

Learning graphical factor models with Riemannian optimization

Hippert-Ferrer, Bouchard, Mian, Vayer, Breloy, arXiv preprint arXiv:2210.11950, 2022

Statistics in signal processing and machine learning

Statistical point of view is ubiquitous:

- **Data** appears as the result of a **random processes** (uncertainties)
- Cast **statistical models** that reasonably fit **empirical histograms**
- Derive **processes** that achieve certain **average performance** for a **task**
(fitting, estimation, detection, classification, prediction)

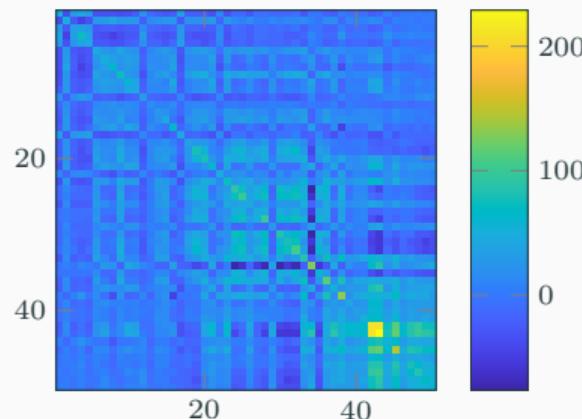
Scharf, Demeure, "Statistical signal processing: detection, estimation, and time series analysis," PrenticeHall, 1991

Hastie, Tibshirani, Friedman, "The Elements of Statistical Learning," Springer-Verlag, 2009

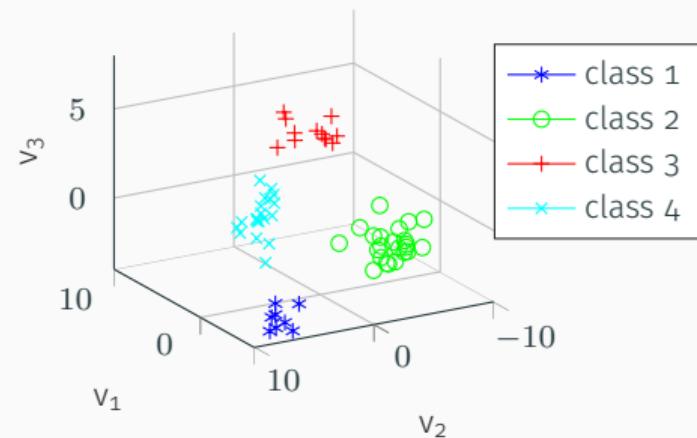
Parametric approach

Represent or analyze the data \mathbf{x} through some statistical parameter θ

Example with $p \simeq 7k$ genes of $n = 63$ patients with $k = 4$ classes [Khan2001] represented by



Covariance of 50 selected genes



3 principal components

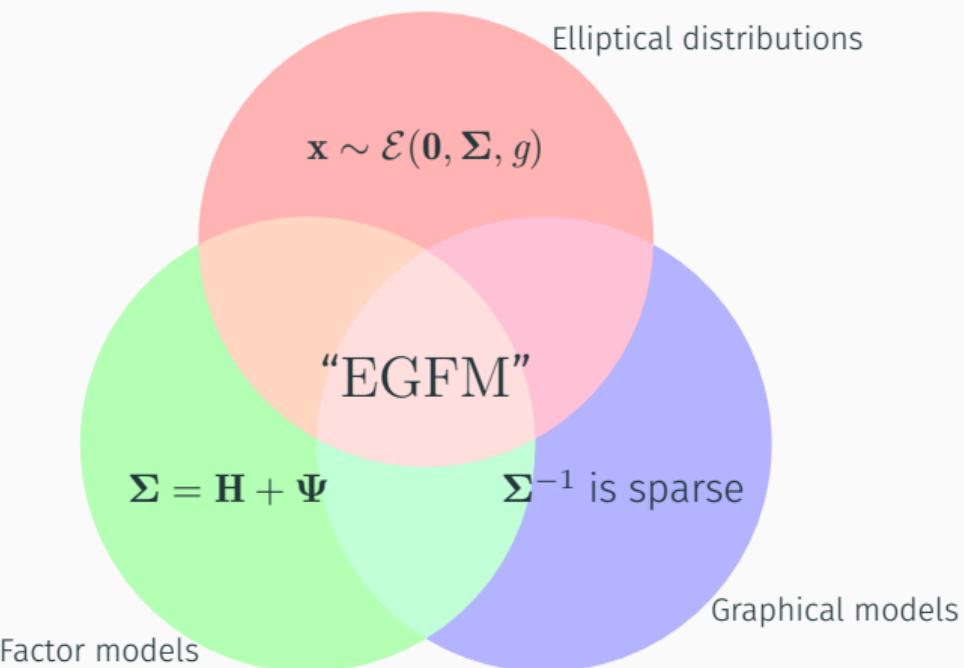
Statistical approach

“Assume $\mathbf{x} \sim f(\mathbf{x}, \boldsymbol{\theta})$, then do stuff”

- **Design** a meaningful pdf f and parameter $\boldsymbol{\theta}$
- **Analyze** model properties, performance bounds...
- **Solve** related optimization problems (MLEs, barycenters...)
- **Apply** the results to a task

Today's talk: **design** and **solve** for “**elliptical graphical factor models**”

WTF is this that?



Outline

- **Design**

- Gaussian Graphical models
- Elliptical models
- Probabilistic PCA and factor models
- Everything together

- **Solve**

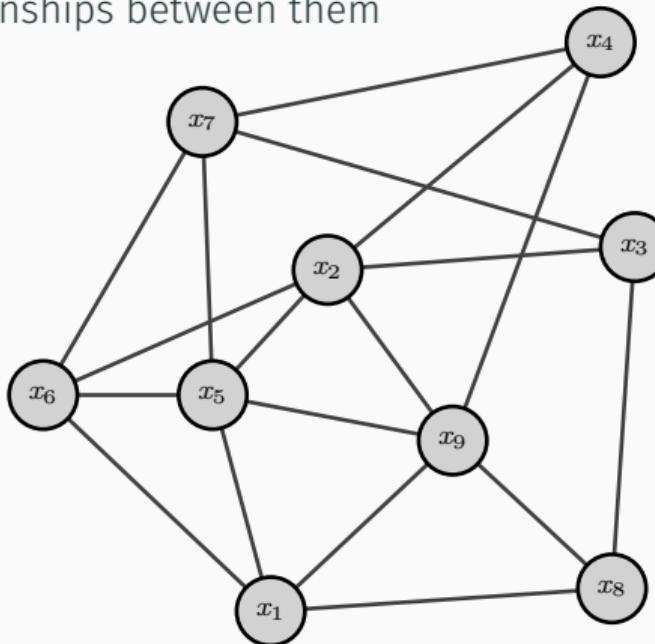
- Manifolds and Riemannian geometry
- Riemannian optimization

- **Apply** on real data examples

Graphical models

Graphs help visualizing **relationships between entities**:

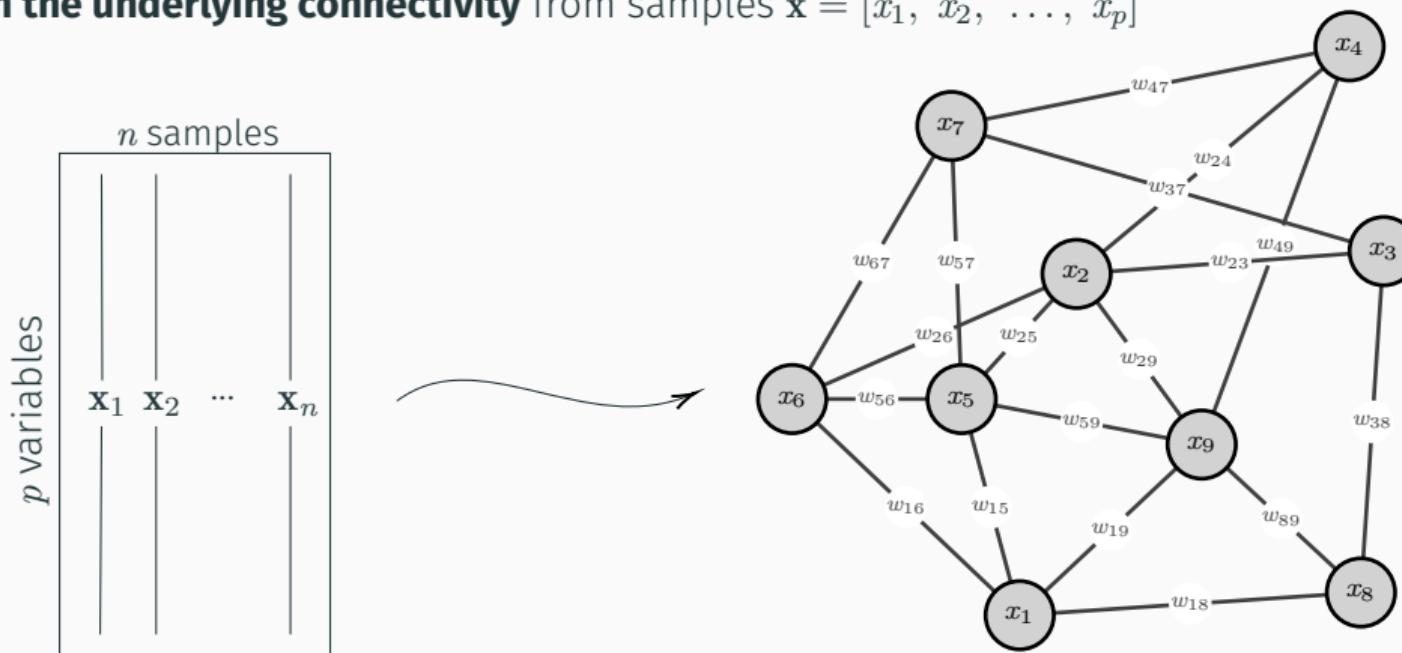
- **Nodes** correspond to entities, or **variables**
- **Edges** encode relationships between them



Graph learning

The graph **topology is unknown** but **each node generates data**

Learn the underlying connectivity from samples $\mathbf{x} = [x_1, x_2, \dots, x_p]$



Graphical model: a statistical point of view

“Connection in the graph = conditional dependence”

For $\mathbf{x} = [\underbrace{x_1, x_2}_{\mathbf{x}_T}, \mathbf{x}_\perp]$, **conditional independence** $x_1 \perp\!\!\!\perp x_2$ holds if $\mathcal{L}(x_1|x_2, \mathbf{x}_\perp) = \mathcal{L}(x_1|\mathbf{x}_\perp)$
“knowing \mathbf{x}_\perp makes x_2 irrelevant for predicting x_1 ”

Assume $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \Sigma)$ with $\Sigma = \begin{bmatrix} \Sigma_{TT} & \Sigma_{T\perp} \\ \Sigma_{\perp T} & \Sigma_{\perp\perp} \end{bmatrix}$ and $\Theta = \Sigma^{-1} = \begin{bmatrix} \Theta_{TT} & \Theta_{T\perp} \\ \Theta_{\perp T} & \Theta_{\perp\perp} \end{bmatrix}$

Then $\mathbf{x}_T|\mathbf{x}_\perp \sim \mathcal{N}(\xi_{T|\perp}, \Sigma_{T|\perp})$ with $\Sigma_{T|\perp} = \Sigma_{TT} - \Sigma_{T\perp}\Sigma_{\perp\perp}^{-1}\Sigma_{\perp T} = \Theta_{TT}^{-1}$

So $x_1 \perp\!\!\!\perp x_2$ (no edge w_{12} on the graph) $\Leftrightarrow \Sigma_{T|\perp}$ is diagonal $\Leftrightarrow \Theta_{12} = 0$

Learning Gaussian graphical models (GGM)

Assume a **Gaussian Markov Random Field** $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \Sigma)$

A **Gaussian graphical model** implies a **sparse precision matrix** $\Theta = \Sigma^{-1}$

Graphical Lasso (GLasso) \Leftrightarrow regularized MLE of Θ

$$\underset{\Theta \in \mathcal{S}_p^{++}}{\text{maximize}} \quad \log \det(\Theta) - \text{Tr}\{\mathbf{S}\Theta\} - \lambda h(\Theta)$$

→ Graph drawn from Θ 's support

Some limitations

- Gaussian model assumption → sensitive to heavy tails
- No structure in Σ → poor estimates when $n \simeq p$ or $n < p$

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Motivation for elliptical distributions

Objective: find a model $f(\mathbf{x}, \theta)$

- \mathbf{x} is a **sample** in \mathbb{R}^p or \mathbb{C}^p (unstructured)
- f is a **pdf**
- θ **parameterizes** the pdf

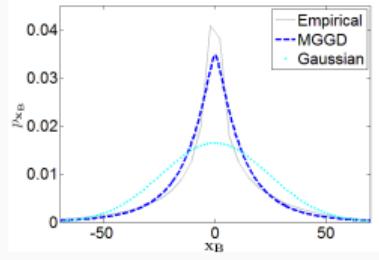
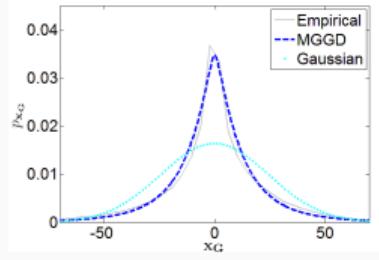
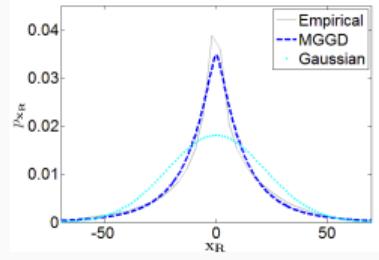
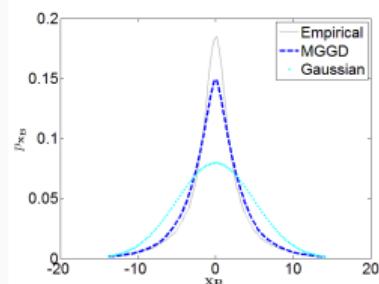
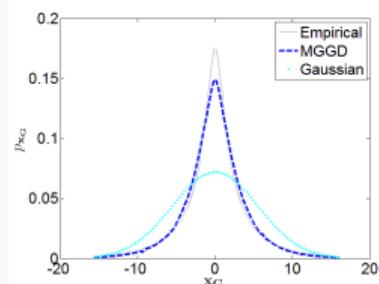
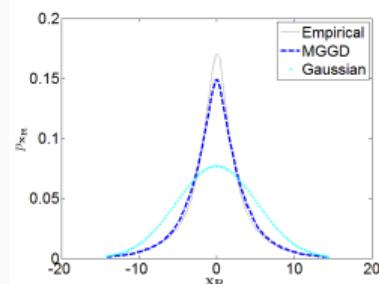
Challenges from real data:

- **Non-Gaussian, heavy-tailed** distributions
- **Outliers**

Elliptical models good entry point for this tutorial =)

- **Large family** that generalizes the multivariate Gaussian distribution
- Still parameterized through **1st and 2nd order moments** (mean, covariance)
- **Better fit** to empirical histograms → **better results**

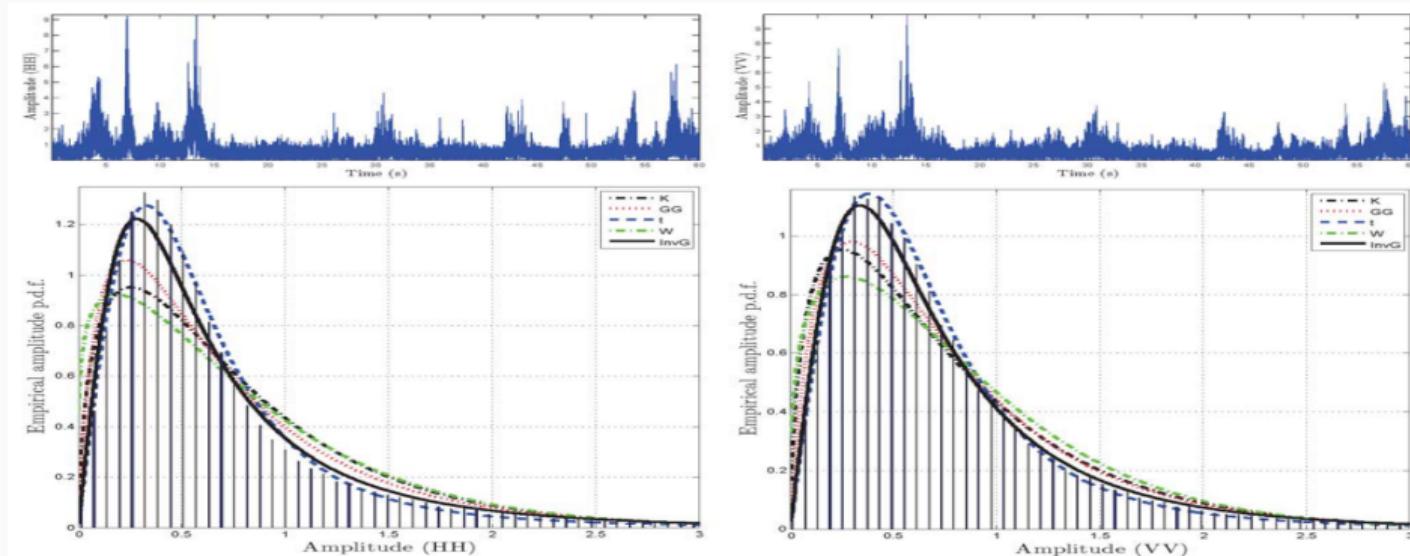
Motivating real-data examples (1/2)



Bark.0000 and Leaves.0008 from VisTex and marginal distributions of wavelet coefficients from RGB channels.

F. Pascal, L. Bombrun, J-Y. Tourneret, Y. Berthonmieu, "Parameter estimation for multivariate generalized Gaussian distributions," IEEE TSP, 2013

Motivating real-data examples (2/2)



Modulus of HH and VV band of Shore of Lake Ontario sensed by McMaster IPIX radar

E. Ollila, D. E. Tyler, V. Koivunen, H. V. Poor, "Complex elliptically symmetric distributions: Survey, new results and applications," IEEE TSP, 2012

Elliptical models

Complex elliptically symmetric distributions (CES)

$\mathbf{x} \sim \mathcal{CES}(\boldsymbol{\mu}, \Sigma, g)$ if its pdf can be written

$$f(\mathbf{x}) \propto |\Sigma|^{-1} g((\mathbf{x} - \boldsymbol{\mu})^H \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})),$$

where $g : [0, \infty) \rightarrow [0, \infty)$ is the **density generator** and

- $\boldsymbol{\mu} \in \mathbb{C}^p$ is the symmetry **center**
- $\Sigma \in \mathcal{H}_p^{++}$ is the **scatter matrix**

If \mathbf{x} has finite 2nd-order moment, the **covariance matrix** is $\mathbb{E} [(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^H] = \alpha \Sigma$

- $\alpha = -2\varphi'(0)$,
- φ is defined by the characteristic function $c_{\mathbf{x}}(\mathbf{t}) = \exp(i\mathbf{t}^H \boldsymbol{\mu}) \varphi(\mathbf{t}^H \Sigma \mathbf{t})$

Practical CES representation

Stochastic representation theorem

$\mathbf{x} \sim \mathcal{CES}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, g)$ iif it admits the stochastic representation

$$\mathbf{x} \stackrel{d}{=} \boldsymbol{\mu} + \sqrt{\mathcal{Q}} \boldsymbol{\Sigma}^{1/2} \mathbf{u}$$

where

- $\mathbf{u} \sim \mathcal{U}(\mathbb{C}S^p)$ follow an uniform distribution on unit complex p -sphere
- \mathcal{Q} is the **2nd-order modular variate**, independent of \mathbf{u} , with pdf

$$p(\mathcal{Q}) = \delta_{p,g}^{-1} \mathcal{Q}^{p-1} g(\mathcal{Q})$$

Interpretation:

- $\boldsymbol{\Sigma}$ pilots the **shape of the ellipsoid** (privileged direction)
- \mathcal{Q} (equivalently g) models **amplitude fluctuations** (possibly heavy tails)

Some remarks on CES properties

1. **One-to-one relation** between pdf of \mathcal{Q} and g
2. **Ambiguity**: (\mathcal{Q}, Σ) and $(c^{-1}\mathcal{Q}, c\Sigma)$, $c > 0$ are valid stochastic representations of \mathbf{x}
 \Rightarrow requires normalization constraint
3. **Covariance matrix**: $\mathbb{E} [(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^H] = \mathbb{E}[\mathcal{Q}]\Sigma/p$, if $\mathbb{E}[\mathcal{Q}]$ exists
4. **Sampling**:
 - Draw a 2nd-order modular variate \mathcal{Q} from its pdf $p()$
 - Draw $\mathbf{n} \sim \mathcal{CN}(\mathbf{0}, \mathbf{I}_p)$, then $\mathbf{u} \stackrel{d}{=} \mathbf{n}/|\mathbf{n}| \mathcal{U} \sim (\mathbb{C}S^p)$
 - Set $\mathbf{x} \stackrel{d}{=} \boldsymbol{\mu} + \sqrt{\mathcal{Q}}\Sigma^{1/2}\mathbf{u}$

Important related distribution families

Compound Gaussian (CG) aka spherically invariant random vectors (SIRV)

$\mathbf{x} \sim \mathcal{CG}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, f_\tau)$ iif it admits the stochastic CG-representation

$$\mathbf{x} \stackrel{d}{=} \boldsymbol{\mu} + \sqrt{\tau} \mathbf{n}$$

where

- $\tau \geq 0$ is called the **texture**, with pdf f_τ that is independent of \mathbf{n}
- $\mathbf{n} \sim \mathbb{C}\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$ is called the **speckle**.

Note: subclass of CES because if $\mathbf{n}_0 \sim \mathbb{C}\mathcal{N}(\mathbf{0}, \mathbf{I})$, then $\mathbf{n}_0 \stackrel{d}{=} \sqrt{s} \mathbf{u}$ with $s \sim \Gamma(1, p)$

Mixture of scaled Gaussian distributions (MSG)

$\mathbf{x}_i \sim \mathbb{C}\mathcal{N}(\mathbf{0}, \tau_i \boldsymbol{\Sigma})$, where τ_i is unknown deterministic

Main examples (1/2)

Multivariate Gaussian distribution

CG: $f_\tau = \delta_1$ (or CES with $\mathcal{Q} \sim \Gamma(1, p)$)

Multivariate t -distribution with degree of freedom ν

CG: $\tau^{-1} \sim \Gamma(\nu/2, 2/\nu)$, where $\nu > 0$

- Encompasses **Complex Cauchy dist.** ($\nu = 1$) and **CN dist.** ($\nu \rightarrow \infty$)
- Finite 2nd-order moment for $\nu > 2$

K -distribution with shape parameter ν

CG: $\tau \sim \Gamma(\nu, 1/\nu)$, where $\nu > 0$

- Encompasses **heavy-tailed dist.** ($\nu \downarrow$) and **CN dist.** ($\nu \rightarrow \infty$)
- $\mathbb{E}[\tau] = 1 \implies \Sigma = \mathbb{E} [\mathbf{x}\mathbf{x}^H]$

Main examples (2/2)

GG distribution with parameters s and η

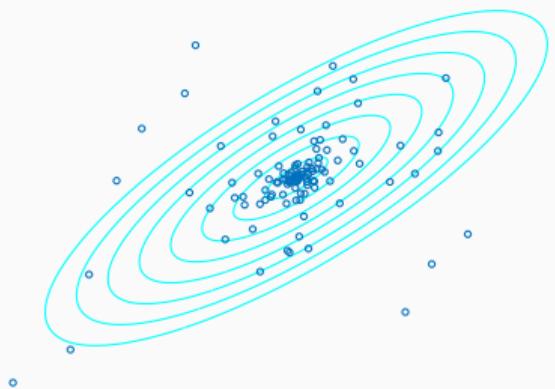
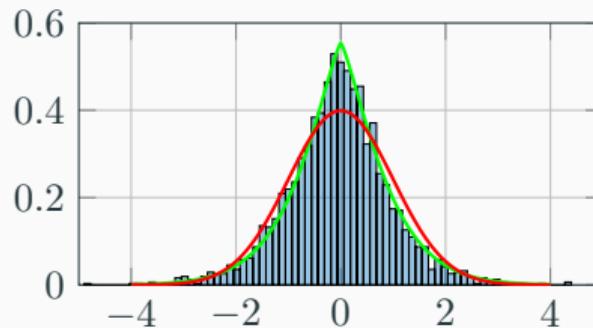
- CES: $\mathcal{Q} =_d G^{1/s}$ where $G \sim \Gamma(m/s, \eta)$, $s, \eta > 0$
- PDF: $f_{\mathbf{x}}(\mathbf{x}) = cte |\Sigma|^{-1} \exp(-(\eta \mathbf{x}^H \Sigma^{-1} \mathbf{x})^s)$
- Complex analog of the [exponential power family](#), also called [Box-Tiao distributions](#)
- Subclass of multivariate [symmetric Kotz-type distributions](#)
- Case $s = 1 \implies$ [CN dist.](#)
- Heavier tailed than normal for $s < 1$ and lighter tailed for $s > 1$
- $s = 1/2 \implies$ generalization of [Laplace dist.](#)

Wrapping-up

Complex elliptically symmetric distributions (CES)

$\mathbf{x} \sim \mathcal{CES}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, g)$ if it has for pdf

$$f(\mathbf{x}) \propto |\boldsymbol{\Sigma}|^{-1} g((\mathbf{x} - \boldsymbol{\mu})^H \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}))$$



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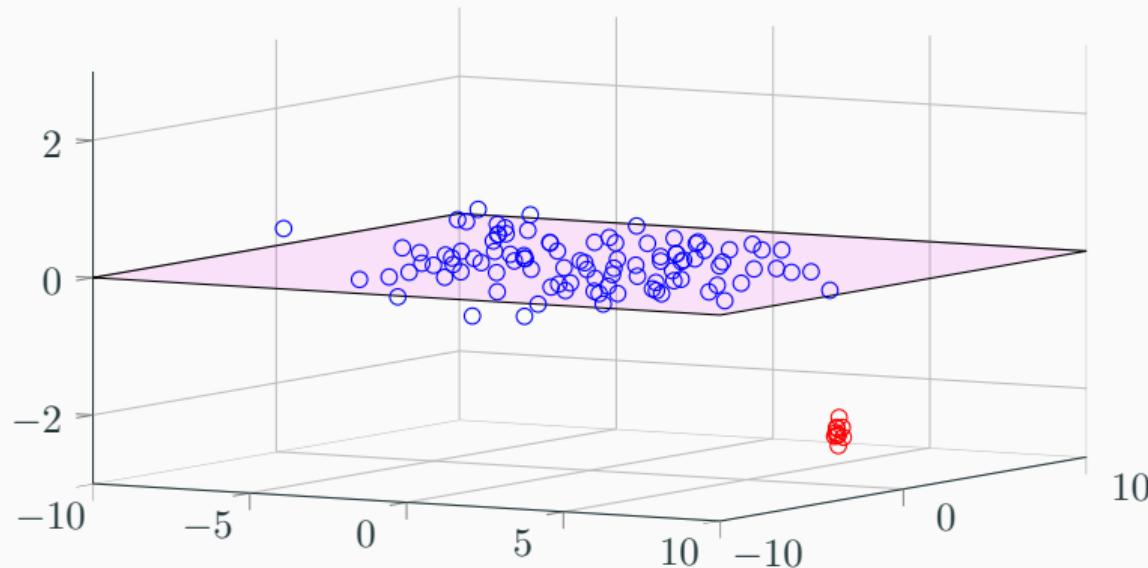
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Subspace learning grounds

$$\mathbf{x}_i \simeq \mathbf{U}\mathbf{U}^H\mathbf{x}_i, \text{ with } \mathbf{U} \in \text{St}(p, k) \triangleq \{\mathbf{U} \in \mathbb{C}^{p \times k} \mid \mathbf{U}^H\mathbf{U} = \mathbf{I}\}$$



Probabilistic PCA and low-rank factor models

- **Probabilistic PCA** in Gaussian model

[Tipping, 1999]

$$\mathbf{x}_i = \mathbf{UD}^{1/2}\mathbf{s}_i + \mathbf{n}_i \quad \text{with} \quad \mathbf{s} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_k) \quad \text{and} \quad \mathbf{n} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_p)$$

ML estimator of \mathbf{U} is the k leading eigenvectors of $\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top \Leftrightarrow \text{PCA}$

- **Factor models** generalizes to $[\mathbf{n}]_j \sim \mathcal{N}(\mathbf{0}, \sigma_j^2)$, resulting in the **covariance structure**

$$\begin{aligned} \mathbb{E}[\mathbf{x}\mathbf{x}^\top] = \boldsymbol{\Sigma} &\in \mathcal{M}_{p,k} = \left\{ \boldsymbol{\Sigma} = \mathbf{H} + \boldsymbol{\Psi}, \mathbf{H} \in \mathcal{S}_{p,k}^+, \boldsymbol{\Psi} \in \mathcal{D}_p^{++} \right\} \\ &= \text{"rank } k \text{ plus diagonal"} \end{aligned}$$

Dimension reduction: from $p(p+1)/2$ to $p(k+1) - k(k-3)/2$ parameters!

Outline

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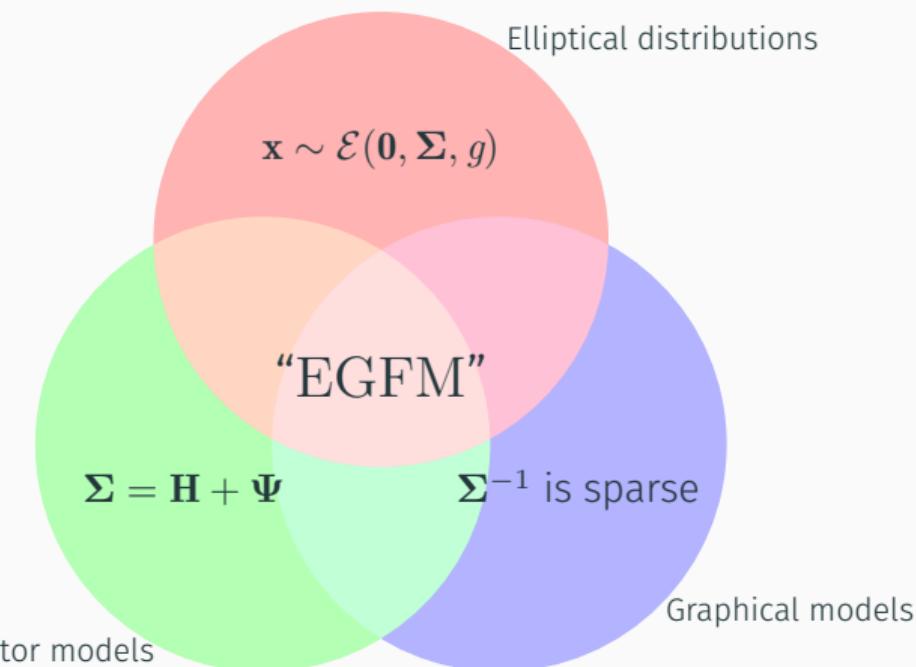
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Putting everything together



Learning EGFM

$$\begin{aligned} & \underset{\Sigma \in \mathcal{S}_p^{++}}{\text{minimize}} \quad \mathcal{L}(\Sigma) + \lambda h(\Sigma) \\ & \text{subject to} \quad \Sigma \in \mathcal{M}_{p,k} \end{aligned}$$

- **Likelihood**

$$\mathcal{L}(\Sigma) \propto \frac{1}{n} \sum_{i=1}^n \rho(\mathbf{x}_i^\top \Sigma^{-1} \mathbf{x}_i) + \frac{1}{2} \log |\Sigma| + \text{const.}$$

e.g., $g(t) = (1 + t/\nu)^{-\frac{\nu+p}{2}}$ for t -distribution

- **Smooth penalty**

$$h(\Sigma) = \sum_{q \neq \ell} \phi([\Sigma^{-1}]_{q\ell})$$

e.g., $\phi(t) = \varepsilon \log(\cosh(t/\varepsilon))$

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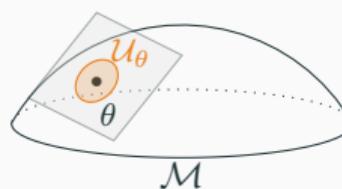
Structured parameter space as a manifold

The **parameter spaces**

- **Covariance matrices:** $\Sigma \in \mathcal{H}_p^{++}$
- **Rank k PSD matrices:** $\mathbf{H} \in \mathcal{S}_{p,k}^+$

turn out to be **manifolds** \mathcal{M} (locally diffeomorphic to \mathbb{R}^d , with $\dim(\mathcal{M}) = d$)

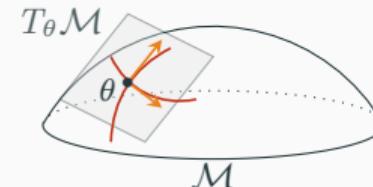
$\forall \theta \in \mathcal{M}, \exists \mathcal{U}_\theta \subset \mathcal{M}$ and $\varphi_\theta : \mathcal{U}_\theta \rightarrow \mathbb{R}^d$, diffeomorphism



Riemannian manifolds (1/2)

Tangent space $T_\theta \mathcal{M}$ at point θ

- Curve $\gamma : \mathbb{R} \rightarrow \mathcal{M}, \gamma(0) = \theta$
- Derivative: $\dot{\gamma}(0) = \lim_{t \rightarrow 0} \frac{\gamma(t) - \gamma(0)}{t}$
- Tangent space $T_\theta \mathcal{M} = \{\dot{\gamma}(0) : \gamma : \mathbb{R} \rightarrow \mathcal{M}, \gamma(0) = \theta\}$

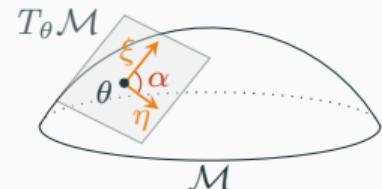


Equip $T_\theta \mathcal{M}$ with a **Riemannian metric** $\langle \cdot, \cdot \rangle_\theta$ yields a **Riemannian manifold**

- $\langle \cdot, \cdot \rangle_\theta : (T_\theta \mathcal{M} \times T_\theta \mathcal{M}) \rightarrow \mathbb{R}$ **inner product** on $T_\theta \mathcal{M}$
(bilinear, symmetric, positive definite)
- defines length and relative positions of tangent vectors

$$\|\xi\|_\theta^2 = \langle \xi, \xi \rangle_\theta$$

$$\alpha(\xi, \eta) = \frac{\langle \xi, \eta \rangle_\theta}{\|\xi\|_\theta \|\eta\|_\theta}$$



Riemannian manifolds (2/2)

The Riemannian metric $\langle \cdot, \cdot \rangle_\theta$ induces **a geometry** for \mathcal{M}

Geodesics $\gamma : [0, 1] \rightarrow \mathcal{M}$

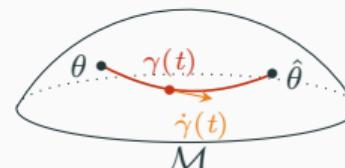
- generalizes straight lines on \mathcal{M}

- curves on \mathcal{M} with zero acceleration: $\frac{D^2\gamma}{dt^2} = 0$

defined by $(\gamma(0), \dot{\gamma}(0))$ or $(\gamma(0), \gamma(1))$

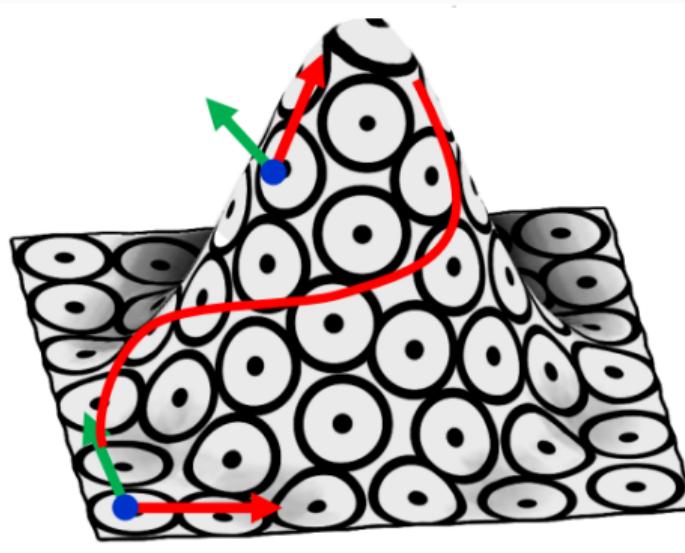
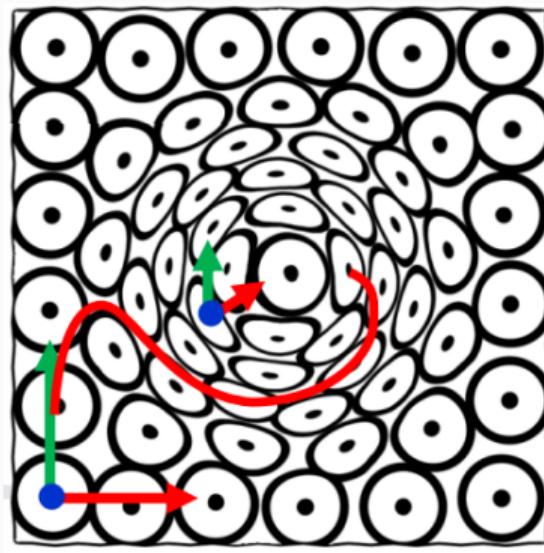
operator $\frac{D^2}{dt^2}$ depends on \mathcal{M} and $\langle \cdot, \cdot \rangle$.

Riemannian distance $\text{dist}(\theta, \hat{\theta}) = \int_0^1 \|\dot{\gamma}(t)\|_{\gamma(t)} dt$



distance = length of γ connecting θ and $\hat{\theta}$

Riemannian geometry – Riemannian metric: intuition



Which metric/geometry to chose ?

The **Fisher information metric** looks like an **ideal driven by the model**

Still, we can chose **alternate metrics suited to some needs**

- Availability (**closed-form**) of theoretical objects
- Interesting **invariance** properties
- **Practical results** of the chosen task

Metric	Geodesics	Distance	Retraction	Completeness	Invariance 1	Invariance 2	Perf.
(a)	✗	✗	✓	✓	✗	✓	82%
(b)	✓	✗	✓	✓	✓	✗	86%
(c)	✓	✓	✓	✗	✗	✓	79%

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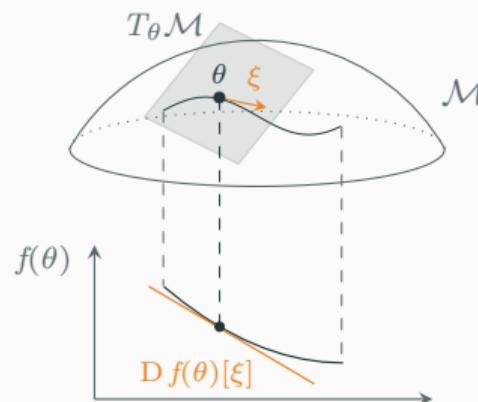
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Riemannian optimization

$$\underset{\theta \in \mathcal{M}}{\text{minimize}} \quad f(\theta)$$

Riemannian optimization: a framework for optimization on \mathcal{M} equipped with $\langle \cdot, \cdot \rangle$.



Descent direction of f at θ :

$$\xi \in T_\theta \mathcal{M}, \quad Df(\theta)[\xi] < 0$$

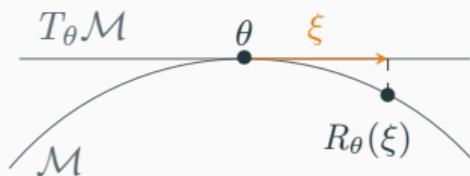
Riemannian gradient of f at θ :

$$\langle \text{grad } f(\theta), \xi \rangle_\theta = Df(\theta)[\xi]$$

Riemannian optimization

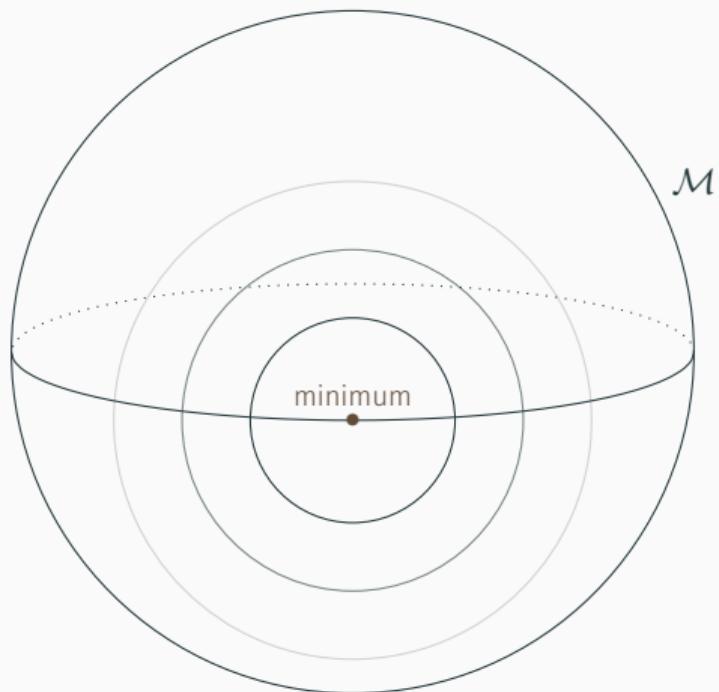
Main ingredients

- Descent direction: $\xi \in T_\theta \mathcal{M}$ so that $\langle \text{grad } f(\theta), \xi \rangle_\theta < 0$
- **Retraction** of ξ on \mathcal{M} (smooth mapping)

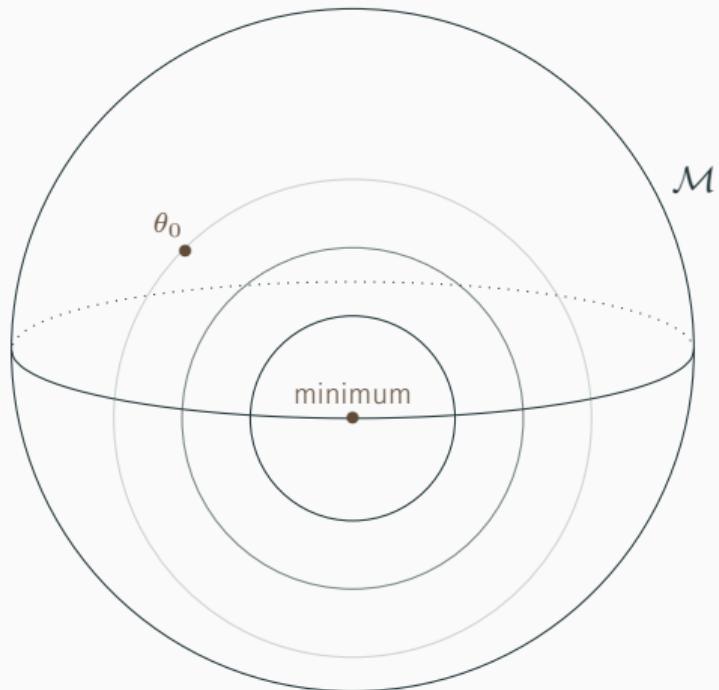


Flexibility: metric, retraction, descent method (gradient, conjugate gradient, BFGS...)

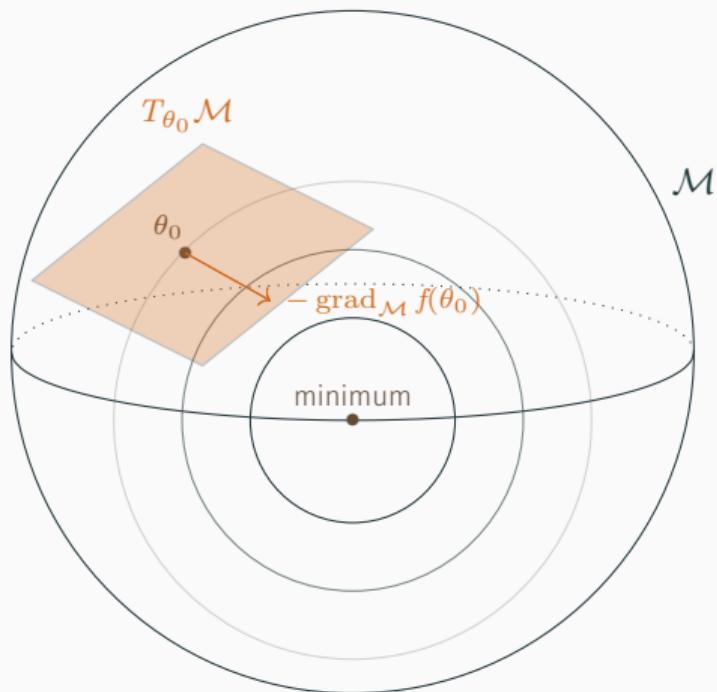
Example: Riemannian gradient descent $\theta_{i+1} = R_{\theta_i}(-t_i \text{grad } f(\theta_i))$



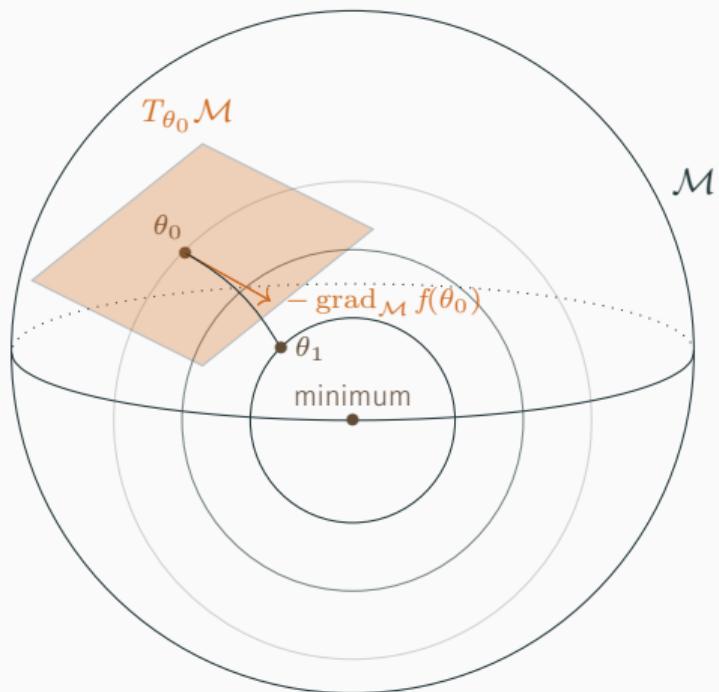
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Optimization on \mathcal{S}_p^{++} and $\mathcal{M}_{p,k}$

Tools for $\Sigma \in \mathcal{S}_p^{++}$

Tangent space $\forall \Sigma \in \mathcal{S}_p^{++}, T_\Sigma \mathcal{S}_p^{++} \simeq \mathcal{S}_p$

Metric $\langle \xi, \eta \rangle_\Sigma = \text{Tr}(\Sigma^{-1} \xi \Sigma^{-1} \eta)$

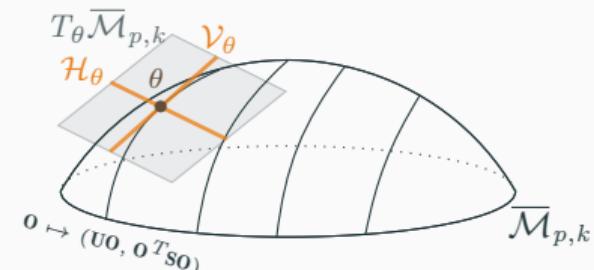
Gradient $\text{grad } f(\Sigma) = \Sigma \text{ sym}(\text{grad}_{\mathcal{S}} f(\Sigma)) \Sigma$

Retraction $R_\Sigma(\xi) = \Sigma + \frac{1}{2} \xi \Sigma^{-1} \xi$

Tools for $\mathbf{H} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^H \in \mathcal{H}_{p,k}^+$ as $(\text{St}(p, k) \times \mathcal{H}_k^{++})/\mathcal{U}_k$

Metric:

$$\langle \bar{\xi}, \bar{\eta} \rangle_{\bar{\theta}} = \underbrace{\Re(\text{Tr}(\xi_{\mathbf{U}}^H (\mathbf{I}_p - \frac{1}{2} \mathbf{U} \mathbf{U}^H) \eta_{\mathbf{U}}))}_{\text{canonical on } \text{St}(p, k)} + \underbrace{\alpha \text{Tr}(\boldsymbol{\Lambda}^{-1} \xi_{\boldsymbol{\Lambda}} \boldsymbol{\Lambda}^{-1} \eta_{\boldsymbol{\Lambda}}) + \beta \text{Tr}(\boldsymbol{\Lambda}^{-1} \xi_{\boldsymbol{\Lambda}}) \text{Tr}(\boldsymbol{\Lambda}^{-1} \eta_{\boldsymbol{\Lambda}})}_{\text{affine invariant on } \mathcal{H}_k^{++}}$$



details in [Bouchard21] =)

Outline

- **Design**

- Gaussian Graphical models
- Elliptical models
- Probabilistic PCA and factor models
- Everything together

- **Solve**

- Manifolds and Riemannian geometry
- Riemannian optimization

- **Apply** on real data examples

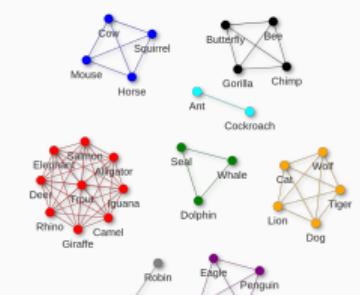
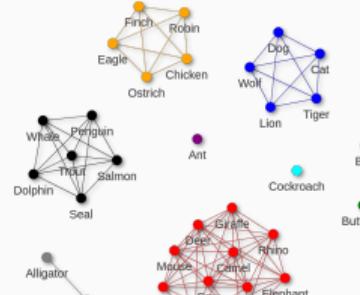
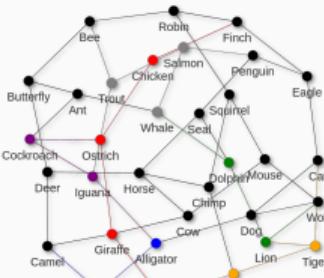
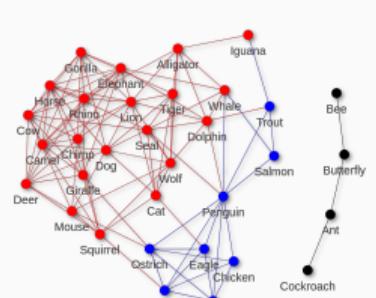
Applications on some data sets

Methods

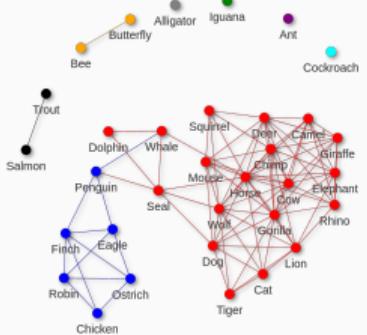
- **GLasso**
- 4 options of **EGFM**: {Gaussian, t -dist.} \times {Full rank, Factor model}
- Laplacian learning: **NGL** (Gauss.), **SGL** (Gauss., K -comp.), **StGL** (t -dist., K -comp.)

Datasets

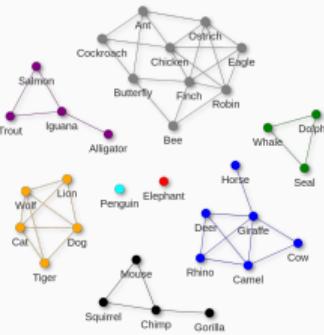
- **Animals**: $p = 33$ animals, $n = 102$ categorical questions
- **GNSS Piton de la Fournaise**: $p = 22$ stations, $n = 1106$ dates
- **Concepts**: $p = 1000$ concepts, $n = 218$ semantic features (5pt scale)



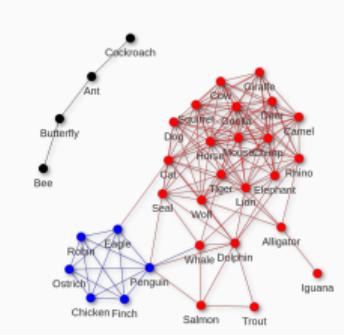
GLasso



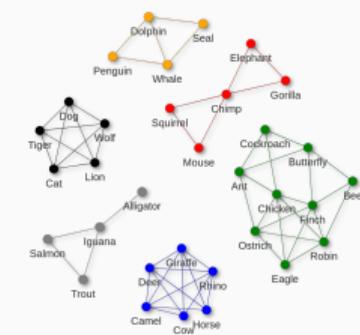
NGL



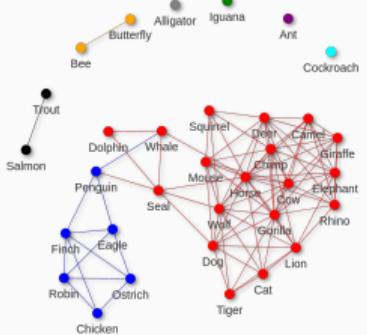
SGL



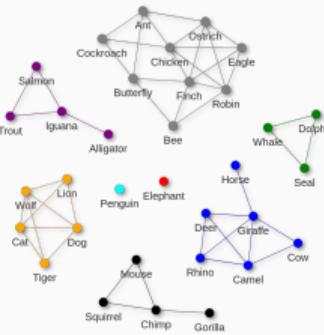
StGL



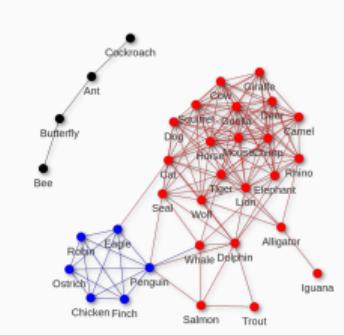
GGM



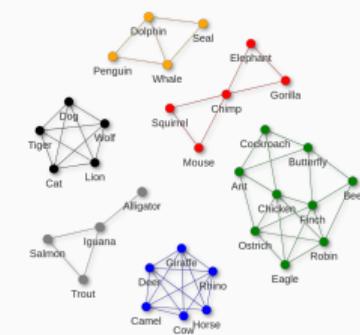
GGFM

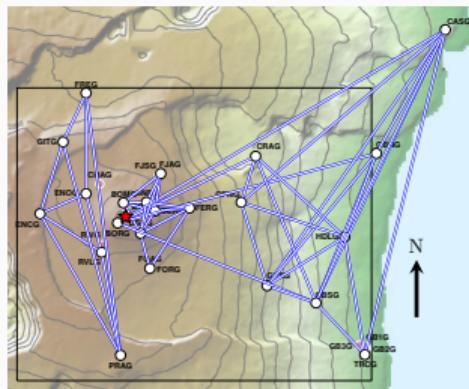


EGM

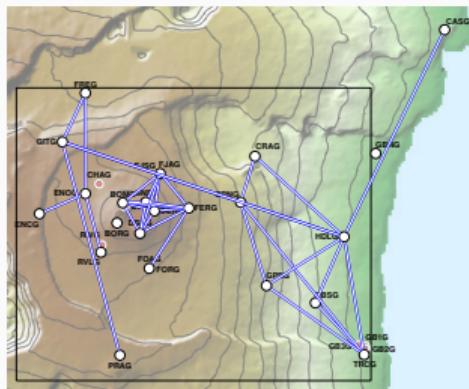


EGFM

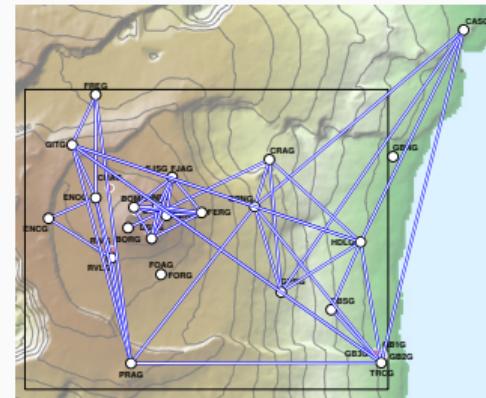




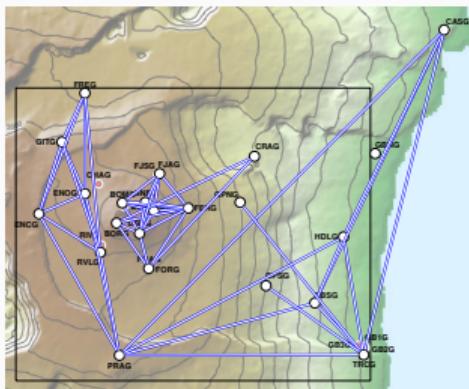
StGL



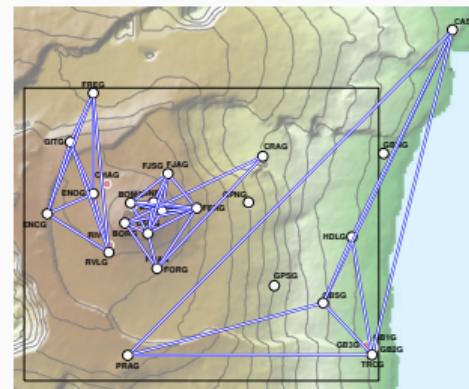
GGM



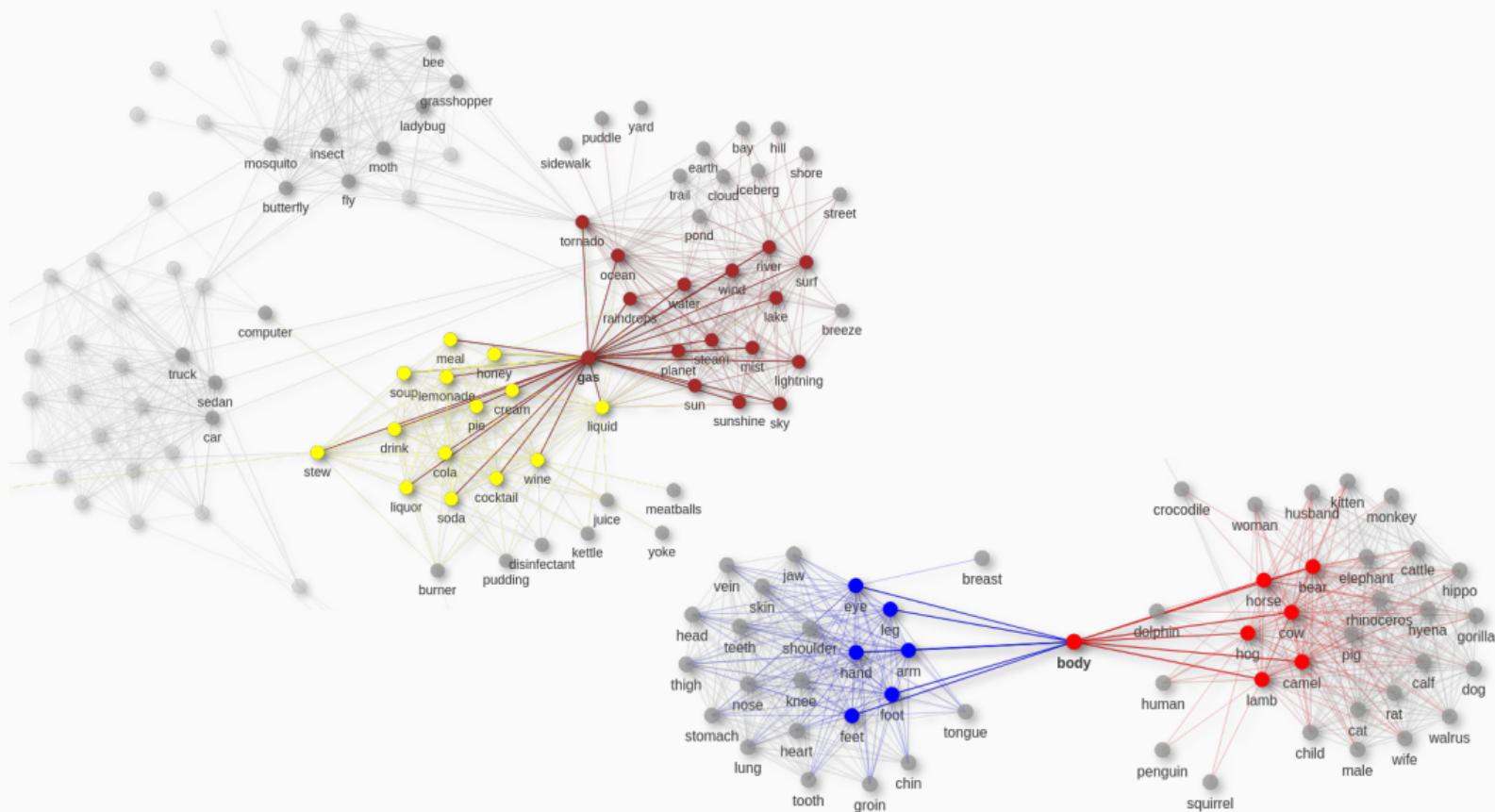
EGM



GGFM



EGFM



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Perspectives

Graph Learning

- Other statistical models \mathcal{L}
- More structures \mathcal{M} (Laplacian, MTP₂, ...)

Geometry of graphs:

- Riemannian geometry of adjacency/Laplacian matrices
- Classify using graphs as features

Links with optimal transport of graphs

Thanks for the invitation! ;D