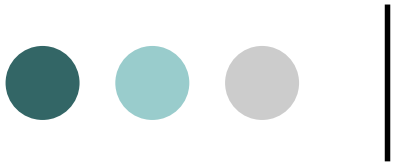

Applications of geometric optimisation techniques to engineering problems

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overview

- **What is geometric optimisation?**

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- **Ex 1: Blind Source Separation (BSS)**

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- What is geometric optimisation?
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- dominant eigenspaces of matrix pencils (LDA)

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- Ex 1: Blind Source Separation (BSS)
- Independent Component Analysis (ICA)
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- Ex 3: time series clustering

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- “on-the-fly” geometry

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- “on-the-fly” geometry
- state of the art and open problems

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What is geometric optimisation?

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Given a real valued function

$$f : M \longrightarrow \mathbb{R},\ x \mapsto f(x)$$

defined on some geometric object M, here a smooth manifold, find a method to compute (if it exists)

$$x_* := \operatorname*{argmin}_{x \in M} f(x)$$

that utilises the (local) geometry of M.

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Ex 1: Blind Source Separation

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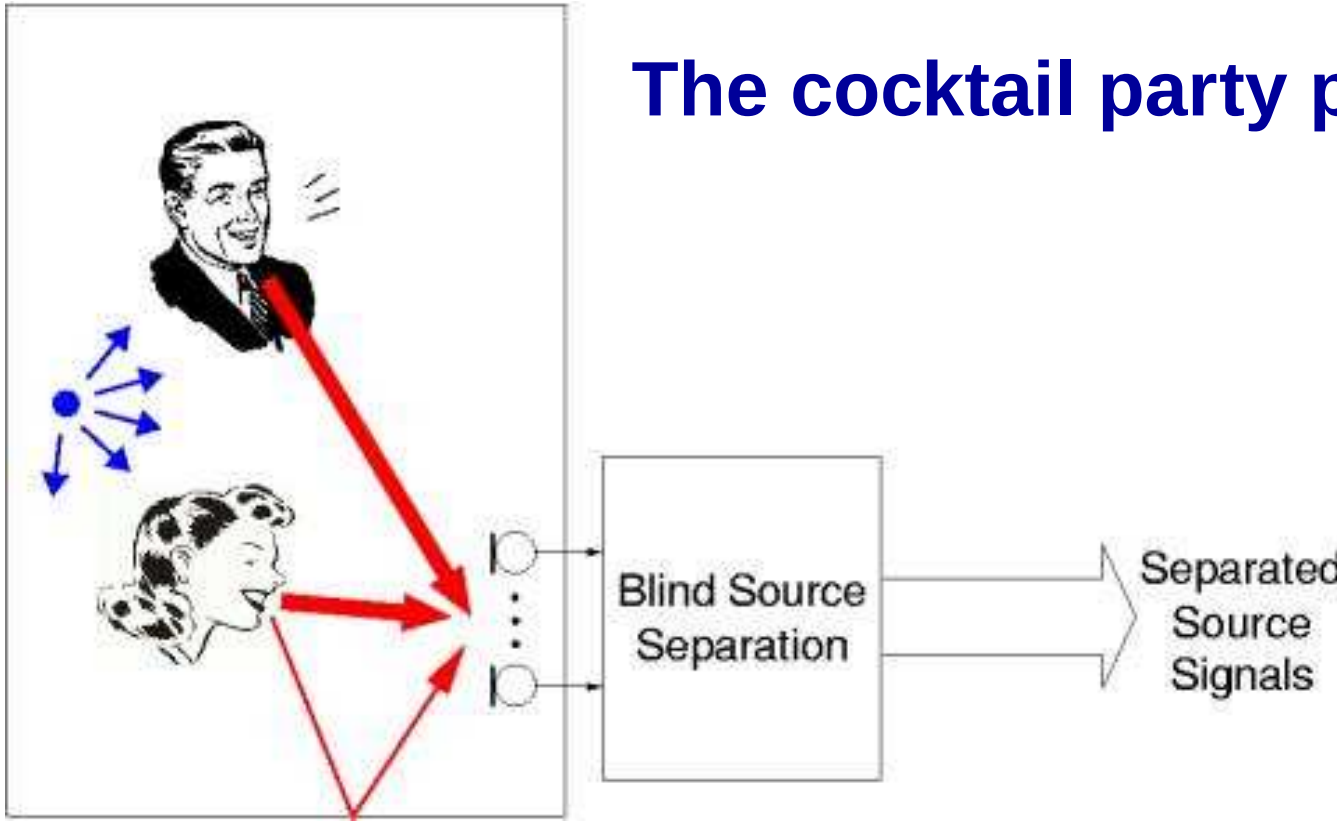

The cocktail party problem.

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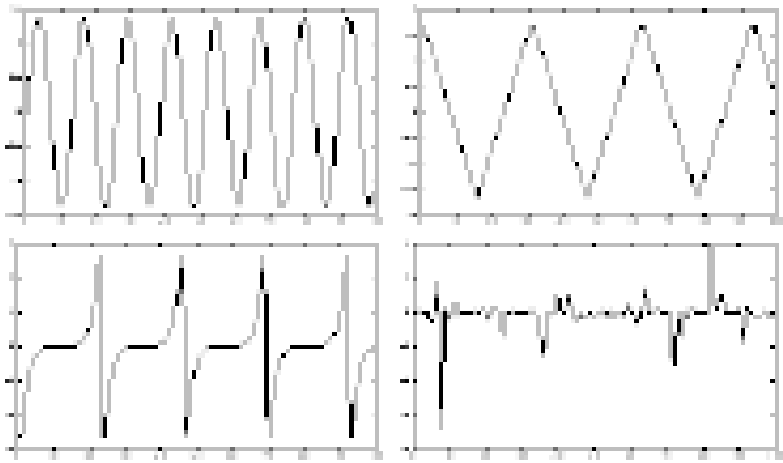
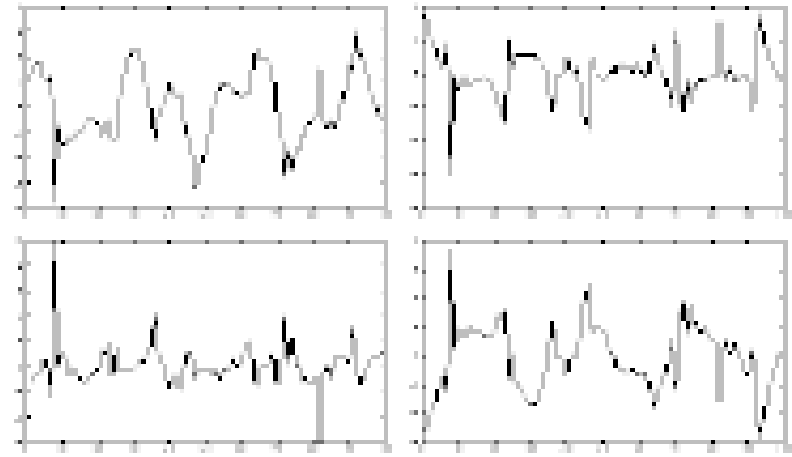
Image: http://www.lnt.de/LMS/research/projects/BSS

Ex 1: Blind Source Separation



source signals



observed mixtures

audio, EEG, MEG, fMRI, wireless, ...

Image: http://www.cis.hut.fi/aapo/papers/NCS99web/node17.html

BSS – the model

Individual signals ($i = 1, \ldots, d$)

$$x_i : [0, T] \longrightarrow \mathbb{R},\ t \mapsto x_i(t)$$

are being uniformly sampled and the samples collected into row vectors

$$x_i = \begin{pmatrix} x_i(t_0) & x_i(t_0 + \Delta) & \ldots & x_i(t_0 + (N-1) \cdot \Delta) \end{pmatrix}$$

which are then stacked into a matrix

$$X = \begin{pmatrix} x_1 \\ \vdots \\ x_d \end{pmatrix} \in \mathbb{R}^{d \times N}.$$

BSS – the model

It is assumed that there are as many source signals as observed signals and that they are related by

$$X_o = M \cdot X_s$$

where $X_o, X_s \in \mathbb{R}^{d \times N}$ **and** $M \in \mathrm{GL}_d(\mathbb{R})$**.**

BSS – the model

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$$X_o = M \cdot X_s$$

where $X_o, X_s \in \mathbb{R}^{d \times N}$ **and** $M \in \mathrm{GL}_d(\mathbb{R})$**.**

Task: Find X_s **(or** M^{-1}**) from knowing** X_o **subject to some plausible criterion.**

BSS as ICA problem

We treat the columns of X_o as i.i.d. samples of an observed random variable vector Y given by

$$Y = M \cdot X$$

where X is the unknown random variable source vector.

BSS as ICA problem

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We treat the columns of X_o as i.i.d. samples of an observed random variable vector Y given by

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where X is the unknown random variable source vector.

The ICA paradigm is now that the components of X, i.e. the individual signals, are mutually independent.

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BSS as ICA problem

Hence, we are trying to find the invertible M that makes the components of the corresponding X "as independent as possible".

BSS as ICA problem

Hence, we are trying to find the invertible M that makes the components of the corresponding X "as independent as possible".

Note: The matrix M in

$$Y = M \cdot X$$

is identifiable up to scaling and permutations if and only if the components of X are mutually independent and at most one of them is Gaussian.

BSS as ICA problem

A computational trick is centering and prewhitening: multiply by the square root of the covariance matrix of Y (assuming finite second moments) to obtain

$$Y = Q \cdot X$$

where $Q \in \mathrm{O}_d(\mathbb{R})$ and X and Y are zero mean and unit variance.

BSS as ICA problem

A computational trick is centering and prewhitening: multiply by the square root of the covariance matrix of Y (assuming finite second moments) to obtain

$$Y = Q \cdot X$$

where $Q \in \mathrm{O}_d(\mathbb{R})$ and X and Y are zero mean and unit variance.

Note: Prewhitening from samples works best in the Gaussian case ...

see IEEE TSP, 53(10):3625–3632, 2005

ICA as geometric optimisation problem

We arrive at the geometric optimisation problem of minimising mutual information between the components of $Q^\top Y$ over $Q \in \mathrm{O}_d(\mathbb{R})$.

ICA as geometric optimisation problem

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One-unit FastICA maximises $\mathbb{E}[G(q^\top Y)]$ over $q \in S^{d-1}$ where $G : \mathbb{R} \longrightarrow \mathbb{R}$, $z \mapsto \frac{1}{a} \log \cosh(az)$ is a contrast function.

The expectation is computed from samples, the optimisation method is an approximate Newton on manifold algorithm.

http://www.cis.hut.fi/aapo/papers/IJCNN99_tutorialweb

Ex 2: face recognition

Image: IEEE TPAMI, 23(2):228–233, 2001

face recognition – the model

An image is represented as a vector $X \in \mathbb{R}^t$. Images are divided in c classes with N_j images X_i^j, $i = 1, \ldots, N_j$ in class $j = 1, \ldots, c$.

face recognition – the model

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Consider the within-class scatter matrix

$$S_w = \sum_{i,j} (X_i^j - \mu_j)(X_i^j - \mu_j)^\top$$

and the between-class scatter matrix

$$S_b = \sum_{j} (\mu_j - \mu)(\mu_j - \mu)^\top.$$

face recognition as LDA problem

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Orthogonally projecting the image vectors into a lower dimensional space $Y = Q^\top X$ yields projected scatter matrices $Q^\top S_{\{w,b\}} Q$.

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face recognition as LDA problem

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The aim is to maximise $\frac{\det(Q^\top S_b Q)}{\det(Q^\top S_w Q)}$ over $Q \in \mathrm{St}(d,t)$, the orthogonal Stiefel manifold.

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This amounts to finding the dominant d-dimensional eigenspace of the pencil (S_b, S_w).

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LDA as geometric optimisation problem

Given a symmetric/positive-definite matrix pencil (A, B) with eigenvalues ($Ax = \lambda Bx$) $\lambda_1 \geq \cdots \geq \lambda_d > \lambda_{d+1} \geq \cdots \geq \lambda_n$ the unique d-dimensional dominant eigenspace is the unique global maximum of

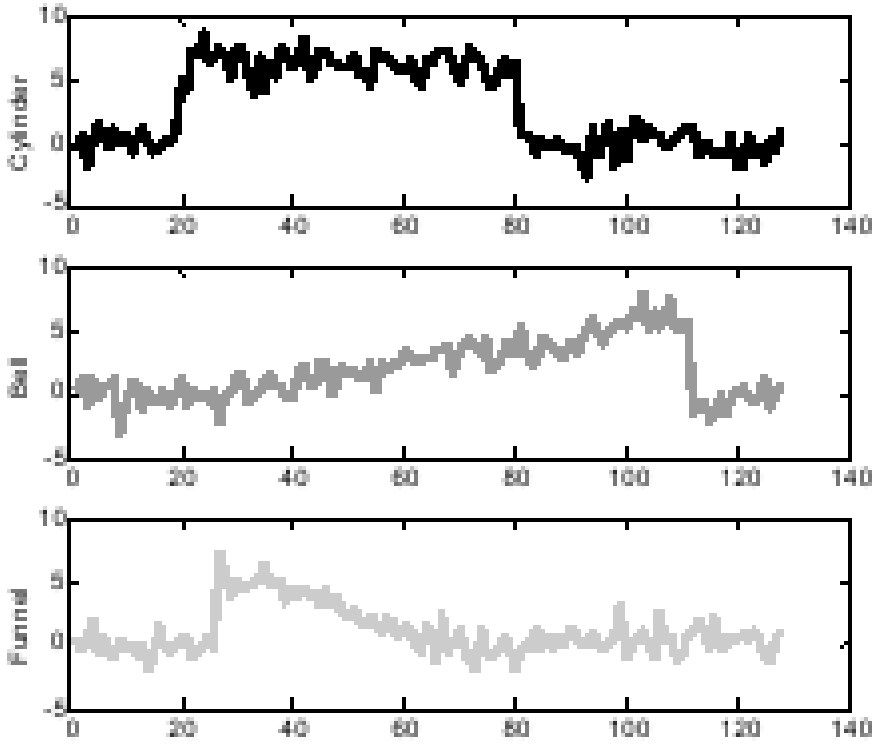
$$f : \mathrm{Grass}(d, n) \longrightarrow \mathbb{R}, \ [Q] \mapsto \mathrm{tr}(Q^\top AQ(Q^T BQ)^{-1})$$

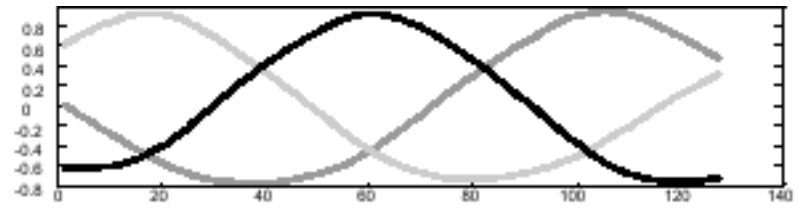
Ex 3: time-series clustering

A time series is a (finite) sequence $\{x_t\}_{t=1,\ldots,N}$ of vectors (in $\mathbb{R}^n$), e.g. arising from (sampling) a trajectory of a dynamical system.
A popular method of time-series clustering works in delay space

$$\left\{ \left(\begin{array}{c} x_p \\ x_{p-1} \\ \vdots \\ x_{p-l+1} \end{array} \right) \middle| \; p = l, \ldots, N \right\}$$

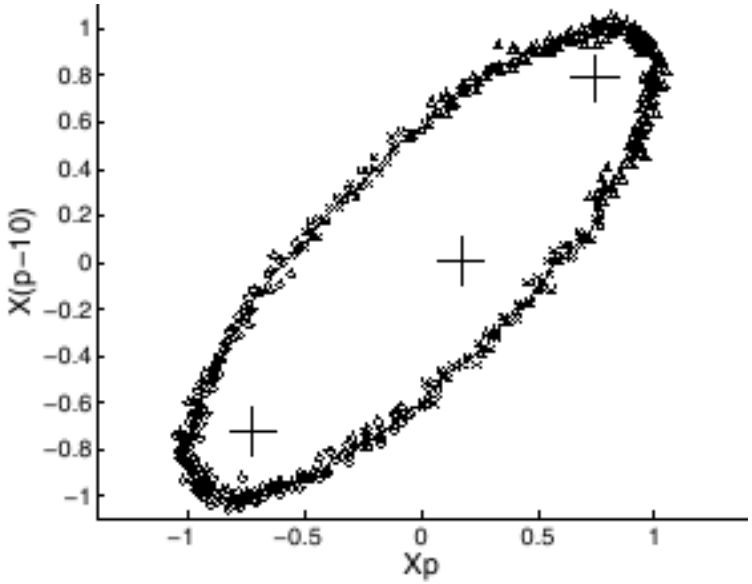
Ex 3: time-series clustering

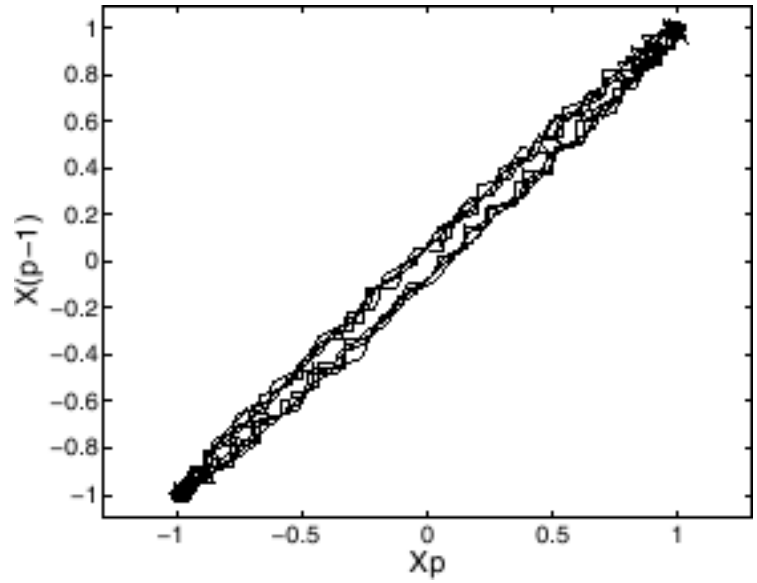




Knowl. Inf. Syst., 8(2):154-177, 2005

Ex 3: time-series clustering





ICDM 2005, pp. 114–121

state of the art

Let $\mathcal{M}$ be a d-dimensional Riemannian manifold and let $f : \mathcal{M} \to \mathbb{R}$ be smooth.

The derivative of f at $x \in \mathcal{M}$ is a linear form

$$\mathrm{D}\, f(x) : T_x\mathcal{M} \to \mathbb{R}$$

A point $x^* \in \mathcal{M}$ is called a critical point of f if

$$\mathrm{D}\, f(x^*)\xi = 0, \qquad \forall \xi \in T_{x^*}\mathcal{M}.$$

state of the art

Fact: $x^* \in \mathcal{M}$ is a strict local minimum of f if

(a) x^* is a critical point of f,

(b) the Hessian form

$$\operatorname{hess} f(x^*) : T_{x^*}\mathcal{M} \times T_{x^*}\mathcal{M} \to \mathbb{R}$$

is positive definite.

state of the art

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Geodesics of $\mathcal{M}$**:** $\forall x \in \mathcal{M}$ **and** $\xi \in T_x\mathcal{M}$

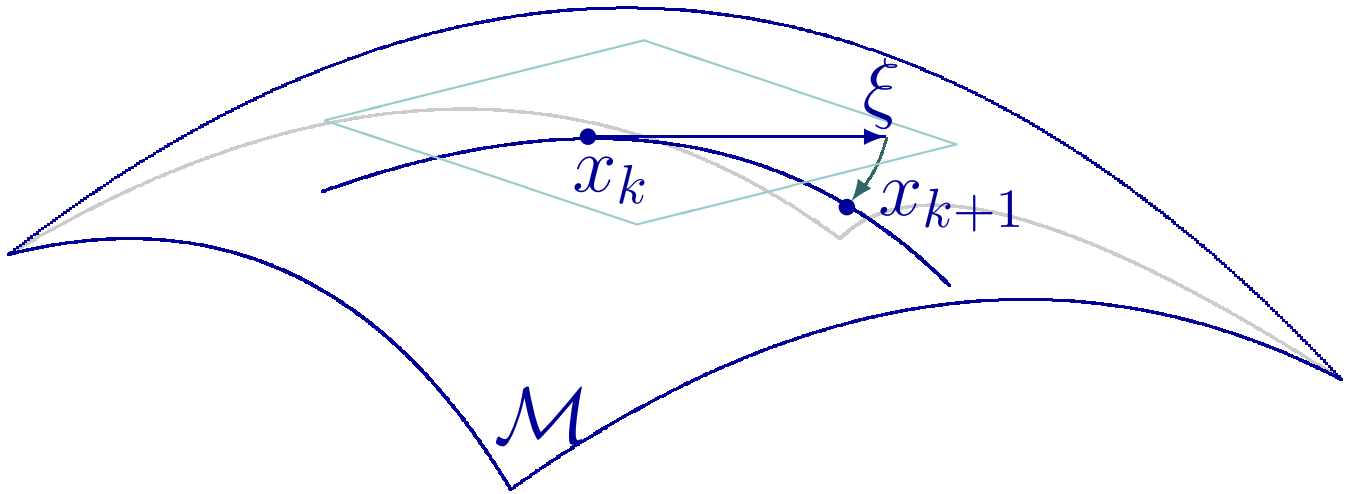
$$\gamma_x : \mathbb{R} \supset (-\varepsilon, \varepsilon) \to \mathcal{M}, \qquad \varepsilon \mapsto \gamma_x(\varepsilon)$$

such that $\gamma_x(0) = x$ **and** $\dot{\gamma}_x(0) = \xi$**.**

state of the art

Riemannian Newton direction $\xi \in T_x\mathcal{M}$ by solving

$$\operatorname{hess} f(x) \cdot \xi = \operatorname{grad} f(x)$$



state of the art

Local parameterisation of $\mathcal{M}$ around $x \in \mathcal{M}$

$$\mu_x : \mathbb{R}^d \to \mathcal{M}, \quad \kappa \mapsto \mu_x(\kappa); \qquad \mu_x(0) = x$$

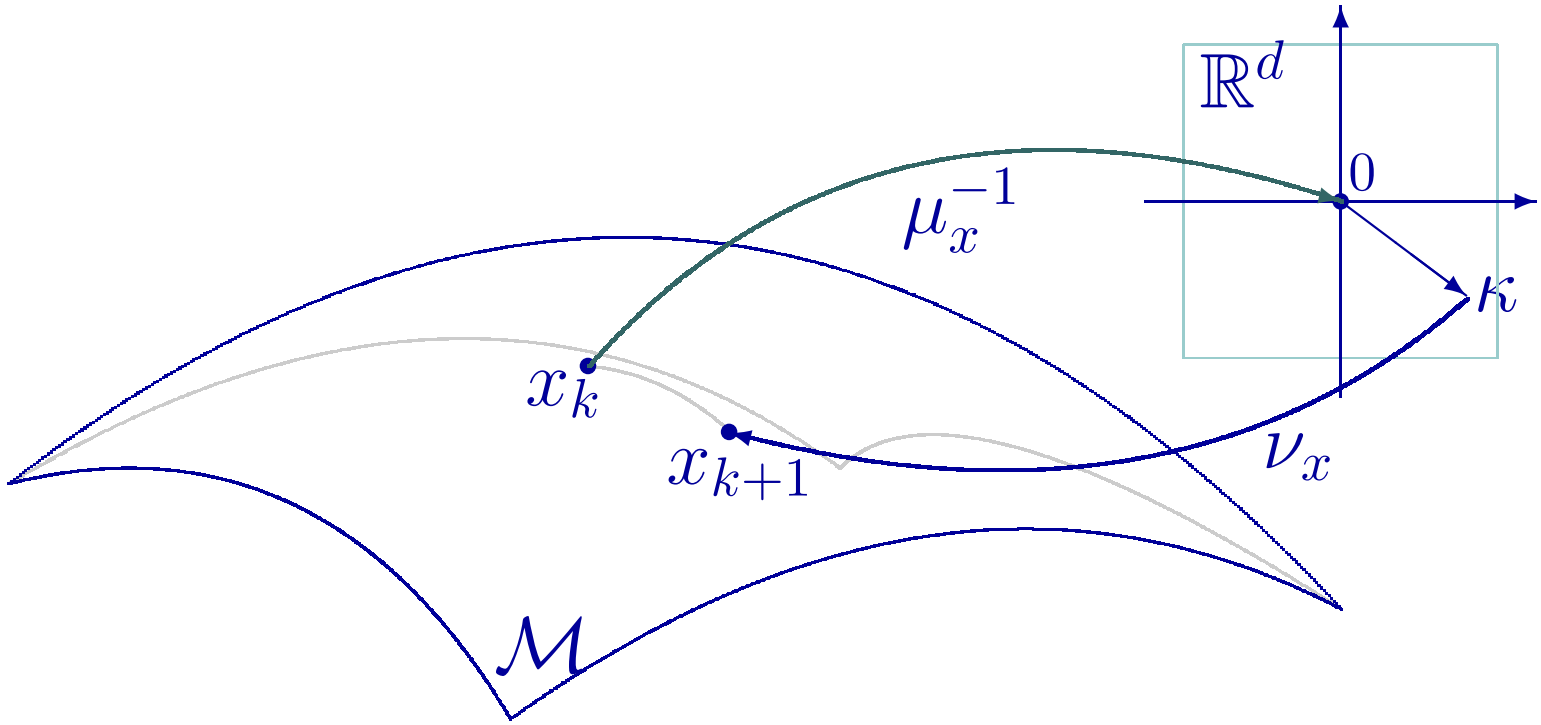
Construct locally

$$f \circ \mu_x : \mathbb{R}^d \to \mathbb{R}$$

Euclidean Newton direction $\kappa \in \mathbb{R}^d$ by solving

$$\mathcal{H}(f \circ \mu_x)(0)\kappa = \nabla(f \circ \mu_x)(0)$$

state of the art



state of the art

Let $x^* \in \mathcal{M}$ be a nondegenerate critical point. Let $\{\mu_x\}_{x\in\mathcal{M}}$ and $\{\nu_x\}_{x\in\mathcal{M}}$ be locally smooth around x^*. Consider the following iteration on $\mathcal{M}$

$$x_0 \in \mathcal{M},\ x_{k+1} = \nu_{x_k}\left(N_{f\circ\mu_{x_k}}(0)\right) \qquad \text{(N)}$$

Theorem: (Hüper-T.) Under the condition

$$\mathrm{D}\,\mu_{x^*}(0) = \mathrm{D}\,\nu_{x^*}(0)$$

there exists an open neighborhood $V \subset \mathcal{M}$ of x^* such that the point sequence generated by (N) converges quadratically to x^* provided $x_0 \in V$.

state of the art

- **know how to construct computable families of coordinate charts for St, Grass**
- **can deal with approximate Newton**
- **local convergence theory for more general iterations (Manton-T.)**
- **some global convergence results of trust region on manifold schemes**

trust-region methods

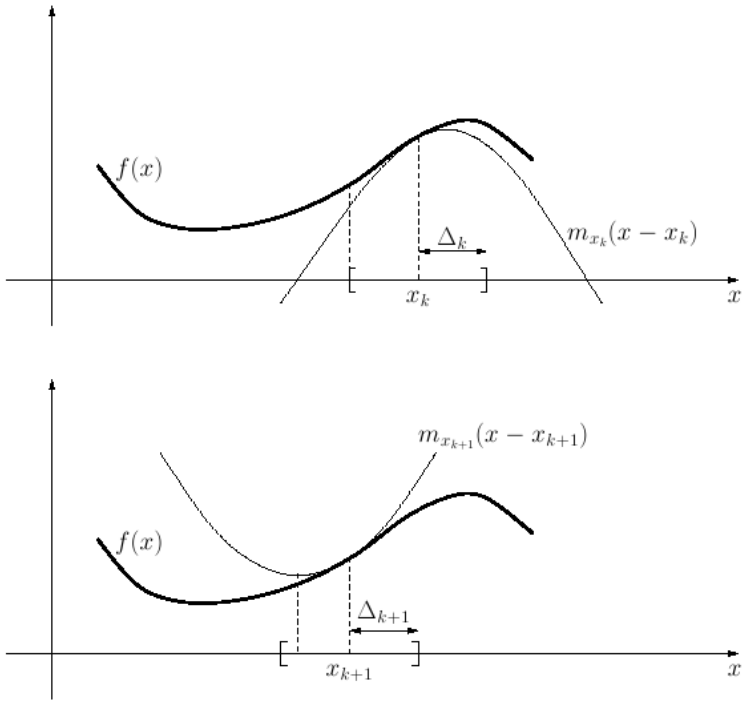


Image: http://www.inma.ucl.ac.be/~blondel/workshops/2004/Absil.pdf

state of the art – ICA

One-unit ICA problem as an optimisation problem on S^{d-1}

$$f : S^{d-1} \to \mathbb{R}, \quad q \mapsto \mathbb{E}[G(q^\top Y)].$$

Geodesics, gradient, Hessian (Hüper-Shen)

$$\gamma_q : \mathbb{R} \to S^{d-1}, \quad \varepsilon \mapsto \exp\left(\varepsilon(\xi q^\top - q\xi^\top)\right) q.$$

$$\operatorname{grad} f(q) = \left(I - qq^\top\right) \mathbb{E}[G'(q^\top Y)\, Y]$$

$$\operatorname{hess} f(q) \cdot \xi = \Big(\underbrace{\mathbb{E}[G''(q^\top Y) Y Y^\top]}_{\in \mathbb{R}^{d\times d}} - \underbrace{\mathbb{E}[G'(q^\top Y) q^\top Y]}_{\in \mathbb{R}}\, I \Big) \cdot \xi$$

state of the art – ICA

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Alternative to geodesics on S^{d-1}

$$\rho_q : \mathbb{R} \to S^{d-1}, \quad \varepsilon \mapsto \frac{q + \varepsilon\xi}{\|q + \varepsilon\xi\|}$$

ANICA as a selfmap on S^{d-1}

$$q \mapsto \frac{\frac{1}{\tau(q)}(\mathbb{E}[G'(q^\top Y)Y] - \mathbb{E}[G''(q^\top Y)]q)}{\|\frac{1}{\tau(q)}(\mathbb{E}[G'(q^\top Y)Y] - \mathbb{E}[G''(q^\top Y)]q)\|},$$

where

$$\tau : S^{d-1} \mapsto \mathbb{R}, \quad \tau(q) := \mathbb{E}[G'(q^\top Y)q^\top Y] - \mathbb{E}[G''(q^\top Y)]$$

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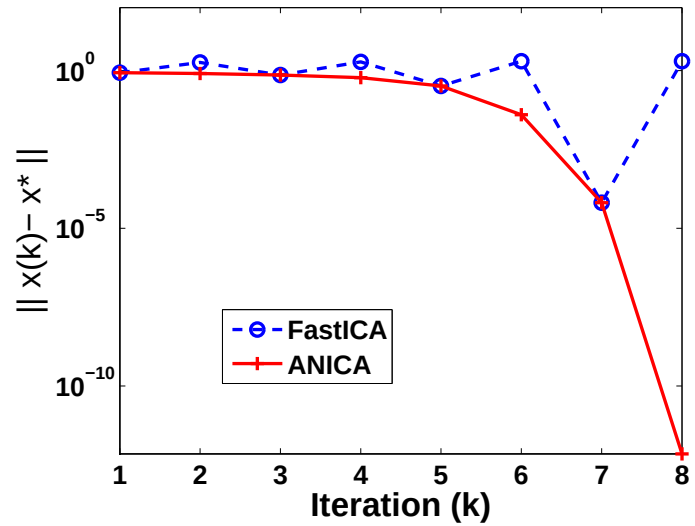
state of the art – ICA

FastICA vs ANICA



state of the art – ICA

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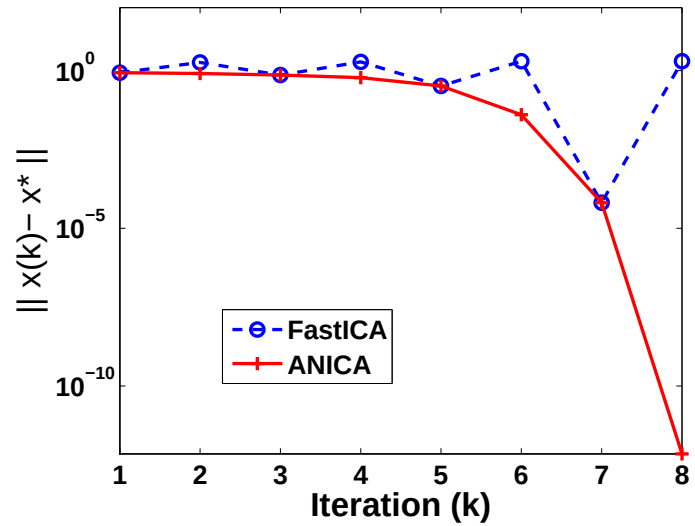
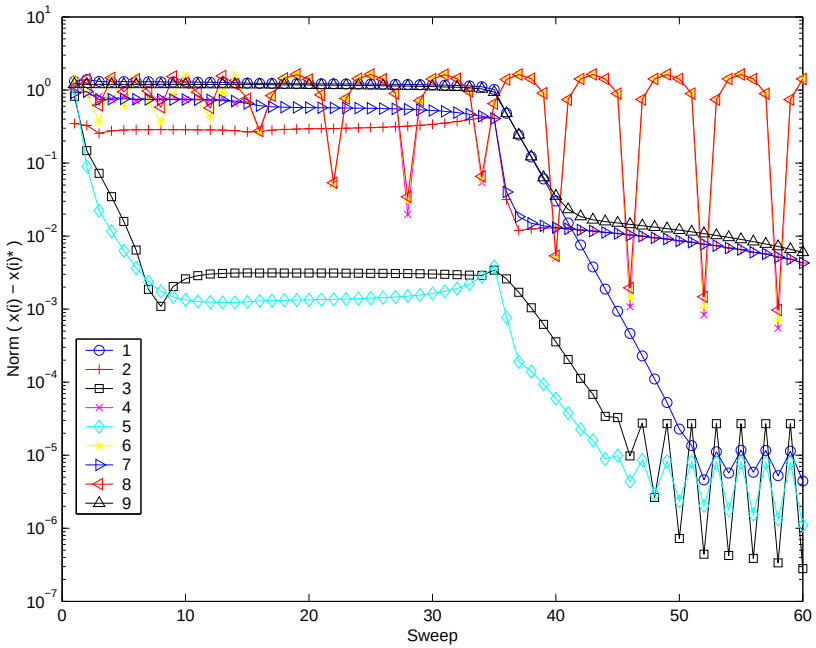
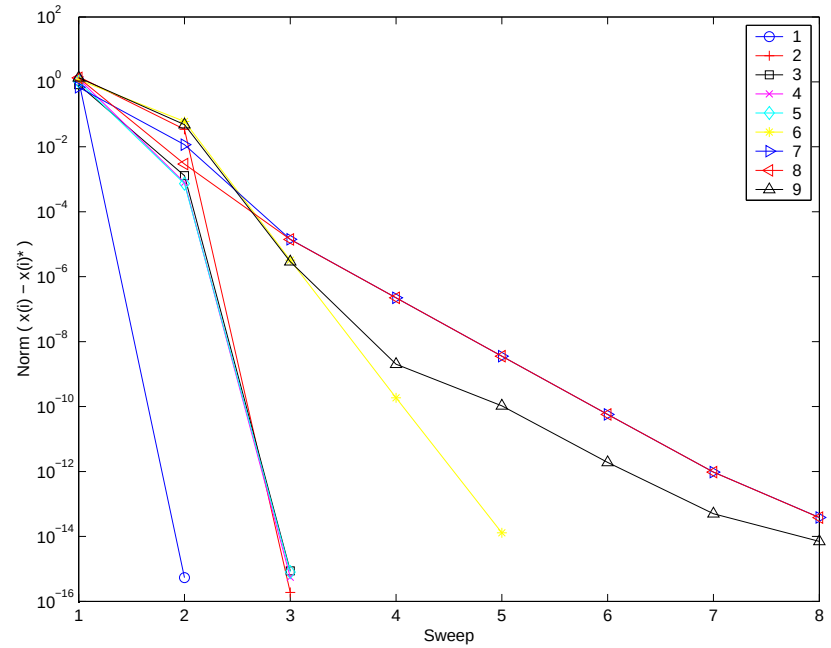


Parallel version (ANLICA, Hüper-Shen) with cost function

$$f : \mathrm{O}_d(\mathbb{R}) \longrightarrow \mathbb{R}, \qquad Q \longmapsto \sum_{i=1}^{m} \mathbb{E}[G(q_i^\top Y)]$$

state of the art – ICA





Parallel FastICA **ANLICA**

the end

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Thank you.

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