eigenvector $\pm v_1$ only.
2. Superlinear (cubic) local convergence to $\pm v_1$.
3. "Matrix-free" (no factorization of A, B)
   but possible use of preconditioner.
4. Minimal storage space required.

Strategy

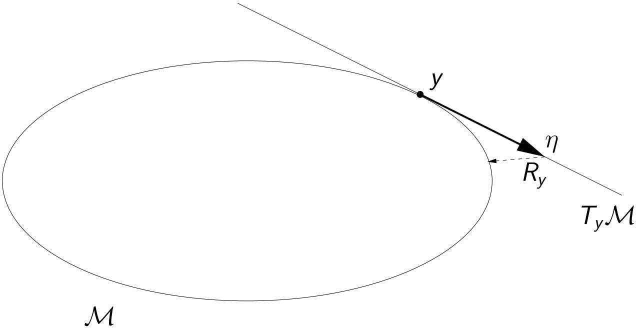
- Rewrite computation of leftmost eigenpair as an optimization problem (on a manifold).
- Use a model-trust-region scheme to solve the problem.
  $\rightsquigarrow$ Global convergence.
- Take the exact quadratic model (at least, close to the solution).
  $\rightsquigarrow$ Superlinear convergence.
- Solve the trust-region subproblems using the (Steihaug-Toint) truncated CG (tCG) algorithm.
  $\rightsquigarrow$ "Matrix-free", preconditioned iteration.
  $\rightsquigarrow$ Minimal storage of iteration vectors.

Iteration on the manifold

Manifold: ellipsoid $\mathcal{M} = \{y \in \mathbb{R}^n : y^T B y = 1\}$.
Cost function: $f : \mathcal{M} \to \mathbb{R} : y \mapsto y^T A y$



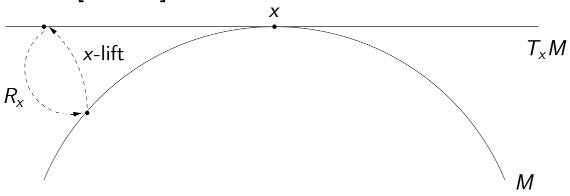
Tangent space and retraction (2D picture)



Tangent space: $T_y\mathcal{M} := \{\eta \in \mathbb{R}^n : y^T B\eta = 0\}$.
Retraction: $R_y\eta := (y+\eta)/\|y+\eta\|_B$.
Lifted cost function: $\hat{f}_y(\eta) := f(R_y\eta) = \frac{(y+\eta)^T A(y+\eta)}{(y+\eta)^T B(y+\eta)}$.

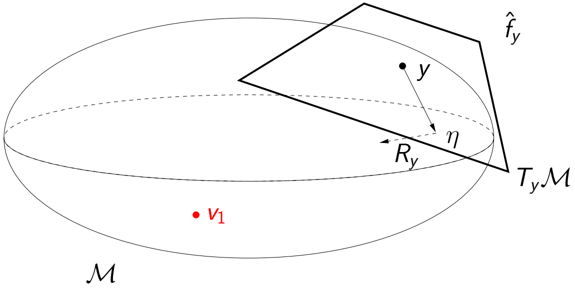
Concept of retraction

Introduced by Shub [Shu86].



1. R_x is defined and one-to-one in a neighbourhood of 0_x in T_xM.
2. $R_x(0_x) = x$.
3. $\mathrm{D}R_x(0_x) = \mathrm{id}_{T_xM}$, the identity mapping on T_xM, with the canonical identification $T_{0_x}T_xM \simeq T_xM$.

Tangent space and retraction



Tangent space: $T_y\mathcal{M} := \{\eta \in \mathbb{R}^n : y^T B\eta = 0\}$.
Retraction: $R_y\eta := (y+\eta)/\|y+\eta\|_B$.
Lifted cost function: $\hat{f}_y(\eta) := f(R_y\eta) = \frac{(y+\eta)^T A(y+\eta)}{(y+\eta)^T B(y+\eta)}$.

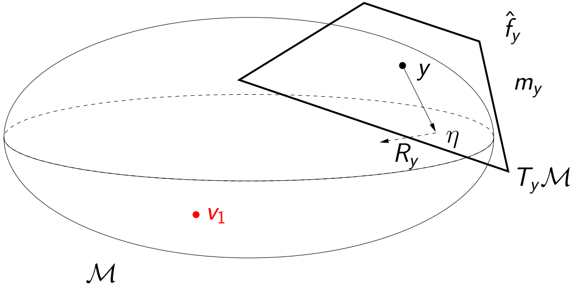
Quadratic model

$$
\begin{aligned}
\hat{f}_y(\eta) &= \frac{y^T A y}{y^T B y} + 2\frac{y^T A \eta}{y^T B y} + \frac{1}{y^T B y}\left(\eta^T A \eta - \frac{y^T A y}{y^T B y}\eta^T B \eta\right) + \dots \\
&= f(y) + 2\langle PAy, \eta\rangle + \frac{1}{2}\langle 2P(A - f(y)B)P\eta, \eta\rangle + \dots
\end{aligned}
$$

where $\langle u, v\rangle = u^T v$ and $P = I - By(y^T B^2 y)^{-1} y^T B$.
Model:

$$
m_y(\eta) = f(y) + 2\langle PAy, \eta\rangle + \frac{1}{2}\langle P(A - f(y)B)P\eta, \eta\rangle, \quad y^T B\eta = 0.
$$

Quadratic model



$$m_y(\eta) = f(y) + 2\langle PAy, \eta\rangle + \frac{1}{2}\langle P(A - f(y)B)P\eta, \eta\rangle, \quad y^T B\eta = 0.$$

Newton vs Trust-Region

Model:

$$m_y(\eta) = f(y) + 2\langle PAy, \eta\rangle + \frac{1}{2}\langle P(A - f(y)B)P\eta, \eta\rangle, \quad y^T B\eta = 0. \quad (7)$$

Newton method: Compute the stationary point of the model, i.e., solve

$$P(A - f(y)B)P\,\eta = -PAy.$$

Instead, compute (approximately) the minimizer of m_y within a trust-region

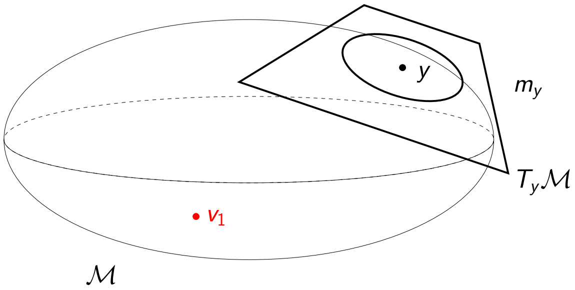
$$\{\eta \in T_x\mathcal{M} : \eta^T\eta \leq \Delta^2\}.$$

Trust-region subproblem

Minimize

$$m_y(\eta) = f(y) + 2\langle PAy, \eta\rangle + \frac{1}{2}\langle P(A - f(y)B)P\eta, \eta\rangle, \quad y^T B\eta = 0.$$

subject to $\eta^T \eta \leq \Delta^2$.



Truncated CG method for the TR subproblem (1)

Let $\langle \cdot, \cdot \rangle$ denote the standard inner product and let $\mathcal{H}_{x_k} := P(A - f(x_k)B)P$ denote the Hessian operator.

Initializations:

Set $\eta_0 = 0$, $r_0 = P_{x_k} A x_k = A x_k - B x_k (x_k^T B^2 x_k)^{-1} x_k^T B A x_k$, $\delta_0 = -r_0$;

Then repeat the following loop on j:

Check for negative curvature

if $\langle \delta_j, \mathcal{H}_{x_k} \delta_j \rangle \leq 0$

Compute τ such that $\eta = \eta_j + \tau \delta_j$ minimizes $m(\eta)$ in (7) and satisfies $\|\eta\| = \Delta$;

return η;

Truncated CG method for the TR subproblem (2)

Generate next inner iterate

Set $\alpha_j = \langle r_j, r_j\rangle / \langle \delta_j, \mathcal{H}_{x_k}\delta_j\rangle$;

Set $\eta_{j+1} = \eta_j + \alpha_j\delta_j$;

Check trust-region

if $\|\eta_{j+1}\| \geq \Delta$

Compute $\tau \geq 0$ such that $\eta = \eta_j + \tau\delta_j$ satisfies $\|\eta\| = \Delta$;

return η;

Truncated CG method for the TR subproblem (3)

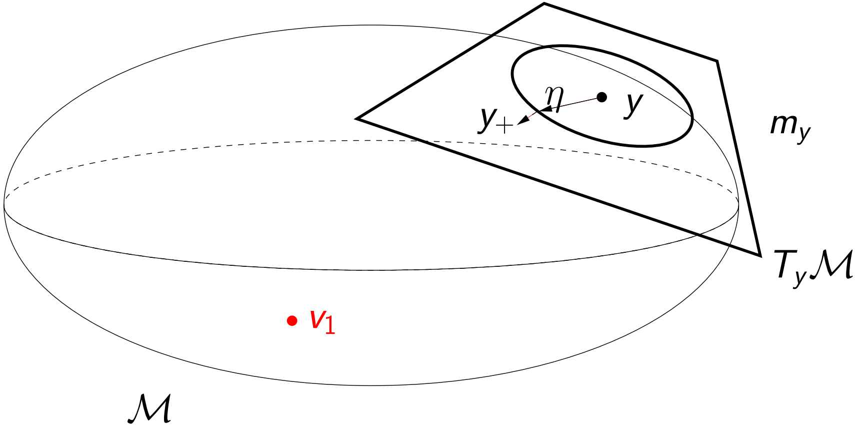
Update residual and search direction

Set $r_{j+1} = r_j + \alpha_j \mathcal{H}_{x_k} \delta_j$;
Set $\beta_{j+1} = \langle r_{j+1}, r_{j+1} \rangle / \langle r_j, r_j \rangle$;
Set $\delta_{j+1} = -r_{j+1} + \beta_{j+1} \delta_j$;
$j \leftarrow j + 1$;

Check residual

If $\|r_j\| \leq \|r_0\| \min\left(\|r_0\|^\theta, \kappa\right)$ for some prescribed θ and κ
return η_j;

Overall iteration



The outer iteration – manifold trust-region (1)

Data: symmetric $n \times n$ matrices A and B, with B positive definite.
Parameters: $\bar{\Delta} > 0$, $\Delta_0 \in (0, \bar{\Delta})$, and $\rho' \in (0, \frac{1}{4})$.
Input: initial iterate $x_0 \in \{y : y^T B y = 1\}$.
Output: sequence of iterates $\{x_k\}$ in $\{y : y^T B y = 1\}$.
Initialization: $k = 0$
Repeat the following:

The outer iteration – manifold trust-region (2)

- Obtain η_k using the Steihaug-Toint truncated conjugate-gradient method to approximately solve the trust-region subproblem

$$\min_{x_k^T B\eta=0} m_{x_k}(\eta) \quad \text{s.t. } \|\eta\| \leq \Delta_k, \tag{8}$$

where m is defined in (7).

The outer iteration – manifold trust-region (3)

- Evaluate
$$\rho_k = \frac{\hat{f}_{x_k}(0) - \hat{f}_{x_k}(\eta_k)}{m_{x_k}(0) - m_{x_k}(\eta_k)} \tag{9}$$
where $\hat{f}_{x_k}(\eta) = \frac{(x_k+\eta)^T A (x_k+\eta)}{(x_k+\eta)^T B (x_k+\eta)}$.
- Update the trust-region radius:
  if $\rho_k < \frac{1}{4}$
  $\Delta_{k+1} = \frac{1}{4}\Delta_k$
  else if $\rho_k > \frac{3}{4}$ **and** $\|\eta_k\| = \Delta_k$
  $\Delta_{k+1} = \min(2\Delta_k, \bar{\Delta})$
  else
  $\Delta_{k+1} = \Delta_k$;

The outer iteration – manifold trust-region (4)

- Update the iterate:
  if $\rho_k > \rho'$
  $$x_{k+1} = (x_k + \eta_k)/\|x_k + \eta_k\|_B; \tag{10}$$
  else
  $x_{k+1} = x_k;$
  $k \leftarrow k + 1$

Strategy

- Rewrite computation of leftmost eigenpair as an optimization problem (on a manifold).
- Use a model-trust-region scheme to solve the problem.
  $\rightsquigarrow$ Global convergence.
- Take the exact quadratic model (at least, close to the solution).
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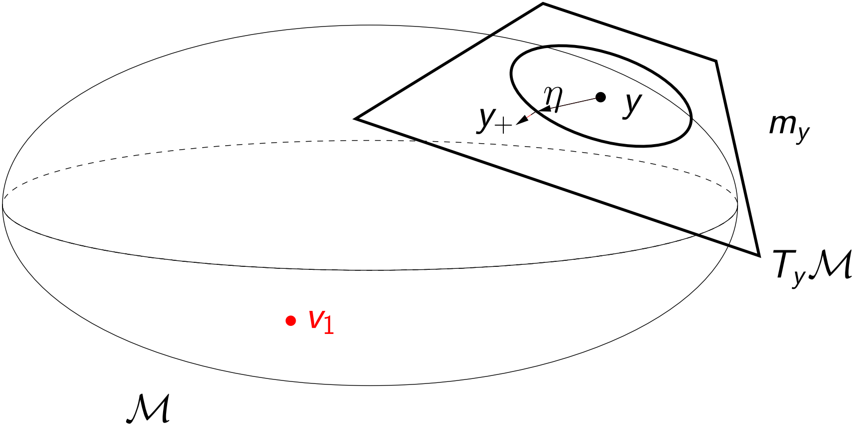
  $\rightsquigarrow$ "Matrix-free", preconditioned iteration.
  $\rightsquigarrow$ Minimal storage of iteration vectors.

Summary

We have obtained a trust-region algorithm for minimizing the Rayleigh quotient over an ellipsoid.

Generalization to trust-region algorithms for minimizing functions on manifolds: the Riemannian Trust-Region (RTR) method [ABG07].

Convergence analysis



Global convergence of Riemannian Trust-Region algorithms

Let $\{x_k\}$ be a sequence of iterates generated by the RTR algorithm with $\rho' \in (0, \frac{1}{4})$. Suppose that f is C^2 and bounded below on the level set $\{x \in M : f(x) < f(x_0)\}$. Suppose that $\|\mathrm{grad}\, f(x)\| \leq \beta_g$ and $\|\mathrm{Hess}\, f(x)\| \leq \beta_H$ for some constants β_g, β_H, and all $x \in M$. Moreover suppose that

$$\|\frac{D}{dt}\frac{d}{dt} Rt\xi\| \leq \beta_D \tag{11}$$

for some constant β_D, for all $\xi \in TM$ with $\|\xi\| = 1$ and all $t < \delta_D$, where $\frac{D}{dt}$ denotes the covariant derivative along the curve $t \mapsto Rt\xi$. Further suppose that all approximate solutions η_k of the trust-region subproblems produce a decrease of the model that is at least a fixed fraction of the Cauchy decrease.

Global convergence (cont'd)

It then follows that

$$\lim_{k \to \infty} \operatorname{grad} f(x_k) = 0.$$

And only the local minima are stable (the saddle points and local maxima are unstable).

Local convergence of Riemannian Trust-Region algorithms

Consider the RTR-tCG algorithm. Suppose that f is a C^2 cost function on M and that

$$\|\mathcal{H}_k - \mathrm{Hess}\,\hat{f}_{x_k}(0_k)\| \leq \beta_{\mathcal{H}} \|\mathrm{grad}\, f(x_k)\|. \tag{12}$$

Let $v \in M$ be a nondegenerate local minimum of f, (i.e., $\mathrm{grad}\, f(v) = 0$ and $\mathrm{Hess}\, f(v)$ is positive definite). Further assume that $\mathrm{Hess}\,\hat{f}_{x_k}$ is Lipschitz-continuous at 0_x uniformly in x in a neighborhood of v, i.e., there exist $\beta_1 > 0$, $\delta_1 > 0$ and $\delta_2 > 0$ such that, for all $x \in B_{\delta_1}(v)$ and all $\xi \in B_{\delta_2}(0_x)$, it holds

$$\|\mathrm{Hess}\,\hat{f}_{x_k}(\xi) - \mathrm{Hess}\,\hat{f}_{x_k}(0_{x_k})\| \leq \beta_{L2} \|\xi\|. \tag{13}$$

Local convergence (cont'd)

Then there exists $c > 0$ such that, for all sequences $\{x_k\}$ generated by the RTR-tCG algorithm converging to v, there exists $K > 0$ such that for all $k > K$,

$$\mathrm{dist}(x_{k+1}, v) \leq c\,(\mathrm{dist}(x_k, v))^{\min\{\theta+1,2\}}, \tag{14}$$

where θ governs the stopping criterion of the tCG inner iteration.

Convergence of trust-region-based eigensolver

Theorem:

Let (A, B) be an $n \times n$ symmetric/positive-definite matrix pencil with eigenvalues $\lambda_1 < \lambda_2 \leq \ldots \leq \lambda_{n-1} \leq \lambda_n$ and an associated B-orthonormal basis of eigenvectors $(v_1, \ldots, v_n)$.

Let $\mathcal{S}_i = \{y : Ay = \lambda_i By,\ y^T By = 1\}$ denote the intersection of the eigenspace of (A, B) associated to λ_i with the set $\{y : y^T By = 1\}$.

...

Convergence (global)

(i) Let $\{x_k\}$ be a sequence of iterates generated by the Algorithm. Then $\{x_k\}$ converges to the eigenspace of (A, B) associated to one of its eigenvalues. That is, there exists i such that $\lim_{k\to\infty} \mathrm{dist}(x_k, \mathcal{S}_i) = 0$.

(ii) Only the set $\mathcal{S}_1 = \{\pm v_1\}$ is stable.

Convergence (local)

(iii) There exists $c > 0$ such that, for all sequences $\{x_k\}$ generated by the Algorithm converging to $\mathcal{S}_1$, there exists $K > 0$ such that for all $k > K$,

$$\mathrm{dist}(x_{k+1}, \mathcal{S}_1) \leq c\,(\mathrm{dist}(x_k, \mathcal{S}_1))^{\min\{\theta+1,2\}} \tag{15}$$

with $\theta > 0$.

Strategy

- Rewrite computation of leftmost eigenpair as an optimization problem (on a manifold).
- Use a model-trust-region scheme to solve the problem.
  $\rightsquigarrow$ Global convergence.
- Take the exact quadratic model (at least, close to the solution).
  $\rightsquigarrow$ Superlinear convergence.
- Solve the trust-region subproblems using the (Steihaug-Toint) truncated CG (tCG) algorithm.
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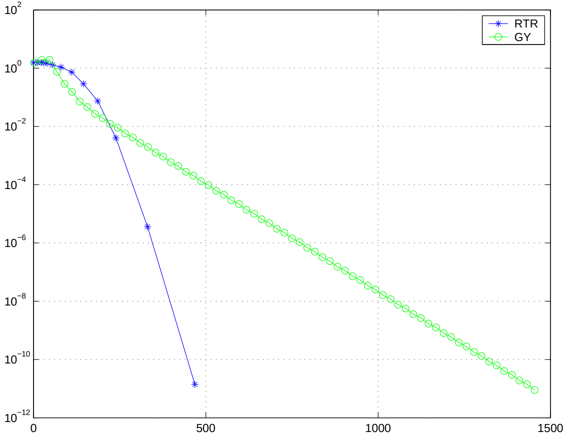
  $\rightsquigarrow$ Minimal storage of iteration vectors.

Numerical experiments: RTR vs Krylov [GY02]



Distance to target versus matrix-vector multiplications.
Symmetric/positive-definite generalized eigenvalue problem.

Conclusion: A Three-Step Approach

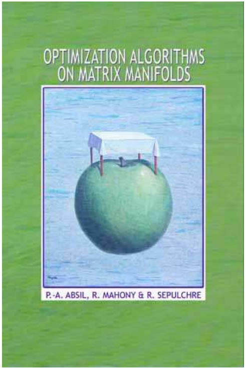
- Formulation of the computational problem as a geometric optimization problem.
- Generalization of optimization algorithms on abstract manifolds.
- Exploit flexibility and additional structure to build numerically efficient algorithms.

A few pointers

- Optimization on manifolds: Luenberger [Lue73], Gabay [Gab82], Smith [Smi93, Smi94], Udrişte [Udr94], Manton [Man02], Mahony and Manton [MM02], PAA *et al.* [ABG04, ABG07]...
- Trust-region methods: Powell [Pow70], Moré and Sorensen [MS83], Moré [Mor83], Conn *et al.* [CGT00].
- Truncated CG: Steihaug [Ste83], Toint [Toi81], Conn *et al.* [CGT00]...
- Retractions: Shub [Shu86], Adler *et al.* [ADM$^+$02]...

THE END

Optimization Algorithms on Matrix Manifolds
P.-A. Absil, R. Mahony, R. Sepulchre
Princeton University Press, January 2008



1. Introduction
2. Motivation and applications
3. Matrix manifolds: first-order geometry
4. Line-search algorithms
5. Matrix manifolds: second-order geometry
6. Newton's method
7. Trust-region methods
8. A constellation of superlinear algorithms

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