Stochastic gradient descent on Riemannian manifolds

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Introduction

- We proposed a stochastic gradient algorithm on a specific manifold for matrix regression in:
- *Regression on fixed-rank positive semidefinite matrices: a Riemannian approach*, Meyer, Bonnabel and Sepulchre, Journal of Machine Learning Research, 2011.
- Compete(ed) with (then) state of the art for low-rank Mahalanobis distance and kernel learning
- Convergence then left as an open question
- The material of today's presentation is the paper *Stochastic gradient descent on Riemannian manifolds*, IEEE Trans. on Automatic Control, in press, preprint on Arxiv.

Outline

1. Stochastic gradient descent
   - Introduction and examples
   - SGD and machine learning
   - Standard convergence analysis (due to L. Bottou)
2. Stochastic gradient descent on Riemannian manifolds
   - Introduction
   - Results
3. Examples

Classical example

Linear regression: Consider the linear model

$$y = x^T w + \nu$$

where $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$.

- examples: $z = (x, y)$
- measurement error (loss):

$$Q(z, w) = (y - \hat{y})^2 = (y - x^T w)^2$$

- cannot minimize total loss $C(w) = \int Q(z, w) dP(z)$
- minimize empirical loss instead $C_n(w) = \frac{1}{n} \sum_{i=1}^{n} Q(z_i, w)$.

Gradient descent

Batch gradient descent : process all examples together

$$w_{t+1} = w_t - \gamma_t \nabla_w \left(\frac{1}{n} \sum_{i=1}^{n} Q(z_i, w_t) \right)$$

Stochastic gradient descent: process examples one by one

$$w_{t+1} = w_t - \gamma_t \nabla_w Q(z_t, w_t)$$

for some random example $z_t = (x_t, y_t)$.

$\Rightarrow$ well known identification algorithm for Wiener systems, ARMAX systems etc.

Stochastic versus online

Stochastic: examples drawn randomly from a finite set

- SGD minimizes the empirical loss

Online: examples drawn with unknown $dP(z)$

- SGD minimizes the expected loss (+ tracking property)

Stochastic approximation: approximate a sum by a stream of single elements

Stochastic versus batch

SGD can converge very slowly: for a long sequence

$$\nabla_w Q(z_t, w_t)$$

may be a very bad approximation of

$$\nabla_w C_n(w_t) = \nabla_w \left(\frac{1}{n} \sum_{i=1}^{n} Q(z_i, w_t) \right)$$

SGD can converge very fast when there is redundancy

- extreme case $z_1 = z_2 = \cdots$

Some examples

Least mean squares: Widrow-Hoff algorithm (1960)

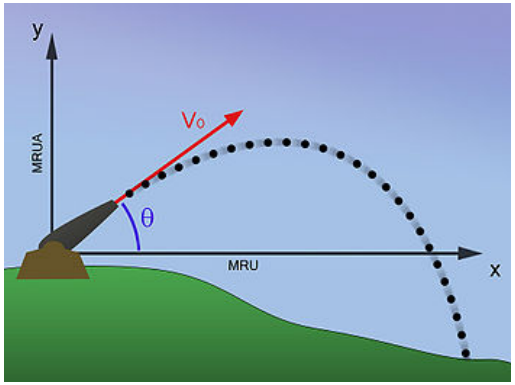
- Loss: $Q(z, w) = (y - \hat{y})^2$
- Update: $w_{t+1} = w_t - \gamma_t \nabla_w Q(z_t, w_t) = w_t - \gamma_t (y_t - \hat{y}_t) x_t$

Robbins-Monro algorithm (1951): C smooth with a unique minimum $\Rightarrow$ the algorithm converges in L^2

k-means: McQueen (1967)

- Procedure: pick z_t, attribute it to w^k
- Update: $w^k_{t+1} = w^k_t + \gamma_t (z_t - w^k_t)$

Some examples



Ballistics example (old). Early adaptive control

- optimize the trajectory of a projectile in fluctuating wind.
- successive gradient corrections on the launching angle
- with $\gamma_t \to 0$ it will stabilize to an optimal value

Filtering approach: tradeoff noise/convergence speed

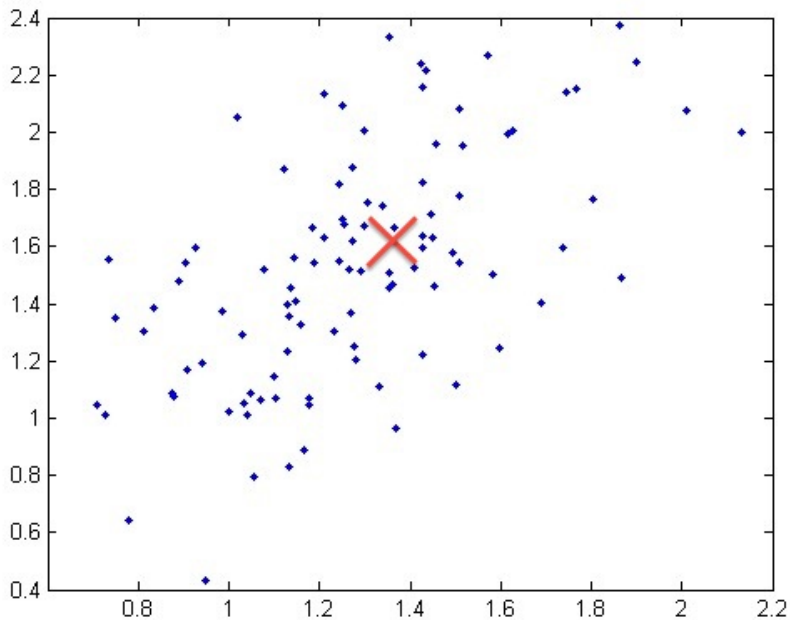
- "Optimal" rate $\gamma_t = 1/t$ (Kalman filter)

Another example: mean

Computing a mean: Total loss $\frac{1}{n}\sum_i \|z_i - w\|^2$

Minimum: $w - \frac{1}{n}\sum_i z_i = 0$ i.e. w is the mean of the points z_i

Stochastic gradient: $w_{t+1} = w_t - \gamma_t(w_t - z_i)$ where z_i randomly picked[2]



[2] what if $\|\|$ is replaced with some more exotic distance ?

Outline

Learning on large datasets

Machine learning problems: in many cases "learn" an input to output function $f : x \mapsto y$ from a training set

Large scale problems: randomly picking the data is a way to handle ever-increasing datasets

Bottou and Bousquet helped popularize SGD for large scale machine learning

Outline

Notation

Expected total loss:

$$C(w) := E_z(Q(z, w)) = \int Q(z, w)dP(z)$$

Approximated gradient under the event z denoted by $H(z, w)$

$$E_z H(z, w) = \nabla(\int Q(z, w)dP(z)) = \nabla C(w)$$

Stochastic gradient update: $w_{t+1} \leftarrow w_t - \gamma_t H(z_t, w_t)$

Convergence results

Convex case: known as Robbins-Monro algorithm. Convergence to the global minimum of $C(w)$ in mean, and almost surely.

Nonconvex case. $C(w)$ is generally not convex. We are interested in proving

- almost sure convergence
- a.s. convergence of $C(w_t)$
- ... to a local minimum
- $\nabla C(w_t) \to 0$ a.s.

Provable under a set of reasonable assumptions

Assumptions

Learning rates: the steps must decrease. Classically

$$\sum \gamma_t^2 < \infty \quad \text{and} \quad \sum \gamma_t = +\infty$$

The sequence $\gamma_t = \frac{1}{t}$ has proved optimal in various applications

Cost regularity: averaged loss $C(w)$ 3 times differentiable (relaxable).

Sketch of the proof

1. confinement: w_t remains a.s. in a compact.
2. convergence: $\nabla C(w_t) \to 0$ a.s.

Confinement

Main difficulties:

1. Only an approximation of the cost is available
2. We are in discrete time

Approximation: the noise can generate unbounded trajectories with small but nonzero probability.

Discrete time: even without noise yields difficulties as there is no line search.

SO ? : confinement to a compact holds under a set of assumptions: well, see the paper[3] ...

[3] L. Bottou: Online Algorithms and Stochastic Approximations. 1998.

Convergence (simplified)

Confinement

- All trajectories can be assumed to remain in a compact set
- All continuous functions of w_t are bounded

Convergence

Letting $h_t = C(w_t) > 0$, second order Taylor expansion:

$$h_{t+1} - h_t \leq -2\gamma_t H(z_t, w_t)\nabla C(w_t) + \gamma_t^2 \|H(z_t, w_t)\|^2 K_1$$

with K_1 upper bound on $\nabla^2 C$.

Convergence (simplified)

We have just proved

$$h_{t+1} - h_t \leq -2\gamma_t H(z_t, w_t)\nabla C(w_t) + \gamma_t^2 \|H(z_t, w_t)\|^2 K_1$$

Conditioning w.r.t. $F_t = \{z_0, \cdots, z_{t-1}, w_0, \cdots, w_t\}$

$$E[h_{t+1} - h_t | F_t] \leq \underbrace{-2\gamma_t \|\nabla C(w_t)\|^2}_{\text{this term} \leq 0} + \gamma_t^2 E_z(\|H(z_t, w_t)\|^2) K_1$$

Assume for some $A > 0$ we have $E_z(\|H(z_t, w_t)\|^2) < A$. Using that $\sum \gamma_t^2 < \infty$ we have

$$\sum E[h_{t+1} - h_t | F_t] \leq \sum \gamma_t^2 A K_1 < \infty$$

As $h_t \geq 0$ from a theorem by Fisk (1965) h_t converges a.s. and $\sum |E[h_{t+1} - h_t | F_t]| < \infty$.

Convergence (simplified)

$$E[h_{t+1} - h_t | F_t] \leq -2\gamma_t \|\nabla C(w_t)\|^2 + \gamma_t^2 E_z(\|H(z_t, w_t)\|^2) K_1$$

Both red terms have convergent sums from Fisk's theorem. Thus so does the blue term

$$0 \leq \sum_t 2\gamma_t \|\nabla C(w_t)\|^2 < \infty$$

Using the fact that $\sum \gamma_t = \infty$ we have[4]

$\nabla C(w_t)$ converges a.s. to 0.

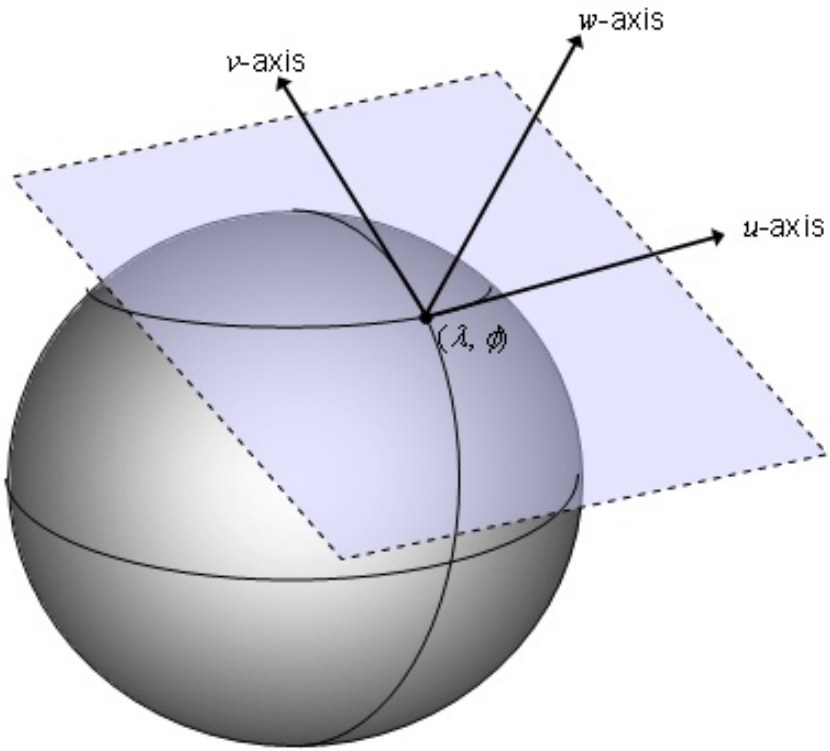
[4] as soon as $\|\nabla C(w_t)\|$ is proved to converge.

Outline

Connected Riemannian manifold

Riemannian manifold: local coordinates around any point

Tangent space:



Riemmanian metric: scalar product $\langle u, v \rangle_g$ on the tangent space

Riemannian manifolds

Riemannian manifold carries the structure of a metric space whose distance function is the arclength of a minimizing path between two points. Length of a curve $c(t) \in \mathcal{M}$

$$L = \int_a^b \sqrt{\langle \dot{c}(t), \dot{c}(t) \rangle_g} dt = \int_a^b \|\dot{c}(t)\| dt$$

Geodesic: curve of minimal length joining sufficiently close x and y.

Exponential map: $\exp_x(v)$ is the point $z \in \mathcal{M}$ situated on the geodesic with initial position-velocity (x, v) at distance $\|v\|$ of x.

Consider $f : \mathcal{M} \to \mathbb{R}$ twice differentiable.

Riemannian gradient: tangent vector at x satisfying

$$\frac{d}{dt}|_{t=0} f(\exp_x(tv)) = \langle v, \nabla f(x) \rangle_g$$

Hessian: operator $\nabla_x^2 f$ such that

$$\frac{d}{dt}|_{t=0} \langle \nabla f(\exp_x(tv)), \nabla f(\exp_x(tv)) \rangle_g = 2\langle \nabla f(x), (\nabla_x^2 f)v \rangle_g.$$

Second order Taylor expansion:

$$f(\exp_x(tv)) - f(x) \leq t\langle v, \nabla f(x) \rangle_g + \frac{t^2}{2}\|v\|_g^2 k$$

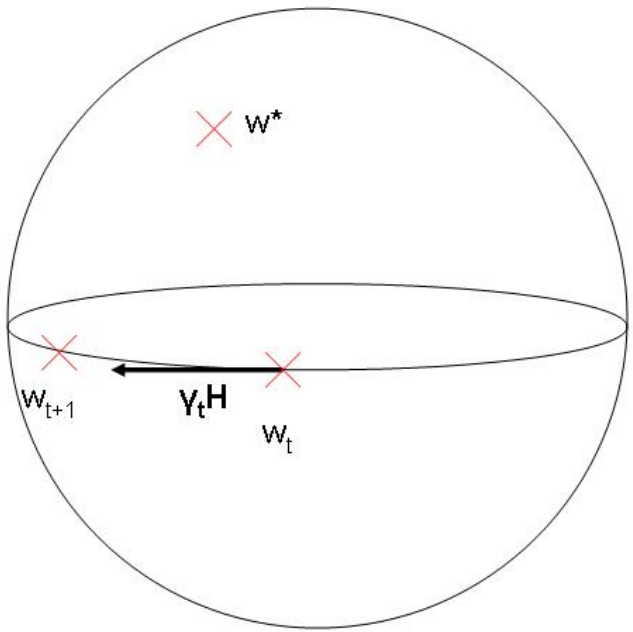
where k is a bound on the hessian along the geodesic.

Riemannian SGD on $\mathcal{M}$

Riemannian approximated gradient: $E_z(H(z_t, w_t)) = \nabla C(w_t)$

Stochastic gradient descent on $\mathcal{M}$: update

$$w_{t+1} \leftarrow \exp_{w_t}(-\gamma_t H(z_t, w_t))$$



Outline

Convergence

Using the same maths but on manifolds, we have proved:

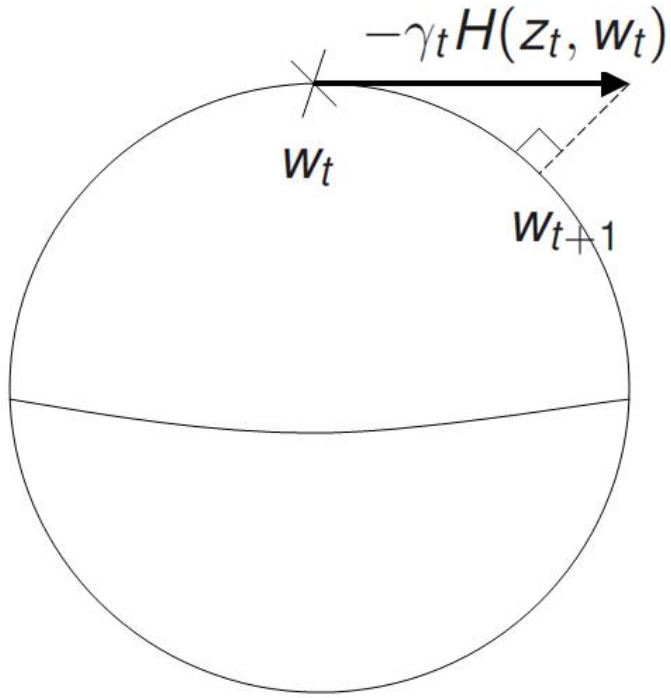
Theorem 1: confinement and a.s. convergence hold under hard to check assumptions linked to curvature.

Theorem 2: if the manifold is compact, the algorithm is proved to a.s. converge under unrestrictive conditions.

Theorem 3: Same as Theorem 2, where a first order approximation of the exponential map is used.

Theorem 3

Example of first-order approximation of the exponential map:



The theory is still valid ! (as the step $\to 0$)

Outline

General method

Four steps:

1. identify the manifold and the cost function involved
2. endow the manifold with a Riemannian metric and an approximation of the exponential map
3. derive the stochastic gradient algorithm
4. analyze the set defined by $\nabla C(w) = 0$.

Considered examples

- Oja algorithm and dominant subspace tracking
- Matrix geometric means
- Amari's natural gradient
- Learning of low-rank matrices
- Consensus and gossip on manifolds

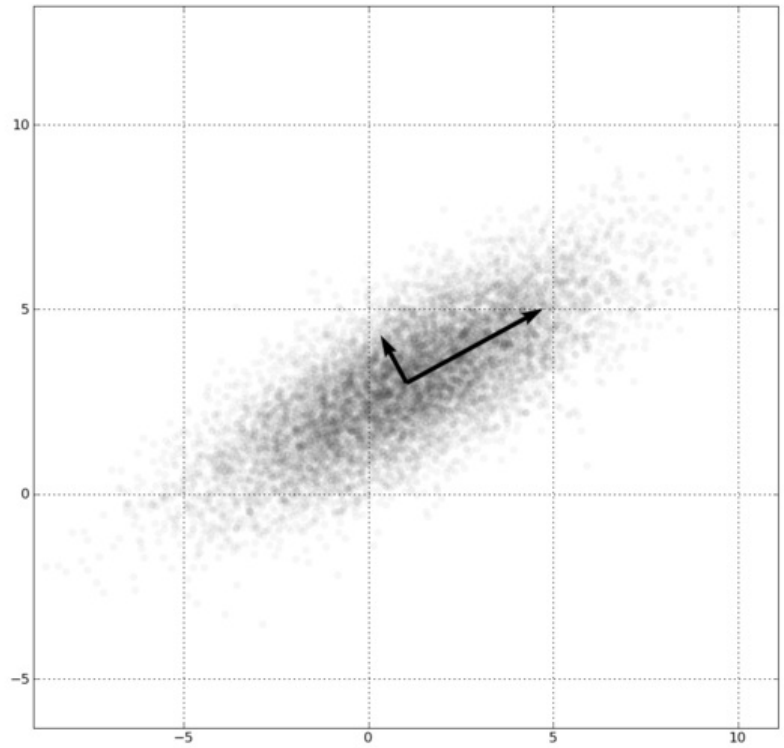
Oja's flow and online PCA

Online principal component analysis (PCA): given a stream of vectors $z_1, z_2, \cdots$ with covariance matrix

$$E(z_t z_t^T) = \Sigma$$

identify online the r-dominant subspace of Σ.

Goal: reduce online the dimension of input data entering a processing system to discard linear combination with small variances. Applications in data compression etc.



Oja's flow and online PCA

Search space: $V \in \mathbb{R}^{r \times d}$ with orthonormal columns. VV^T is a projector identified with an element of the Grassman manifold possessing a natural metric.

Cost: $C(V) = -\mathrm{Tr}(V^T \Sigma V) = E_z \| VV^T z - z \|^2 + cst$

Riemannian gradient: $(I - V_t V_t^T) z_t z_t^T V_t$

Exponential approx: $R_V(\Delta) = V + \Delta$ plus orthonormalisation

Oja flow for subspace tracking is recovered

$V_{t+1} = V_t - \gamma_t (I - V_t V_t^T) z_t z_t^T V_t$ plus orthonormalisation.

Convergence is recovered within our framework (Theorem 3).

Considered examples

- Oja algorithm and dominant subspace tracking
- Positive definite matrix geometric means
- Amari's natural gradient
- Learning of low-rank matrices
- Decentralized covariance matrix estimation

Filtering in the cone $P^+(n)$

Vector-valued image and tensor computing

Results of several filtering methods on a 3D DTI of the brain[5]:

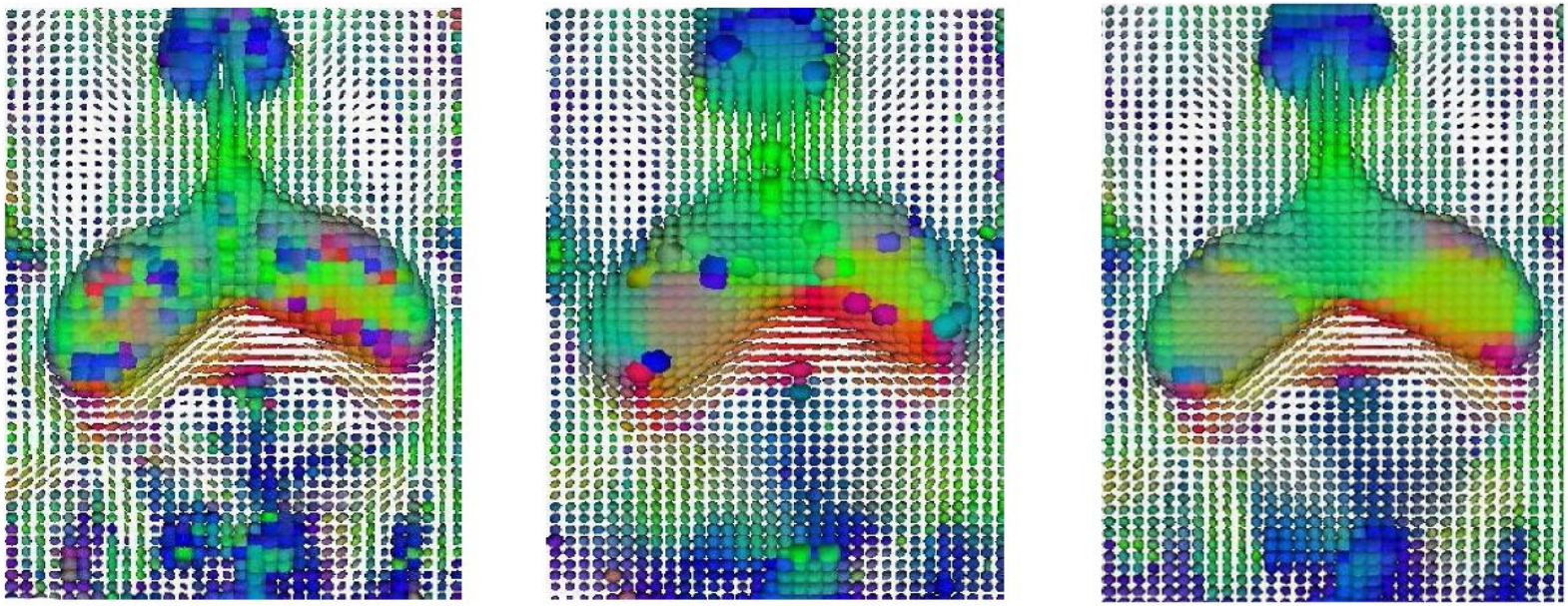


Figure: Original image “Vectorial" filtering “Riemannian" filtering

[5] Courtesy from Xavier Pennec (INRIA Sophia Antipolis)

Riemannian mean in the cone[6]

Right notion of mean in the cone ? Essential to optimization, filtering, interpolation, fusion, completion, learning, ..

Natural metric of the cone allows to define an interesting geometric mean as the midpoint of the geodesics

Generalization to the mean of N positive definite matrices $Z_1, \cdots Z_N$?

Karcher mean: minimizer of $C(W)=\sum_{i=1}^{N} d^2(Z_i, W)$ where d is the geodesic distance.

[6] Ando et al. (2004), Moakher (2005), Petz and Temesi (2005), Smith (2006), Arsigny et al. (2007), Barbaresco (2008), Bhatia (2006) . . .

Matrix geometric means

No closed form solution of the Karcher mean problem.

A Riemannian SGD algorithm was recently proposed[7].

SGD update: at each time pick Z_i and move along the geodesic with intensity $\gamma_t d(W, Z_i)$ towards Z_i

Critical points of ∇C: the Karcher mean exists and is unique under a set of assumptions.

Convergence can be recovered within our framework.

[7] Arnaudon, Marc; Dombry, Clement; Phan, Anthony; Yang, Le *Stochastic algorithms for computing means of probability measures* Stochastic Processes and their Applications (2012)

Considered examples

- Oja algorithm and dominant subspace tracking
- Positive definite matrix geometric means
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Amari's natural gradient

Natural gradient works efficiently in learning
SI **Amari** - Neural computation, 1998 - MIT Press
When a parameter space has a certain underlying structure, the ordinary **gradient** of a function does not represent its steepest direction, but the **natural gradient** does. Inform geometry is used for calculating the **natural** gradients in the parameter space of ...
Cité 1358 fois - Autres articles - Les 19 versions

Considered problem: z_t are realizations of a parametric model with parameter $w \in \mathbb{R}^n$ and joint pdf $p(z, w)$. Let

$$Q(z, w) = l(z, w) = -\log(p(z, w))$$

Cramer-Rao bound: let $\hat{w}$ be an estimator of the true parameter w^* based on k realizations $z_1, \cdots, z_k$. We have

$$\mathbb{E}[(\hat{w} - w^*)(\hat{w} - w^*)^T] \geq \frac{1}{k} G(w^*)^{-1}$$

with G the FIM $G(w) = -\mathbb{E}_z[(\nabla_w^E l(z, w))(\nabla_w^E l(z, w))^T]$

Amari's natural gradient

Riemannian manifold: $\mathcal{M} = \mathbb{R}^n$.

Fisher Information (Riemannian) Metric at w:

$$\langle u, v \rangle = u^T G(w) v$$

Riemannian gradient of $Q(z, w)$

$$\nabla_w(l(z, w)) = G^{-1}(w) \nabla_w^E l(z, w)$$

Exponential approximation: simple addition $R_w(u) = w + u$.
Taking $\gamma_t = 1/t$ we recover the celebrated

Amari's natural gradient: $w_{t+1} = w_t - \frac{1}{t} G^{-1}(w_t) \nabla_w^E l(z_t, w_t)$.

Amari's gradient: conclusion

- Amari's main result: natural gradient is a simple method that asympt. achieves statistical efficiency (i.e. reaches Cramer Rao bound)
- Amari's gradient fits in our framework
- a.s. convergence is recovered
- This completes our results in this specific case.

Considered examples

- Oja algorithm and dominant subspace tracking
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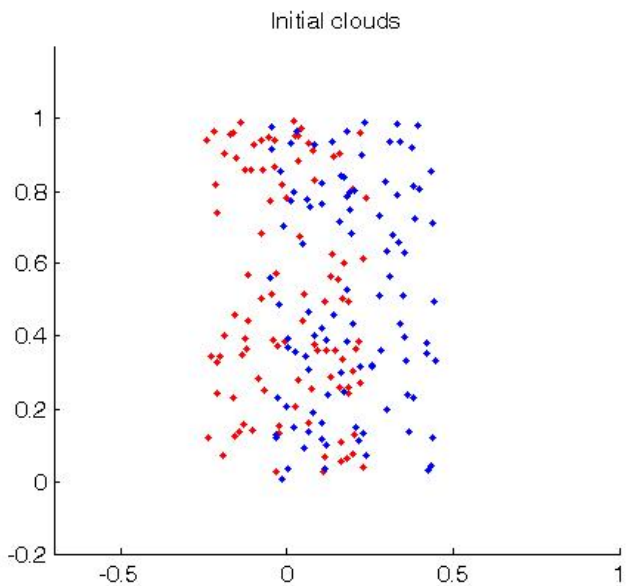
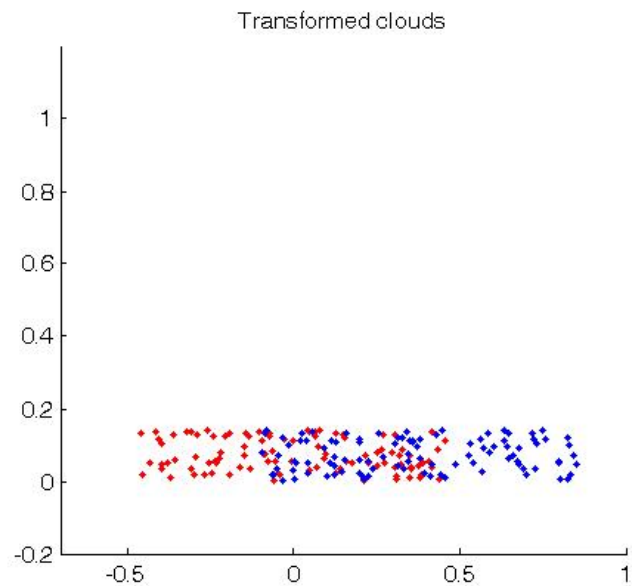
Mahalanobis distance: parameterized by a positive semidefinite matrix W

$$d_W^2(x_i, x_j) = (x_i - x_j)^T W (x_i - x_j)$$

Statistics: W is the inverse of the covariance matrix

Learning: Let $W = GG^T$. Then d_W^2 simple Euclidian squared distance for transformed data $\tilde{x}_i = Gx_i$. Used for classification

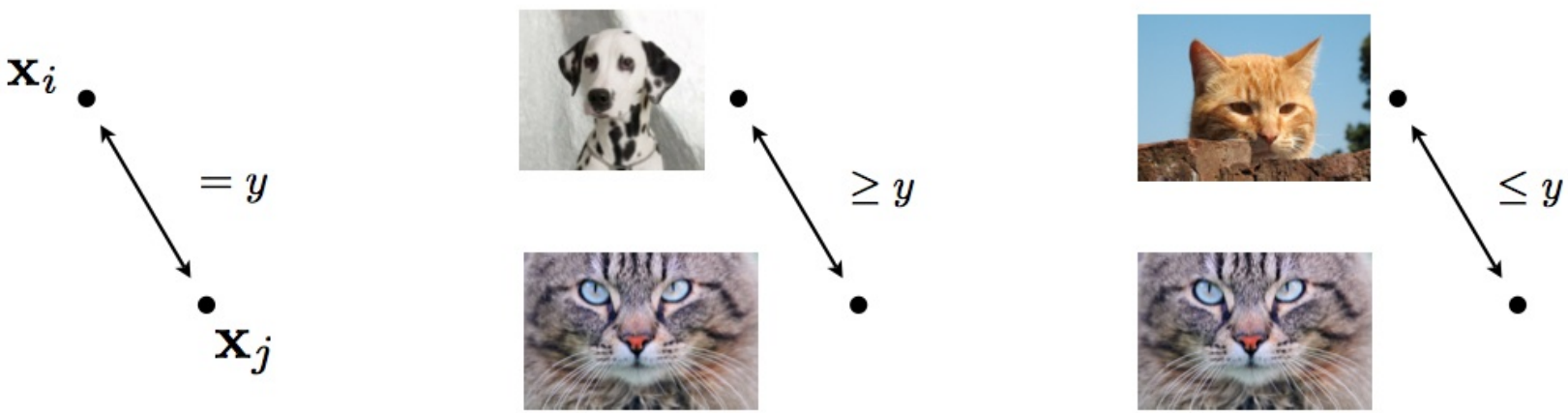




Mahalanobis distance learning

Goal: integrate new constraints to an existing W

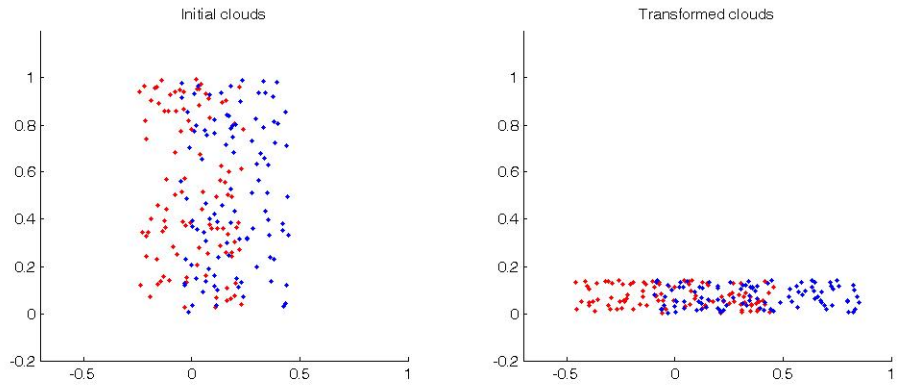
- equality constraints: $d_W(x_i, x_j) = y$
- similarity constraints: $d_W(x_i, x_j) \leq y$
- dissimilarity constraints: $d_W(x_i, x_j) \geq y$



Computational cost significantly reduced when W is low rank !

Interpretation and method

One could have projected everything on a horizontal axis ! For large datasets low rank allows to derive algorithm with linear complexity in the data space dimension d.



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Geometry of $S^+(d, r)$

Semi-definite positive matrices of fixed rank

$$S^+(d, r) = \{W \in \mathbb{R}^{d \times d}, W = W^T, W \succeq 0, \text{rank W} = r\}$$

Problem formulation: $y_t = d_W(x_i, x_j)$, loss: $E((\hat{y} - y)^2)$

Problem: $W - \gamma_t \nabla_W((\hat{y} - y)^2)$ has NOT same rank as W.

Remedy: work on the manifold !

Considered examples

- Oja algorithm and dominant subspace tracking
- Positive definite matrix geometric means
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- Decentralized covariance matrix estimation

Decentralized covariance estimation

Set up: Consider a sensor network, each node i having computed its own empirical covariance matrix $W_{i,0}$ of a process.

Goal: Average out the fluctuations by finding an average covariance matrix.

Constraints: limited communication, bandwith etc.

Gossip method: two random neighboring nodes communicate and set their values equal to the average of their current values.
$\Rightarrow$ should converge to a meaningful average.

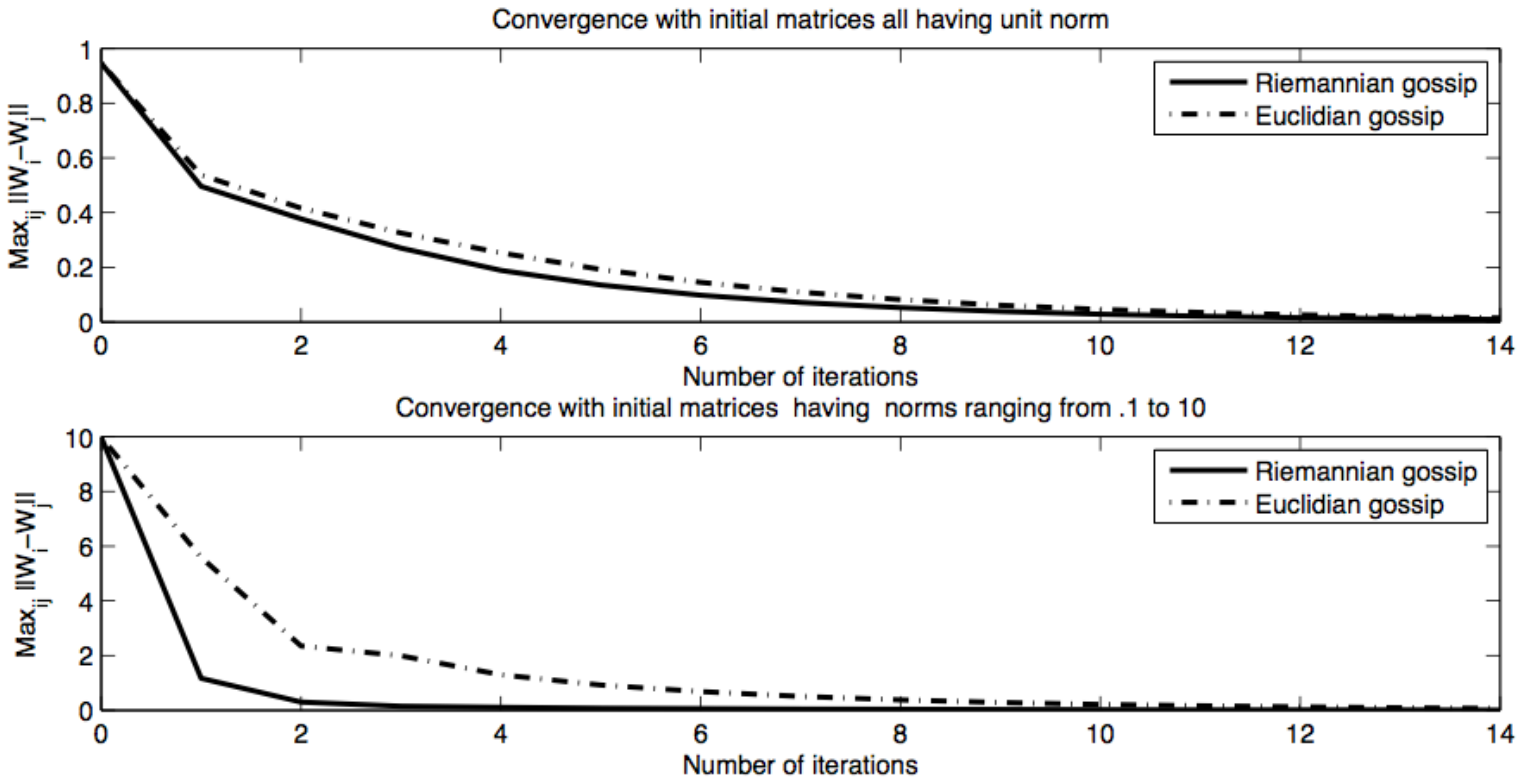
Alternative average why not the midpoint in the sense of Fisher-Rao distance (leading to Riemannian SGD)

$$d(\Sigma_1, \Sigma_2) \approx KL(\mathcal{N}(0, \Sigma_1) \,||\, \mathcal{N}(0, \Sigma_2))$$

Example: covariance estimation

Conventional gossip at each step the usual average $\frac{1}{2}(W_{i,t} + W_{j,t})$ is a covariance matrix, so the algorithms can be compared.

Results: the proposed algorithm converges much faster !



Conclusion

We proposed an intrinsic SGD algorithm. Convergence was proved under reasonable assumptions. The method has numerous applications.

Future work includes:

- better understand consensus on hyperbolic spaces
- adapt several results of the literature to the manifold SGD case: speed of convergence, case of a strongly convex cost, non-differentiability of the cost, search for global minimum etc.
- tackle new applications