A Riemannian BFGS Method for Nonconvex Optimization Problems

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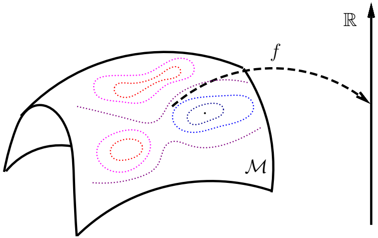
Riemannian Optimization

Constrained Problem: Given $f(x) : \mathcal{M} \to \mathbb{R}$, solve

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

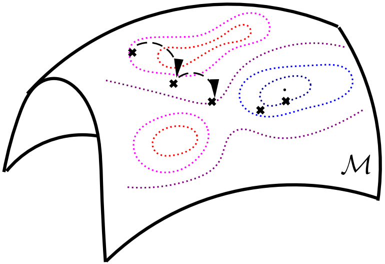
where $\mathcal{M}$ is a Riemannian manifold.

Goal Adapt unconstrained Euclidean algorithms to function on $\mathcal{M}$.

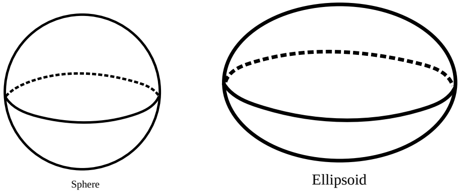


Comparison with Constrained Optimization

- All iterates on the manifold
- Convergence properties of unconstrained optimization algorithms
- No need to consider Lagrange multipliers or penalty functions
- Explore the structure of the constrained set



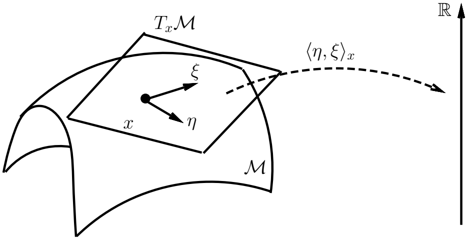
Examples of Manifolds



- Stiefel manifold: $\mathrm{St}(p, n) = \{X \in \mathbb{R}^{n \times p} | X^T X = I_p\}$
- Grassmann manifold: Set of all p-dimensional subspaces of $\mathbb{R}^n$
- Set of fixed rank matrices
- So on

Riemannian Manifolds

Roughly, a Riemannian manifold $\mathcal{M}$ is a smooth set with a smoothly-varying inner product on the tangent spaces.



An Application: Independent Component Analysis

- Determine a few independent components from a large number of samples
- Joint diagonalization on the Stiefel manifold [TCA09]

$$\min_{X \in \mathrm{St}(p,n)} f(X) = \min_{X \in \mathrm{St}(p,n)} -\sum_{i=1}^{N} \|\mathrm{diag}(X^T C_i X)\|_2^2,$$

where $\mathrm{St}(p,n) = \{X \in \mathbb{R}^{n \times p} | X^T X = I_p\}$, $\mathrm{diag}(M)$ denotes a vector formed by the diagonal entry of matrix M and $\| \cdot \|_2$ denotes the 2-norm

- $C_1, \ldots, C_N$ are covariance matrices.

Line search-based Methods

Consider the following generic update for a Euclidean line search-based optimization algorithm:

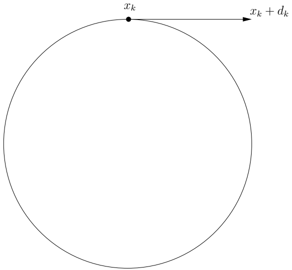
$$x_{k+1} = x_k + \alpha_k d_k \ .$$

This iteration is implemented in numerous ways, e.g.:

- Steepest descent: $d_k = -\nabla f(x_k)$
- Newton's method: $d_k = -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$

Riemannian Manifolds Provide

- Riemannian concepts describing directions and movement on the manifold
- Riemannian analogues for gradient and Hessian

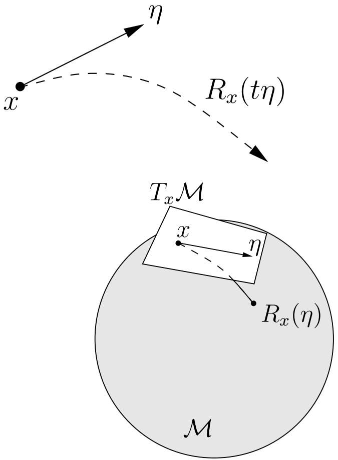


Retractions

Definition

A retraction is a mapping R from TM to M satisfying the following:

- R is continuously differentiable
- $R_x(0) = x$
- $\mathrm{D}\, R_x(0)[\eta] = \eta$



- maps tangent vectors back to the manifold
- defines curves in a direction

Euclidean	Riemannian
$x_{k+1} = x_k + \alpha_k d_k$	$x_{k+1} = R_{x_k}(\alpha_k \eta_k)$

Riemannian line search-based Methods

Riemannian Optimization Algorithm

1. At iterate $x \in M$
2. Find $\eta \in T_x M$ which satisfies certain condition.
3. Choose new iterate $x_+ = R_x(\alpha\eta)$.
4. Goto step 1.

- Riemannian steepest descent [AMS08]: $\eta = -\mathrm{grad}\, f(x)$
- Riemannian Newton [AMS08]: $\eta = -\mathrm{Hess}\, f(x)^{-1} \mathrm{grad}\, f(x)$

Riemannian Methods

In different tangent spaces

- Conjugate gradient method: $\eta_{x_{k-1}}$ and $\mathrm{grad}\, f(x_k)$
- Quasi-Newton method:
  $\mathrm{grad}\, f(x_{k-m}), \mathrm{grad}\, f(x_{k-m+1}), \ldots, \mathrm{grad}\, f(x_k)$

Vector Transport

- Vector transport: Transport a tangent vector from one tangent space to another
- $\mathcal{T}_{\eta_x}\xi_x$, denotes transport of ξ_x to tangent space of $R_x(\eta_x)$. R is a retraction associated with $\mathcal{T}$
- Isometric vector transport $\mathcal{T}_{\mathrm{S}}$ preserve the length of tangent vector

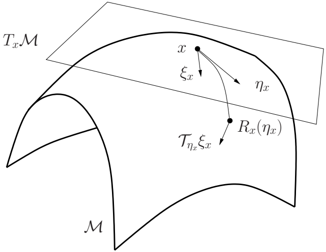


Figure: Vector transport.

BFGS methods

Results of Euclidean BFGS method:

- Converge globally to a stationary point for a strongly convex cost function
- Locally and superlinearly converge to a non-degenerate minimizer, i.e.,

$$\lim_{k\to\infty} \frac{\|x_{k+1} - x_*\|}{\|x_k - x_*\|} = 0.$$

Riemannian BFGS methods

RBFGS method by Qi [Qi11]
specific pair of retraction and vector transport
RBFGS method by Ring and Wirth [RW12]
the expression for $\mathcal{T}_{R_{\eta_x}}$
RBFGS method by Huang et. al [HGA15]
$\mathcal{T}_{R_{\eta_x}} \eta_x$ given η_x

} require

- a convex cost function
- Isometric vector transport

Vector transport by differentiated retraction

Vector transport by differentiated retraction denoted by $\mathcal{T}_R$ is defined by $\mathcal{T}_{R_{\eta_x}} \xi_x := \frac{d}{dt} R_x(\eta_x + t\xi_x)|_{t=0}$.

A New Riemannian BFGS Method

Goal

Develop a Riemannian BFGS method that does not need vector transport by differentiated retraction and convexity of the cost function.

Riemannian BFGS framework

1. At iterate $x \in M$
2. Find $\eta = -\mathcal{B}_k^{-1} \mathrm{grad}\, f(x_k) \in T_x M$, where $\mathcal{B}_k$ is updated by a formula $\mathcal{B}_{k+1} = \psi(\mathcal{B}_k, y_k, s_k)$ (See [HGA15] for details), where $y_k, s_k \in T_{x_k}\mathcal{M}$. (Euc: $y_k = \mathrm{grad}\, f(x_{k+1}) - \mathrm{grad}\, f(x_k)$, $s_k = x_{k+1} - x_k$)
3. Choose new iterate $x_+ = R_x(\alpha\eta)$, where α is a step size satisfying certain condition.
4. Goto step 1.

A New Riemannian BFGS Method

- Why is $\mathcal{T}_R$ used?

  Line search: $h(t) = f(R_x(t\eta_x))$, $h'(t) = \langle \mathrm{grad}\, f(R_x(t\eta_x)), \mathcal{T}_{R_{t\eta_x}} \eta_x \rangle$

- Line search: [BN89, (3.2), (3.3)] require the step size α_k satisfy either

$$h_k(\alpha_k) - h_k(0) \leq -\chi_1 \frac{h_k'(0)^2}{\|\eta_k\|^2} \quad (1)$$

or

$$h_k(\alpha_k) - h_k(0) \leq \chi_2 h_k'(0), \quad (2)$$

where $h_k(t) = f(R_{x_k}(t\eta_k))$, χ_1 and χ_2 are positive constants.

A New Riemannian BFGS Method: Avoid $\mathcal{T}_R$

- If the gradient of f is Lipschitz continuous [AMS08, Definition 7.4.1], then above line search condition is implied by, e.g.,
    - The Goldstein condition
    - The Wolfe condition
    - The Armijo-Goldstein condition

A New Riemannian BFGS Method: For nonconvex problem

- Is a modification on Riemannian BFGS method required for nonconvex problem?

  Yes, an example is given in [Dai13], which shows that BFGS method fails to converge for a nonconvex cost function.

- How to make Riemannian BFGS method work for nonconvex problem?

  Multiple ideas exist for Euclidean BFGS, e.g., [LF01a, LF01b].

A New Riemannian BFGS Method: For nonconvex problem

- For BFGS method, a Riemannian version of [Pow76, Lemma 2] holds, i.e.,

$$\frac{\|y_k\|^2}{\langle y_k, s_k \rangle} \text{ is bounded above} \Rightarrow \liminf_{k \to \infty} \|\mathrm{grad}\, f(x_k)\| = 0.$$

- For nonconvex problem, $\frac{\|y_k\|^2}{\langle y_k, s_k \rangle}$ is not bounded above in general.
- Cautious BFGS update: [LF01b]

$$\mathcal{B}_{k+1} = \begin{cases} \psi(\mathcal{B}_k, y_k, s_k), & \text{if } \frac{\langle y_k, s_k \rangle}{\|s_k\|^2} \geq \vartheta(\|\mathrm{grad}\, f(x_k)\|) \\ \mathcal{T}_{S_{s_k}} \circ \mathcal{B}_k \circ \mathcal{T}_{S_{s_k}}^{-1} \text{ or id}, & \text{otherwise}, \end{cases} \tag{3}$$

where ϑ is a monotone increasing function satisfying $\vartheta(0) = 0$ and ϑ is strictly increasing at 0.

A New Riemannian BFGS Method: Theoretical Results

Global convergence

Under some reasonable assumptions, the iterates $\{x_k\}$ generated by the RBFGS method satisfies

$$\liminf_{k\to\infty} \|\mathrm{grad}\, f(x_k)\| = 0.$$

Superlinear convergence

Under some reasonable assumptions, the cautious BFGS update reduces to ordinary BFGS update around a non-degenerate minimizer and the superlinear convergence holds, i.e.,

$$\lim_{k\to\infty} \frac{\mathrm{dist}(x_{k+1}, x_*)}{\mathrm{dist}(x_k, x_*)} = 0.$$

A New Riemannian BFGS Method

Summary:

- Vector transport by differentiated retraction is not required
- Global convergence is guaranteed for nonconvex cost function
- Superlinear convergence is guaranteed

Limited memory version of this Riemannian BFGS (LRBFGS) can be obtained.

Experiments

Problem: Joint diagonalization on the Stiefel manifold [TCA09]

$$\min_{X \in \mathrm{St}(p,n)} -\sum_{i=1}^{N} \|\mathrm{diag}(X^T C_i X)\|_2^2.$$

- Riemannian BFGS with the Armijo-Goldstein condition

$$h_k(\alpha_k) \leq h_k(0) + \sigma \alpha_k h_k'(0),$$

  where α_k is the largest value in the set $\{1, \varrho, \varrho^2, \varrho^3, \ldots\}$, $0 < \varrho < 1$ and $0 < \sigma < 0.5$.
    - An isometric vector transport is sufficient.
    - isometric vector transport [HGA15, Section 4.1]
    - The implementation of this vector transport is identity

Experiments

- Riemannian BFGS with the Wolfe condition [HGA15]

$$h_k(\alpha_k) \leq h_k(0) + c_1 \alpha_k h_k'(0)$$
$$h_k'(\alpha_k) \geq c_2 h_k'(0)$$

  where $0 < c_1 < 0.5 < c_2 < 1$.

  - The isometric vector transport is required to satisfies $\mathcal{T}_{\mathrm{S}_\xi} \xi = \beta \mathcal{T}_{R_\xi} \xi, \quad \beta = \frac{\|\xi\|}{\|\mathcal{T}_{R_\xi} \xi\|}, \forall \xi \in T_x \mathcal{M}$
  - isometric vector transport [HGA15, Sections 2.3.1 and 5]
  - The implementation of this vector transport is a rank-two update

Parameters and Settings

$$\min_{X \in \mathrm{St}(p,n)} -\sum_{i=1}^{N} \|\mathrm{diag}(X^T C_i X)\|_2^2,$$
$$\mathrm{St}(p,n) = \{X \in \mathbb{R}^{n\times p} | X^T X = I_p\}.$$

- $p = 8$, and $n = 12$
- Stopping criterion: $\|\mathrm{grad}\, f(x_k)\| / \|\mathrm{grad}\, f(x_0)\| < 10^{-6}$
- C++ with compiler g++-4.7 on 64 bit Ubuntu platform with 3.6GHz CPU

Results

Table: An average of 1000 random runs of RBFGS. LS denotes line search condition. VT denotes vector transport

N	LS	VT	iter	nf	ng	nV	t (millisecond)
32	Armijo	identity	183	198	184	365	9.89
	Armijo	rank-2	133	150	134	266	12.3
	Wolfe	rank-2	129	146	132	390	13.1
128	Armijo	identity	190	207	191	380	25.7
	Armijo	rank-2	141	159	142	281	25.8
	Wolfe	rank-2	137	156	141	414	25.8
512	Armijo	identity	196	216	197	393	90.9
	Armijo	rank-2	148	167	149	295	77.7
	Wolfe	rank-2	143	164	148	432	75.8

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The relative efficiency depends on the relative cost on vector transport and cost function evluation

Conclusion

- Combine the line search in [BN89] and the cautious BFGS update in [LF01b] and generalize them to the Riemannian setting.
- Global convergence for a nonconvex cost function
- Superlinear convergence rate
- Vector transport by differentiated retraction not required
- Code: `www.math.fsu.edu/~whuang2/ROPTLIB`

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