Optimization on manifolds

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Optimization On Manifolds

What ?

Why ?

How ?

Optimization On Manifolds

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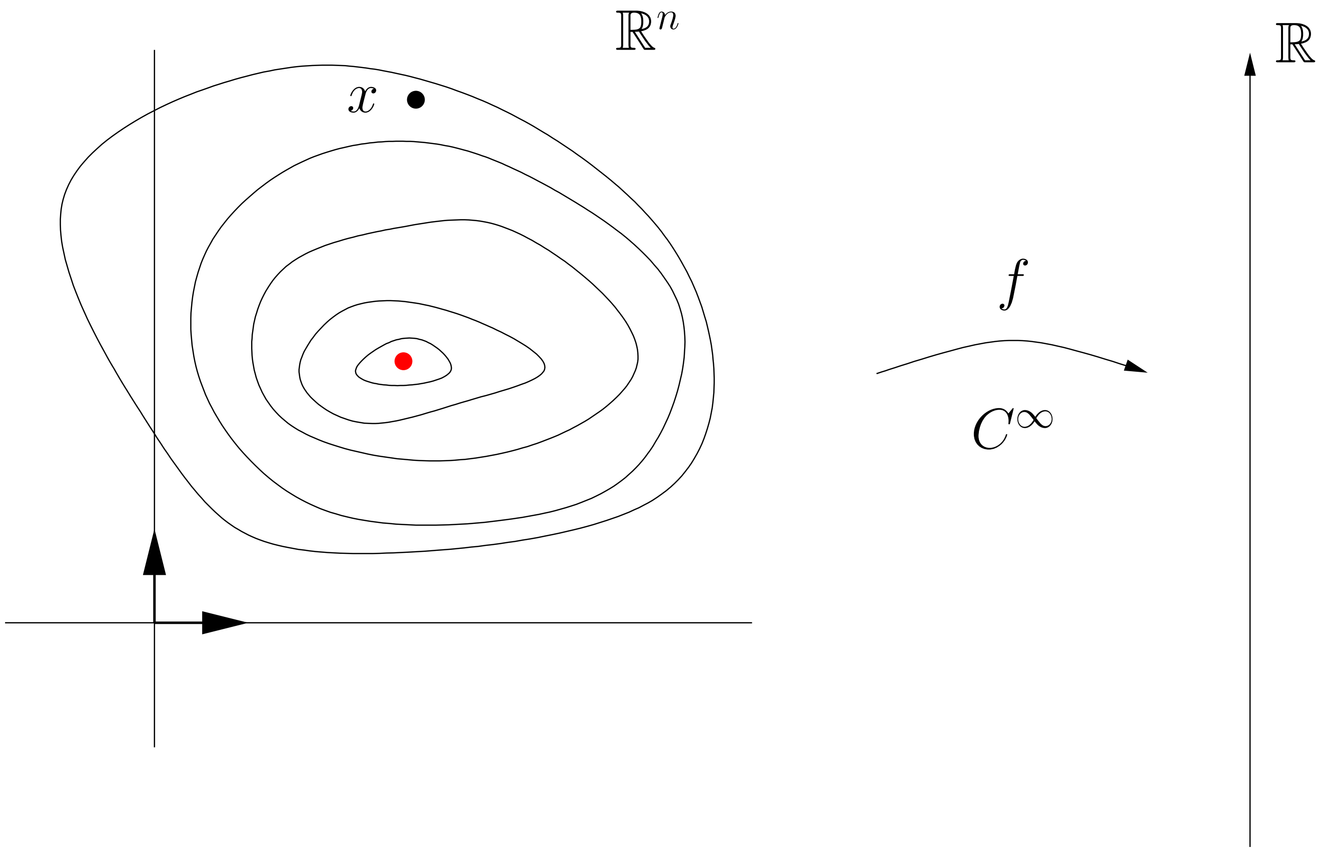
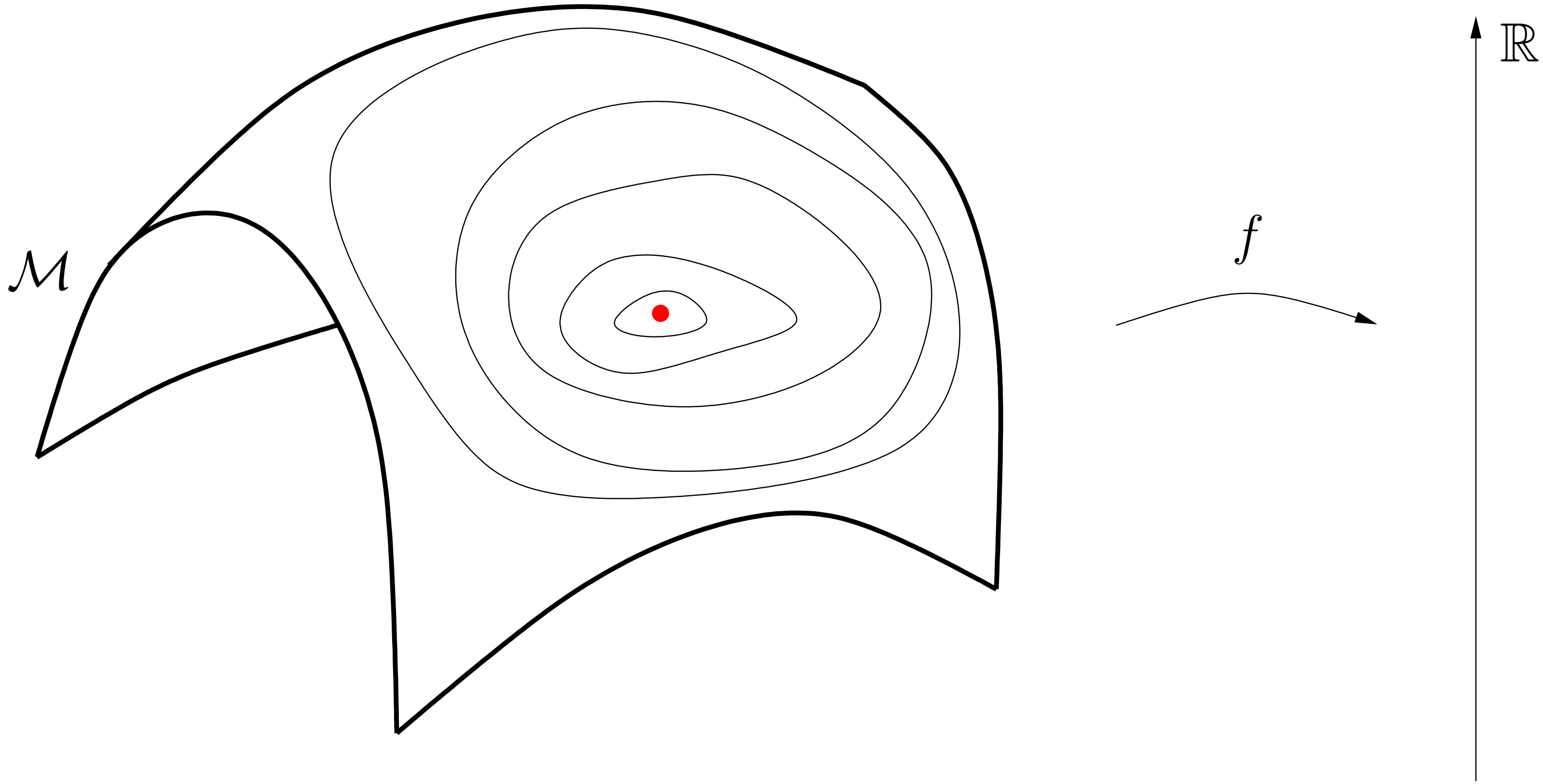
Smooth optimization in $\mathbb{R}^n$



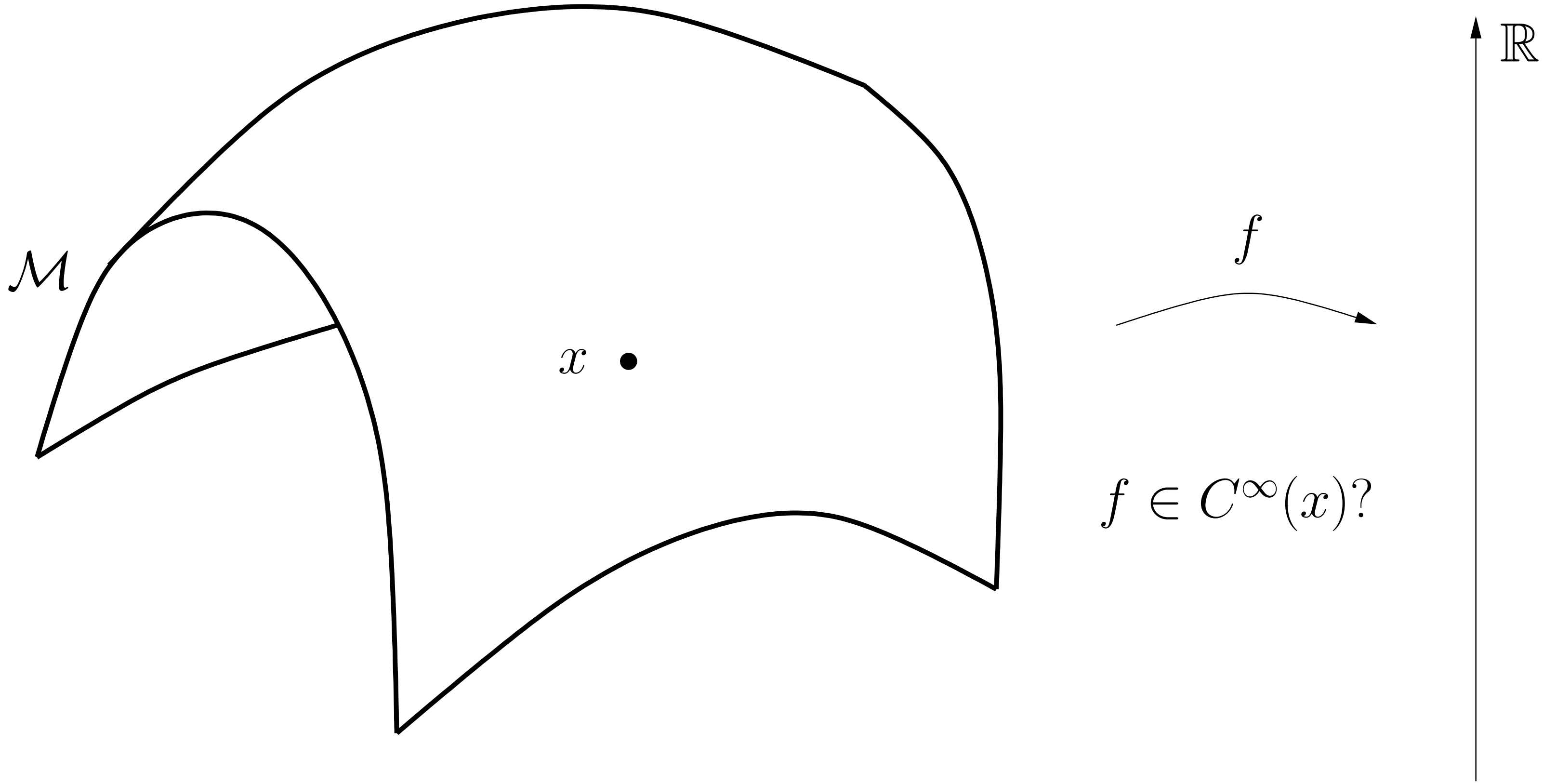
Optimization on "a set"

Differentiability? Generalization went too far!

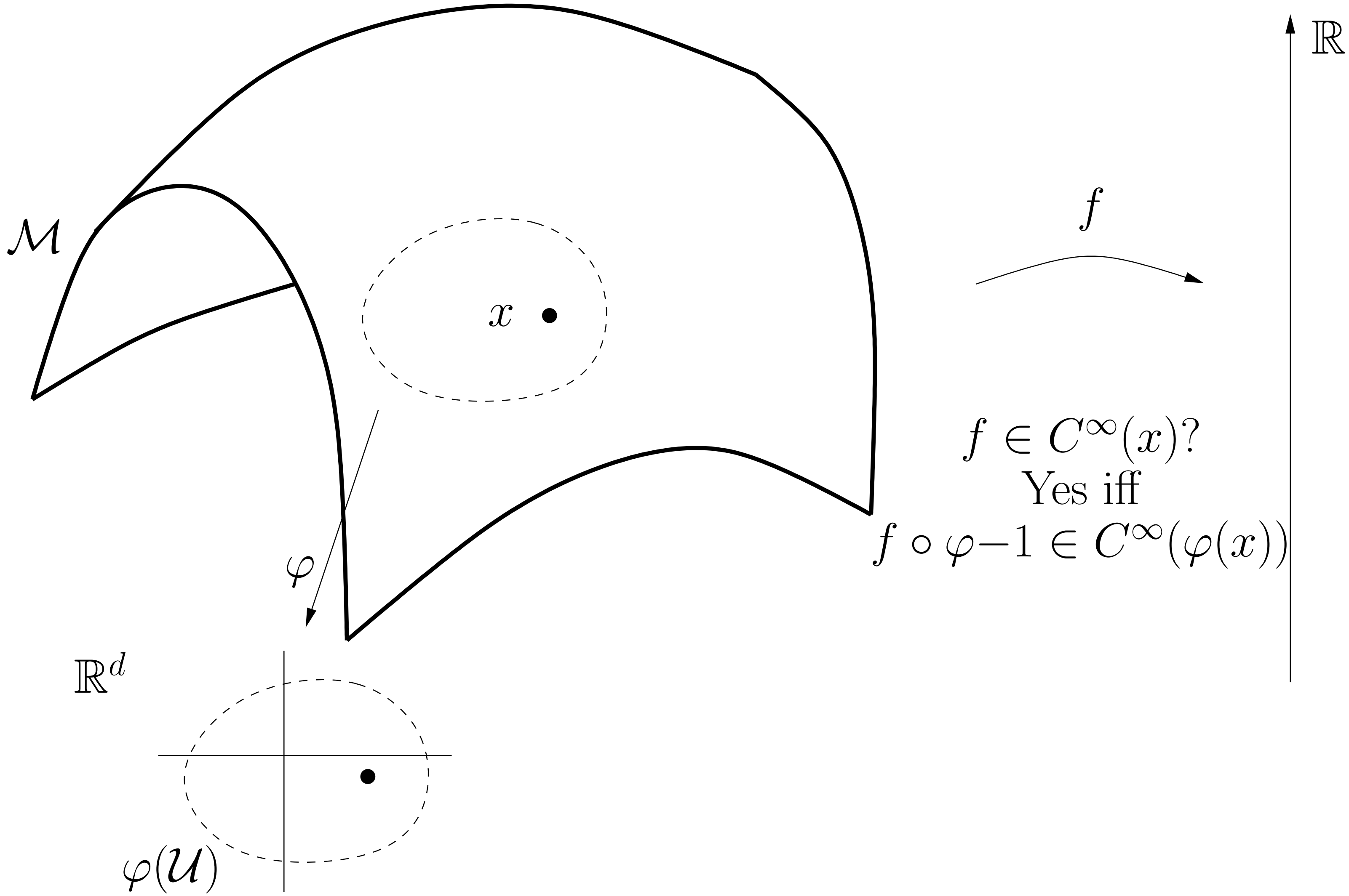
Smooth optimization on a manifold



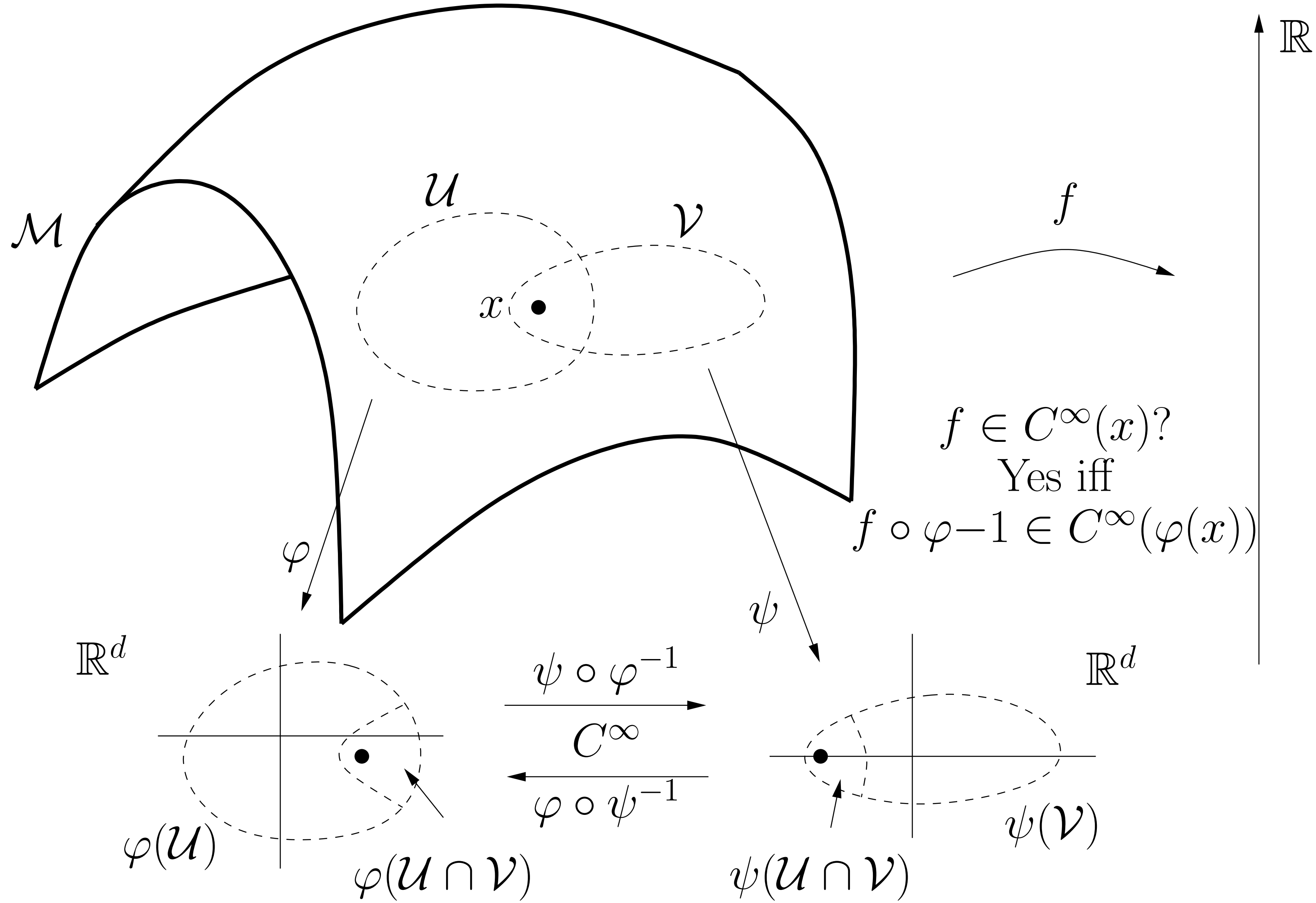
Smooth optimization on a manifold: what “smooth” means



Smooth optimization on a manifold: what "smooth" means



Smooth optimization on a manifold: what "smooth" means



Smooth optimization on a manifold: what "smooth" means

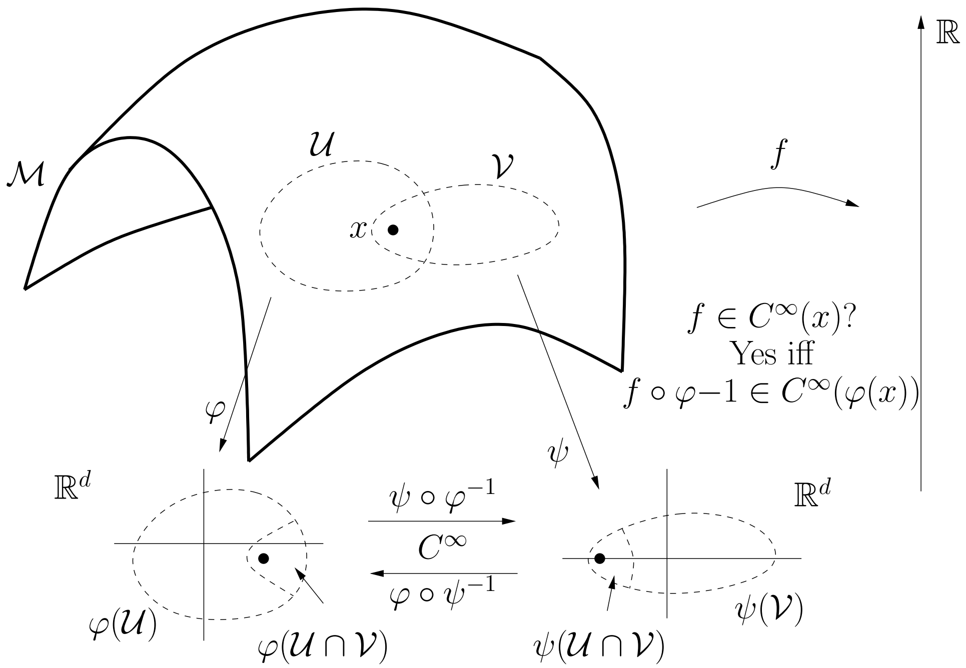
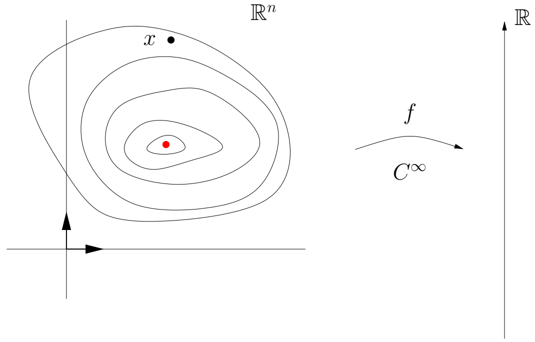


Chart: $\mathcal{U} \xrightarrow[\text{bij.}]{\varphi} \varphi(\mathcal{U})$

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

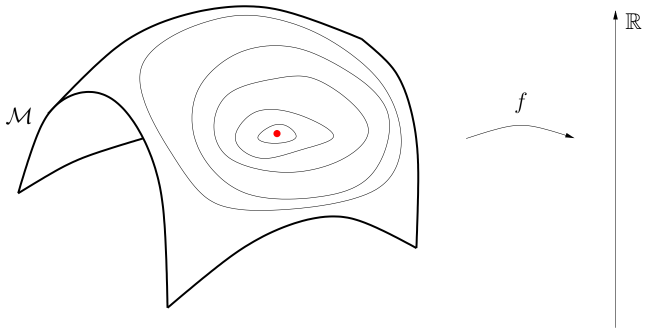
Manifold: Set with an atlas

(Highly Questionable) Summary



Optimization in $\mathbb{R}^n$: too easy

Optimization on arbitrary sets: too difficult



Optimization on manifolds: just right!

(Less Questionable) Summary

Smooth Optimization On Manifolds is a natural generalization of smooth optimization in $\mathbb{R}^n$.

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

Optimization On Manifolds

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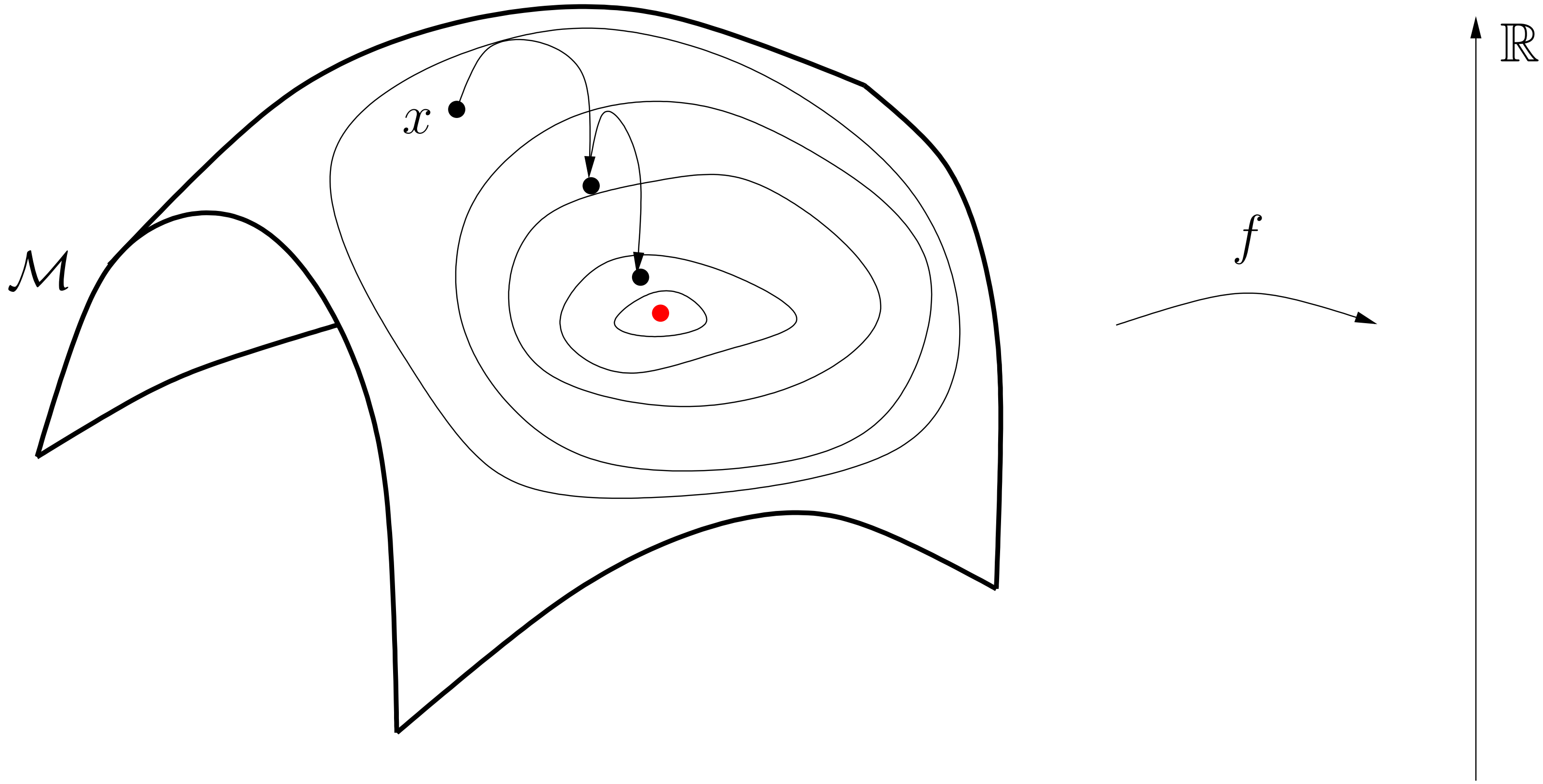
Optimization On Manifolds in one picture



Optimization On Manifolds

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Why?

Two examples of computational problems that can (should) be phrased as problems of Optimization On Manifolds:

- mechanical vibrations
- independent component analysis (ICA)

Mechanical vibrations

Stiffness matrix $A = A^T$, mass matrix $B = B^T \succ 0$.

Equation of vibrations (for undamped discretized linear structures):

$$Ax = \lambda Bx$$

where

- $\lambda = \omega^2$, ω angular frequency of vibration
- x is the corresponding mode of vibration.

Task: find lowest mode of vibration.

Generalized eigenvalue problem (GEP)

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 λ_1 and v_1.

We assume that $\lambda_1 < \lambda_2$ (simple eigenvalue).

GEP: optimization in $\mathbb{R}^n$

$$Av_i = \lambda_i B v_i$$

Cost function: Rayleigh quotient

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

Minimizers of $\tilde{f}$: αv_1, for all $\alpha \neq 0$.

The minimizers of $\tilde{f}$ yield the lowest mode of vibration.

The minimizers are not isolated.

GEP: optimization in $\mathbb{R}^n$

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

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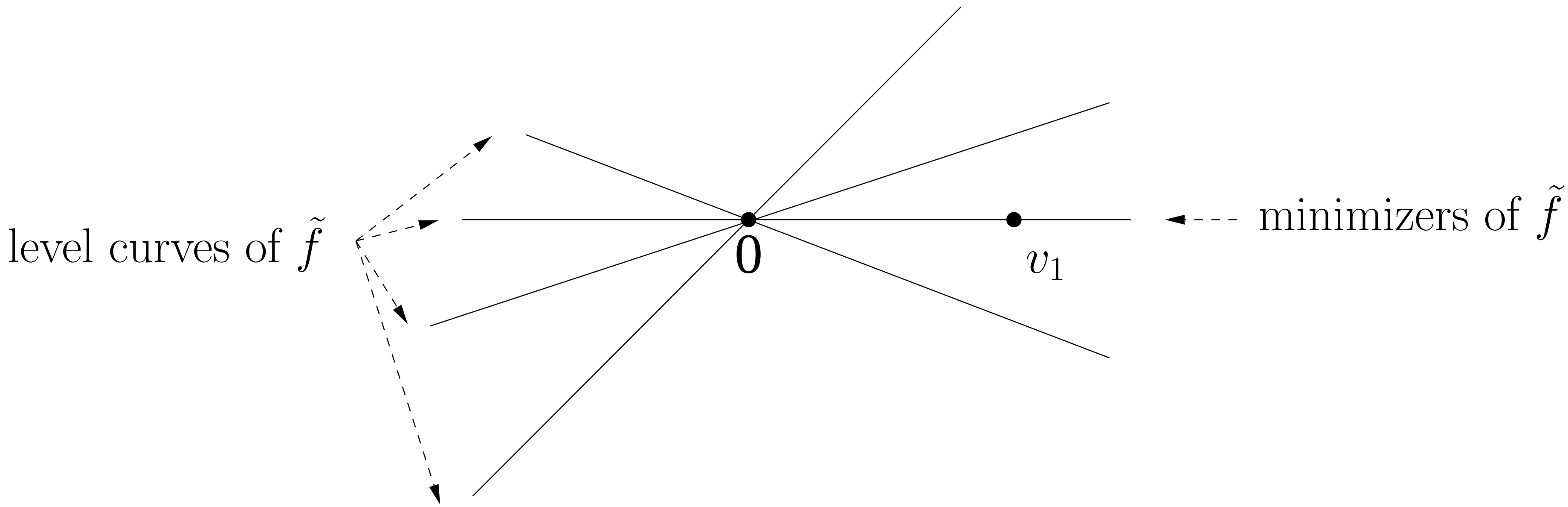
The minimizers of $\tilde{f}$ yield the lowest mode of vibration.

The minimizers are not isolated.

Invariance property: $\tilde{f}(\alpha y) = \tilde{f}(y)$. Idea: exploit the invariance property $\rightsquigarrow$ Optimization On Manifold.

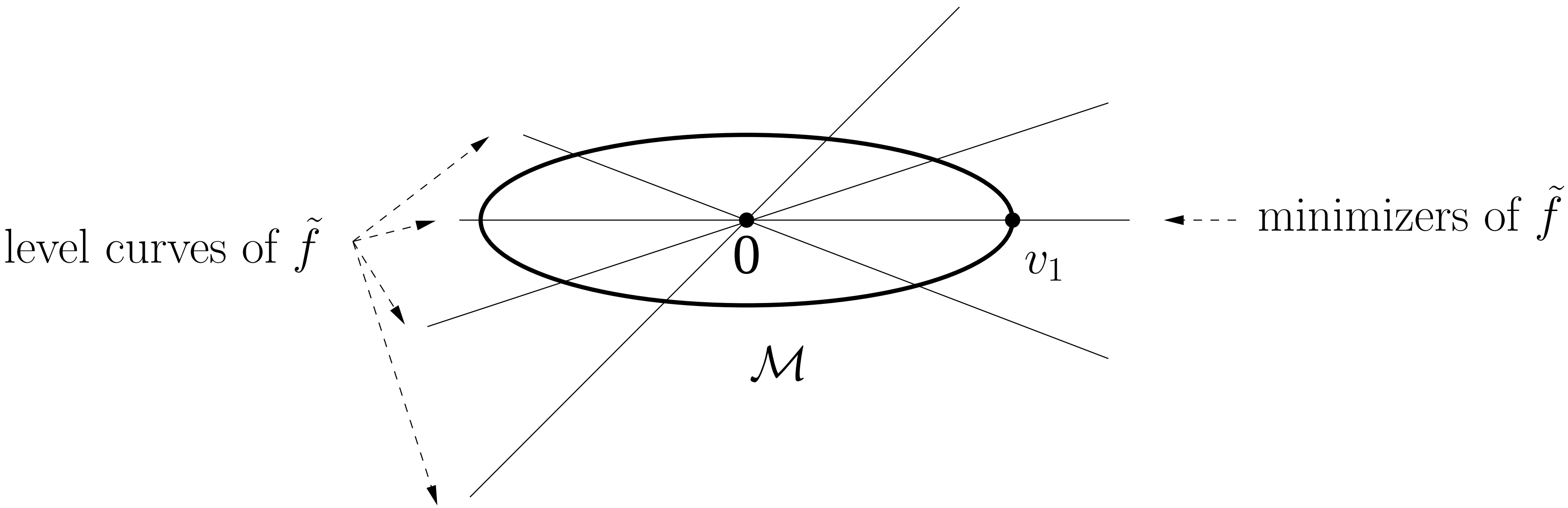
GEP: invariance by scaling

$$\tilde{f}(\alpha y) = \tilde{f}(y).$$



GEP: optimization on ellipsoid

$$\tilde{f}(\alpha y) = \tilde{f}(y).$$



GEP: 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:

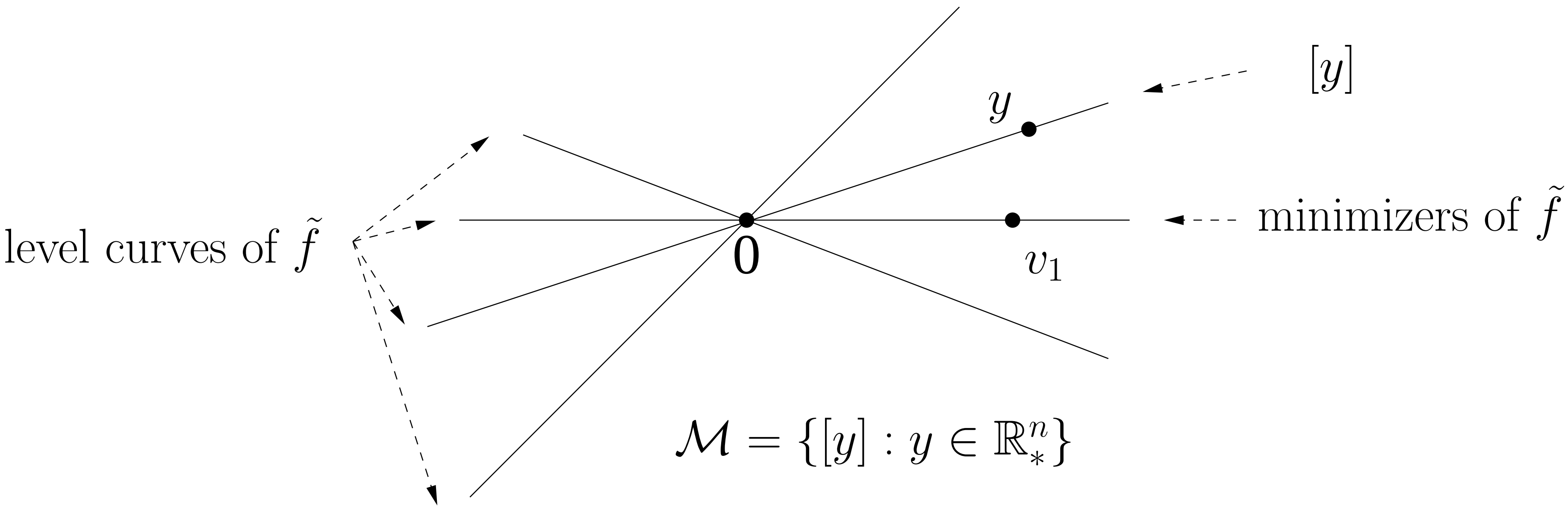
- $\mathcal{M} := \{y \in \mathbb{R}^n : y^T B y = 1\}$, *submanifold* of $\mathbb{R}^n$.
- $f : \mathcal{M} \to \mathbb{R} : f(y) = y^T A y$.

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

Minimizers of f: $\pm v_1$.

GEP: optimization on projective space

$$\tilde{f}(\alpha y) = \tilde{f}(y).$$



$$\mathcal{M} = \{[y] : y \in \mathbb{R}^n_*\}$$

GEP: 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: $[v_1]$.

Block algorithm for GEP: optimization on Grassmann manifold

Goal: compute the p lowest modes simulateously.

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

Invariance: $\tilde{f}(YR) = \tilde{f}(Y)$ for all nonsing. $p \times p$ matrices R.

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

Stationary points of f: $\operatorname{span}\{v_{i_1}, \ldots, v_{i_p}\}$.

Minimizer of f: $[Y] = \operatorname{span}\{v_1, \ldots, v_p\}$.

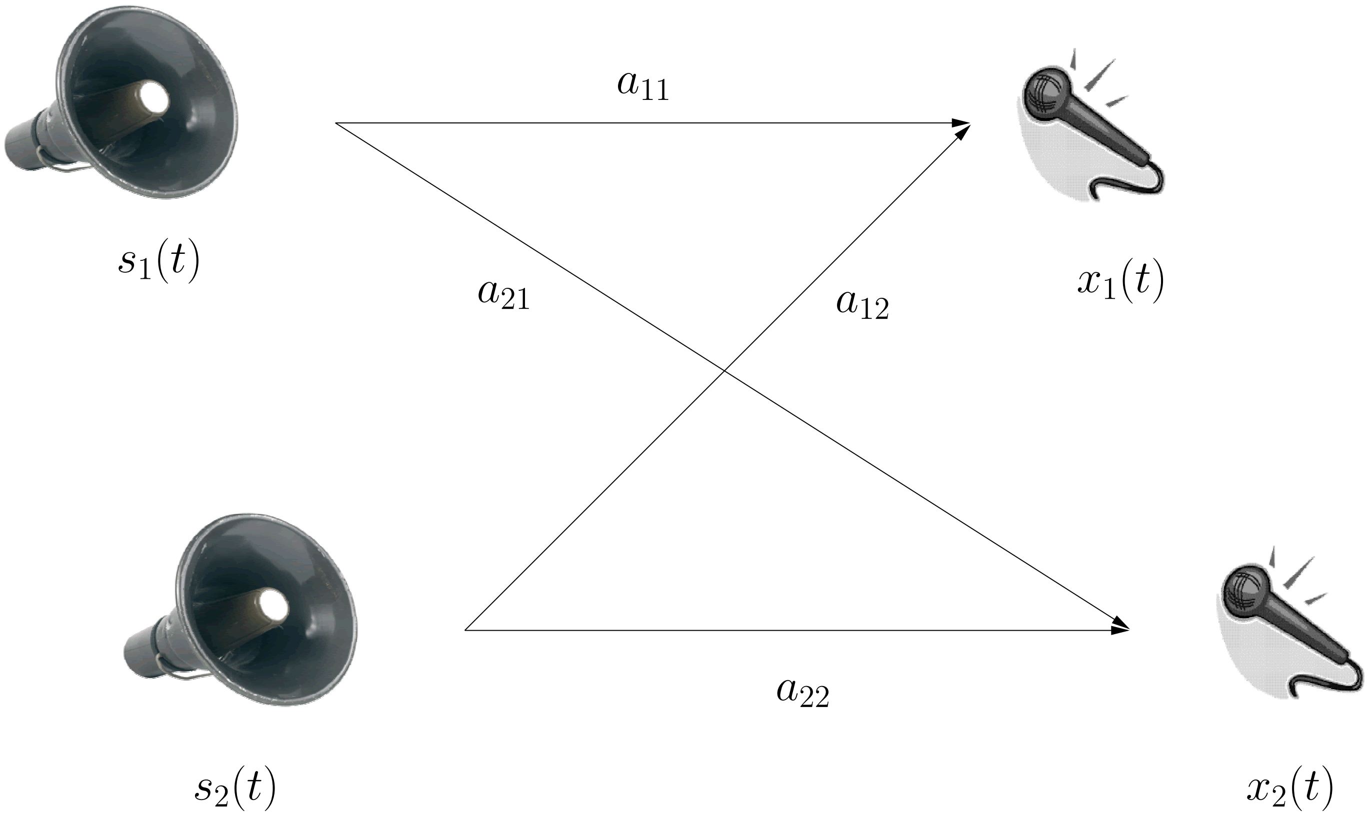
Why?

Two examples of computational problems that can (should) be phrased as problems of Optimization On Manifolds:

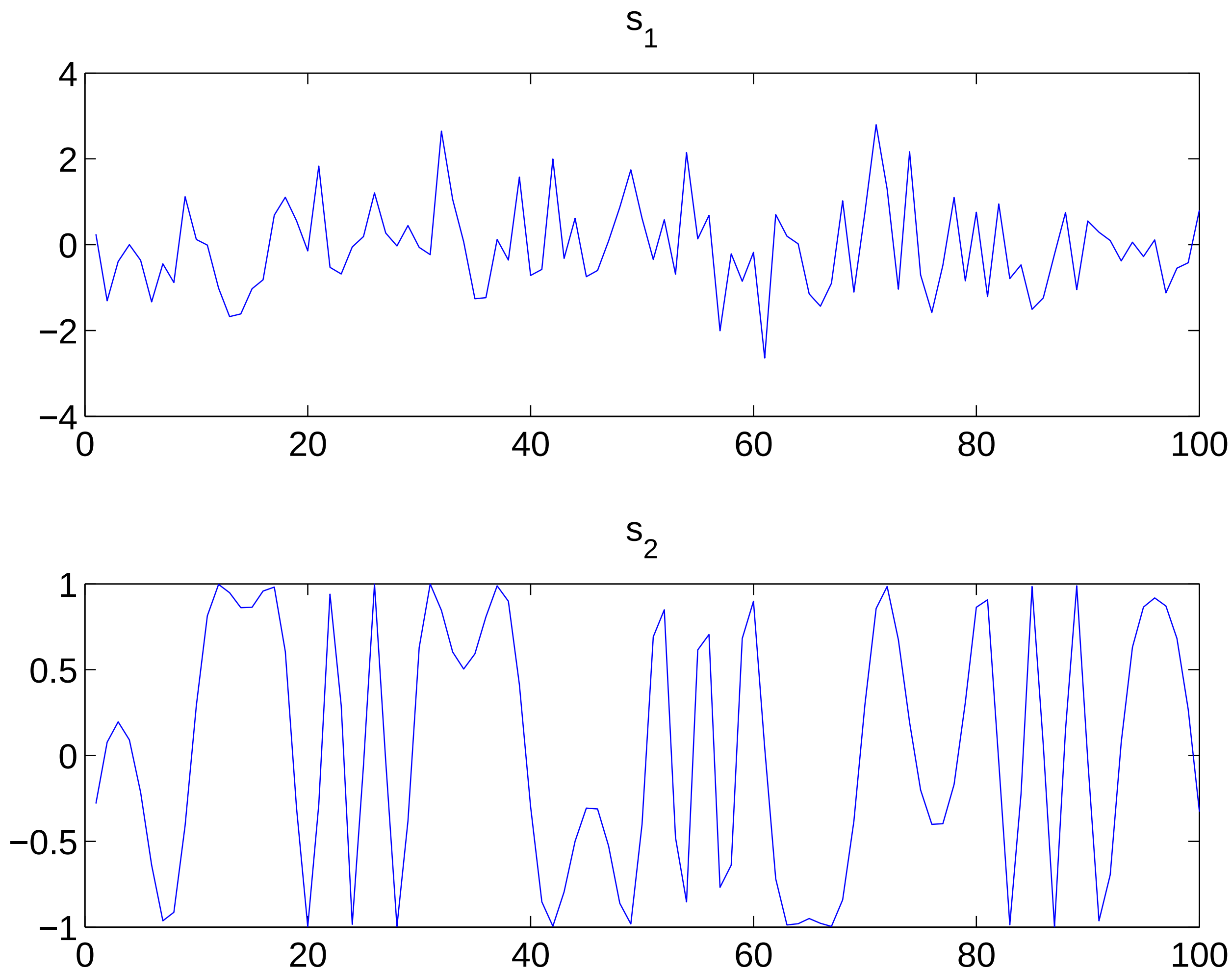
- mechanical vibrations
- independent component analysis (ICA)

Independent Component Analysis (ICA)

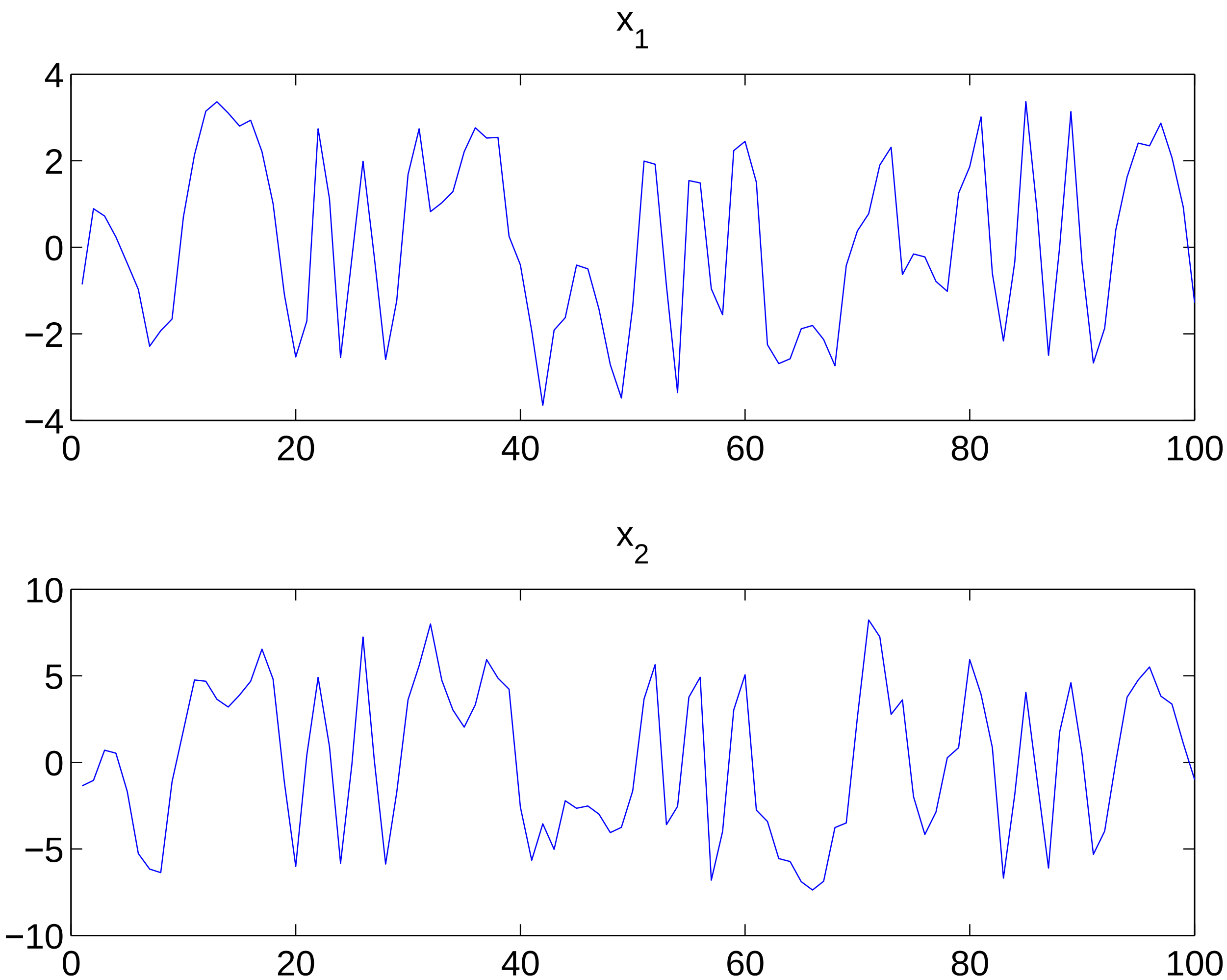
Cocktail party problem



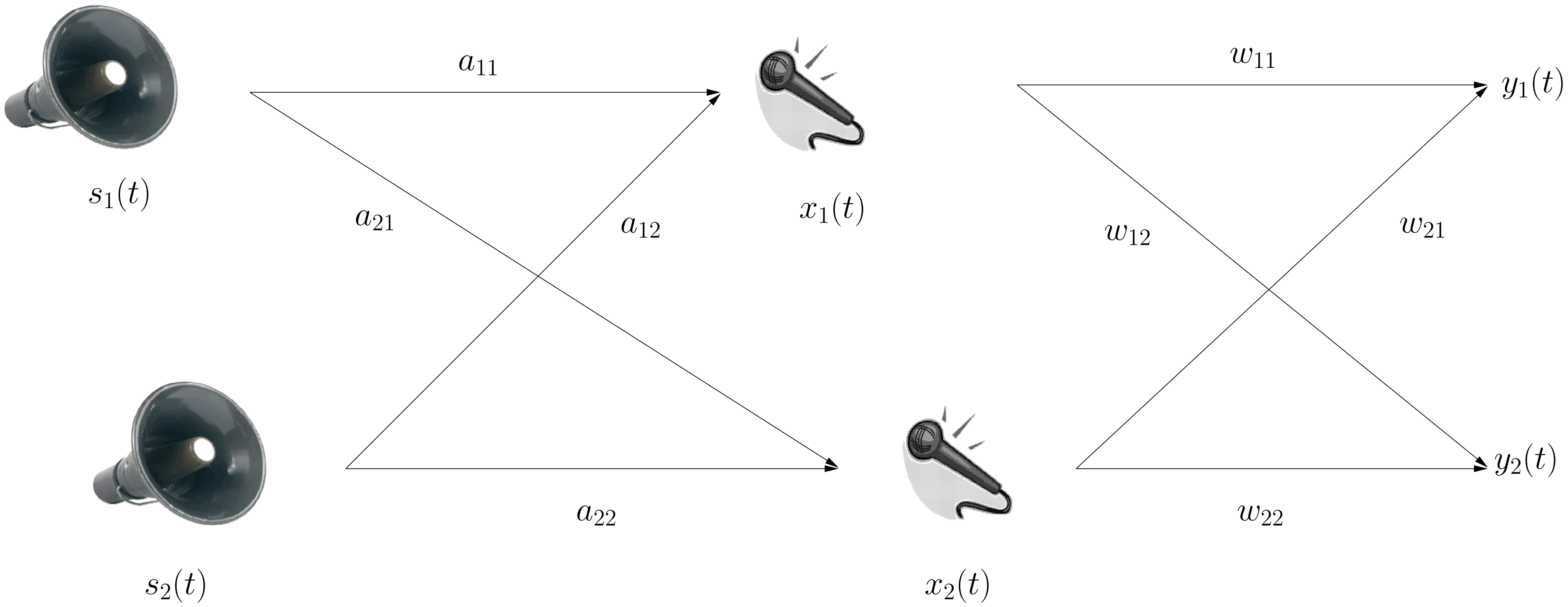
Independent Component Analysis (ICA)



Independent Component Analysis (ICA)



Independent Component Analysis (ICA)



ICA via Joint Diagonalization (JD)

$$y(t) = W^T x(t), \qquad x(t) = As(t)$$

Covariance matrices: $R_u(\tau) := E[u(t+\tau)u^T(t)]$.

Pick lags $\tau_1, \ldots, \tau_N$. It holds

$$R_y(\tau_1) = W^T R_x(\tau_1) W$$

$$\vdots$$

$$R_y(\tau_N) = W^T R_x(\tau_N) W.$$

Task: Select W to make $R_y(\tau_1), \ldots, R_y(\tau_N)$ "as diagonal as possible".

JD as optimization problem

Notation: $C_i := R_x(\tau_i)$.

Task: Make $W^T C_i W$, $i = 1, \ldots, N$, "as diagonal as possible".

Choose cost function to define the "best" joint diagonalization.

$$\tilde{f}(W) := \sum_{i=1}^{N} \left(\log\det \operatorname{ddiag}(W^T C_i W) - \log\det(W^T C_i W) \right).$$

Invariance property: $\tilde{f}(WD) = \tilde{f}(W)$ for all nonsingular diagonal matrix D.

Difficulty: The minimizers are not isolated.

JD as optimization on manifold

$$\tilde{f}(W) := \sum_{i=1}^{N} \left(\log \det \operatorname{ddiag}(W^T C_i W) - \log \det(W^T C_i W) \right).$$

Invariance $\tilde{f}(WD) = \tilde{f}(W)$, hence minimizers not isolated.

Two remedies:

1. Submanifold approach: restrict W to the *oblique manifold*

$$\mathcal{OB} := \{W \in \mathbb{R}^{n \times p} : \operatorname{ddiag}(W^T W) = I_p\}.$$

2. Quotient manifold approach: work on $\mathbb{R}^{n \times p}/\mathcal{D}$, the set of equivalence classes $[W] := W\mathcal{D} := \{WD : D \text{ diagonal}\}$.

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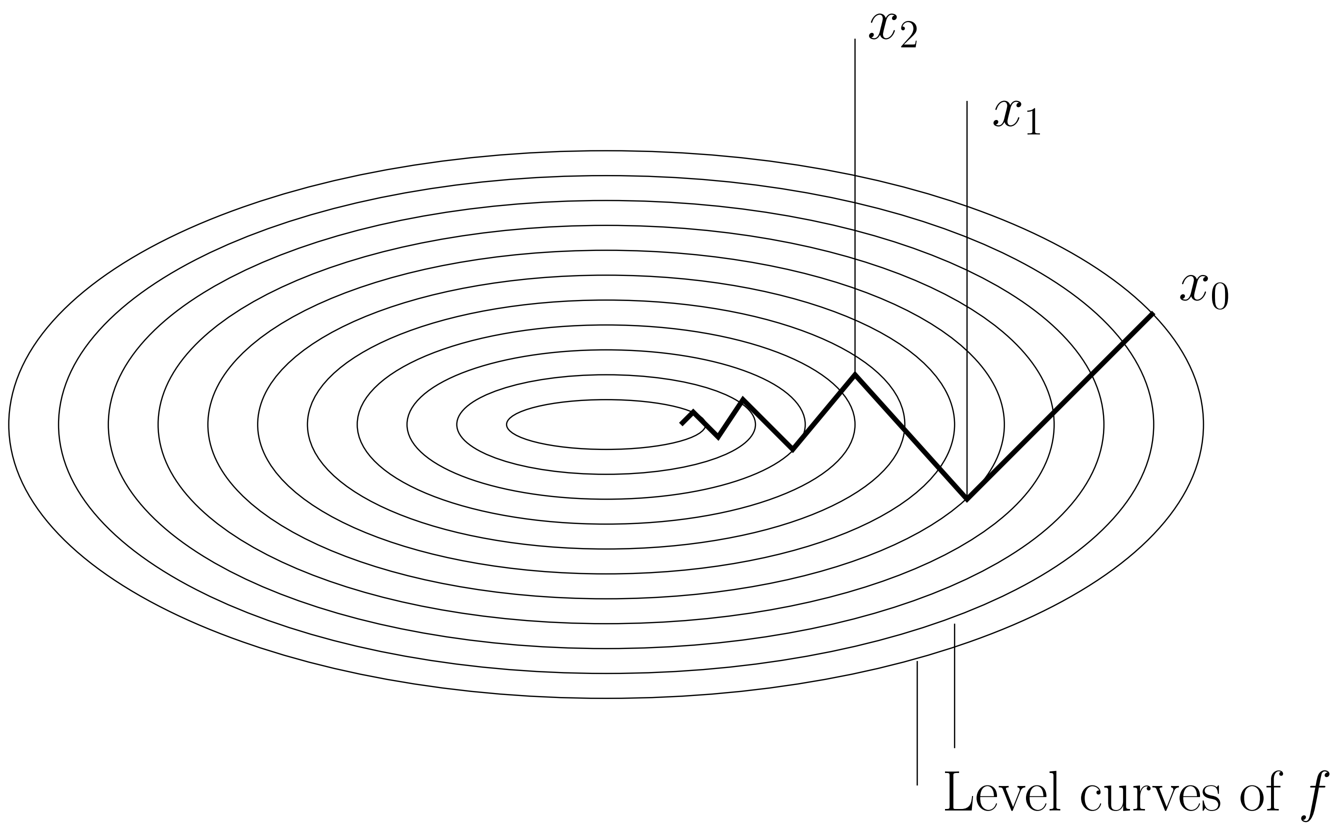
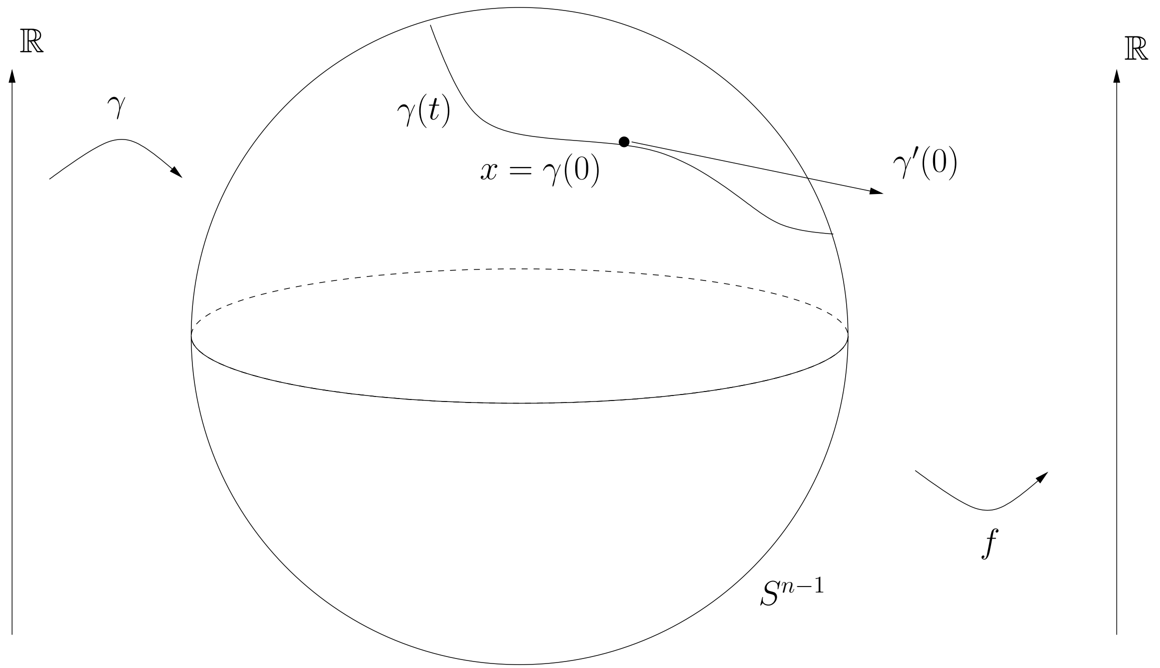
Steepest-descent in $\mathbb{R}^n$

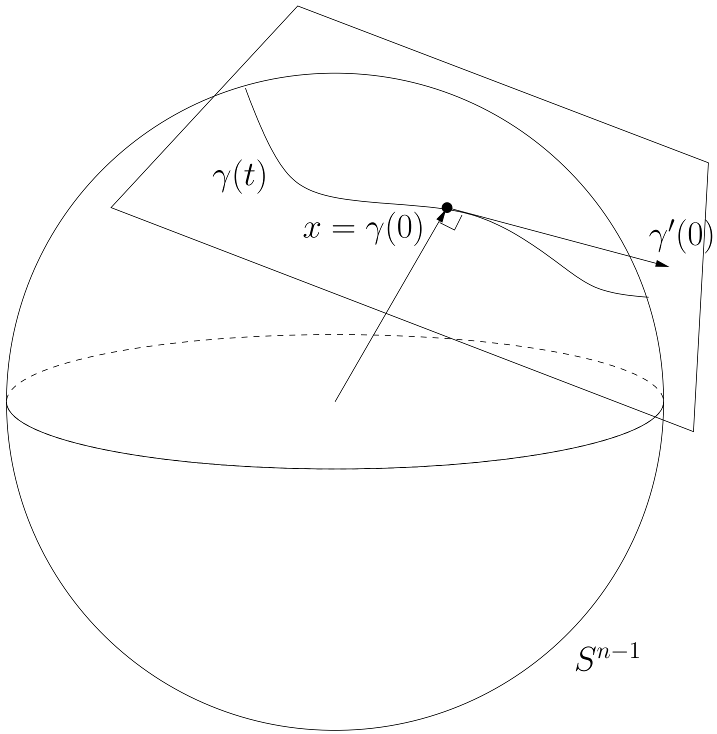


Steepest-descent on manifolds – Tangent vectors



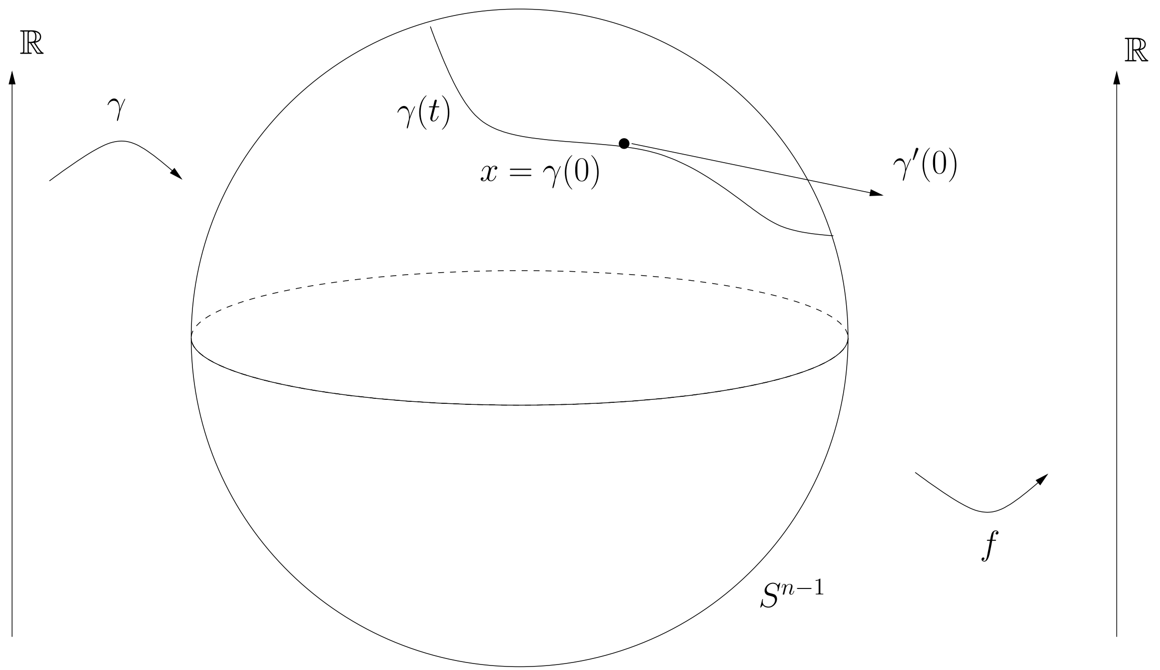
$$\gamma'(0): \quad f \in C^{\infty}(x) \quad \mapsto \quad \frac{\mathrm{d}}{\mathrm{d}t} f(\gamma(t))\big|_{t=0} \in \mathbb{R}$$

Steepest-descent on manifolds – Tangent space



$$T_x\mathcal{M} = \{\gamma'(0) : \gamma \text{ curve in } \mathcal{M},\ \gamma(0) = x\}$$

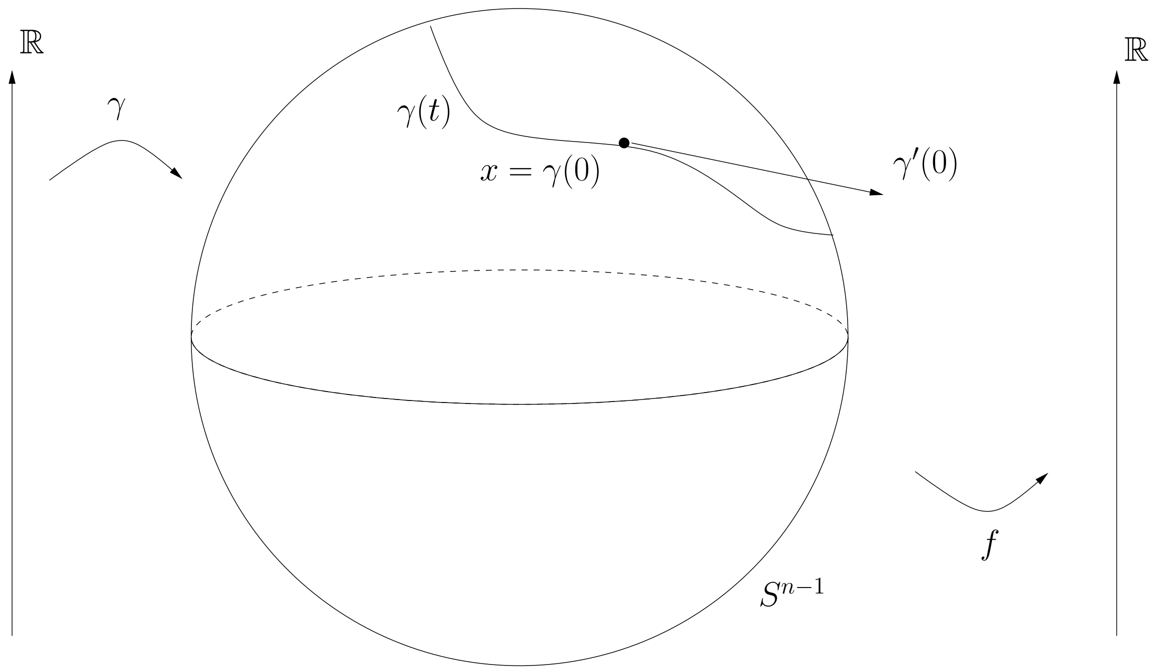
Steepest-descent on manifolds – Descent directions



$\gamma'(0)$ is a *descent direction* for f at x if

$$\gamma'(0)f := \frac{\mathrm{d}}{\mathrm{d}t} f(\gamma(t))|_{t=0} \quad < 0$$

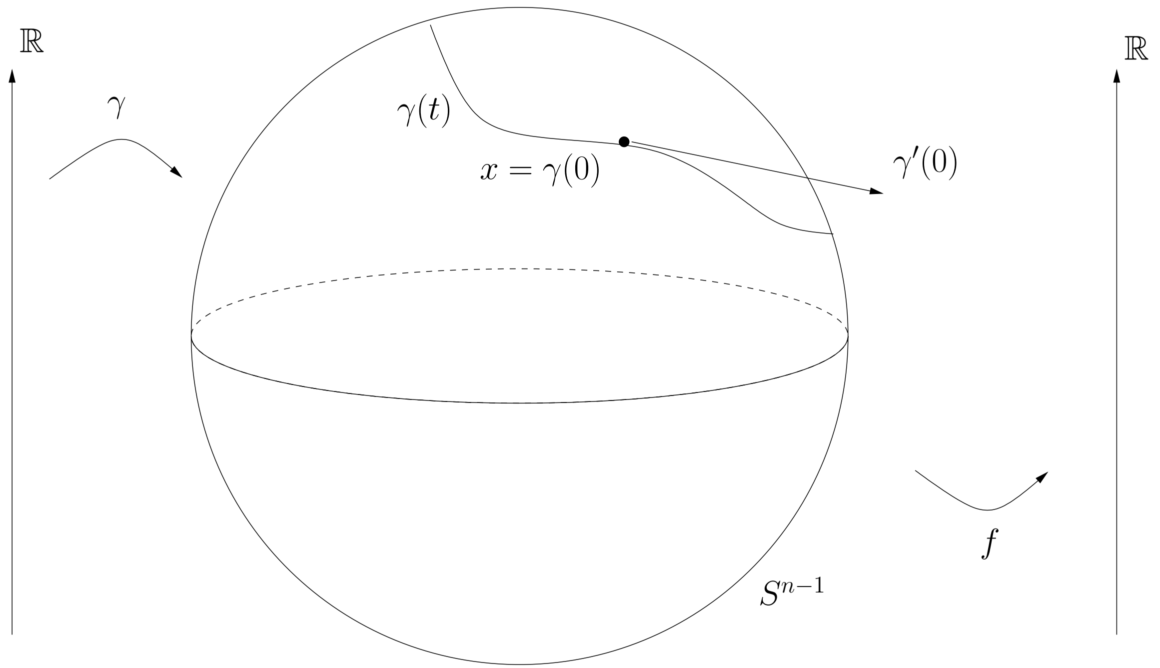
Steepest-descent on manifolds – Steepest descent direction



Define inner product $\langle \cdot, \cdot \rangle_x$ on the tangent space $T_x\mathcal{M}$. Then $\mathcal{M}$ is a *Riemannian manifold*.

Length of a tangent vector: $\|\gamma'(0)\|_x := \sqrt{\langle \gamma'(0), \gamma'(0) \rangle_x}$.

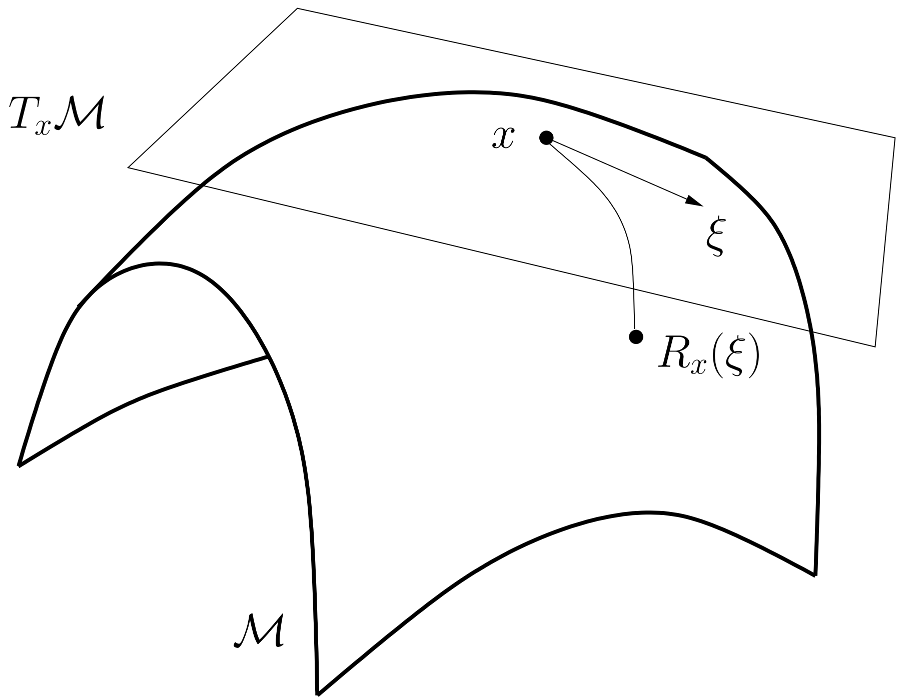
Steepest-descent on manifolds – Steepest descent direction



Steepest-descent direction along $\arg\min_{\xi \in T_x\mathcal{M},\ \|\xi\|_x = 1} \xi f$.

The steepest-descent direction is along the opposite of the *gradient* of f.

Steepest-descent on manifolds – Retraction



$$R_x(0_x) = x, \qquad \frac{\mathrm{d}}{\mathrm{d}t} R_x(t\xi)\Big|_{t=0} = \xi$$

Steepest-descent on manifolds – Summary

Let $\mathcal{M}$ be a Riemannian manifold with a retraction R. Let f be a cost function on $\mathcal{M}$. Let $x_0 \in \mathcal{M}$ be the initial iterate.

For $k = 0, 1, \ldots$:

1. Compute $\operatorname{grad} f(x_k)$.
2. Choose $x_{k+1} = R_{x_k}(-t \operatorname{grad} f(x_k))$ where $t > 0$ is chosen to satisfy a "sufficient decrease" condition.

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A few pointers

- Optimization on manifolds in general: Luenberger [Lue73], Gabay [Gab82], Smith [Smi93, Smi94], Udrişte [Udr94], Manton [Man02], Mahony and Manton [MM02], PAA *et al.* [ABG06b]...
- Stiefel and Grassmann manifolds: Edelman *et al.* [EAS98], PAA *et al.* [AMS04]...
- Retractions: Shub [Shu86], Adler *et al.* [ADM+02]...

- Eigenvalue problem: Chen and Amari [CA01], Lundström and Eldén [LE02], Simoncinin and Eldén [SE02], Brandts [Bra03], Absil *et al.* [AMSV02, AMS04, ASVM04, ABGS05, ABG06a] and Baker *et al.* [BAG06]

- Independent component analysis: Amari *et al.* [ACC00], Douglas [Dou00], Rahbar and Reilly [RR00], Pham [Pha01], Joho and Mathis [JM02], Joho and Rahbar [JR02], Nikpour *et al.* [NMH02], Afsari and Krishnaprasad [AK04], Nishimori and Akaho [NA05], Plumbley [Plu05], PAA and Gallivan [AG06], Shen *et al.* [SHS06], Hüeper *et al.* [HSS06]...

- Pose estimation: Ma *et al.* [MKS01], Lee and

Moore [LM04], Liu *et al.* [LSG04], Helmke *et al.* [HHLM07]

- Various matrix nearness problems: Trendafilov and Lippert [TL02], Grubisic and Pietersz [GP05]...

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Course

"Optimization algorithms on matrix manifolds"

in the Graduate School on Systems, Optimization, Control and Networks (2007-2008)

Lecturers: PAA, Rodolphe Sepulchre

Advertisement # 2: forthcoming book

"Optimization algorithms on matrix manifolds"

by PAA, R. Mahony and R. Sepulchre, to appear (around December 2007)

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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