Model selection for simplicial approximation

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Summary

Outline

1. Motivations
2. Model selection and simplicial complexes
3. Experimental results
4. Discussion

Principal Component Analysis

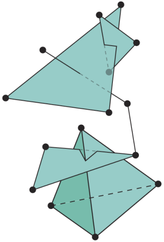
- Observations $X_1, \ldots, X_n \in \mathbb{R}^D$.
- probabilist version of PCA :

  Model : $x_i = z_i + \varepsilon_i$ where $z_i \in E_d$ affine subspace of R^Q

  PCA : least square minimization to find E_d.
- Main limitation : linearity of E_d.
- Extension : principal curves.

Data analysis with simplicial complexes

- Simplicial complex (s.c.) $\mathcal{C}$:
  - Any face of a simplex from $\mathcal{C}$ is also in $\mathcal{C}$.
  - The intersection of any two simplices s_1, $s_2 \in \mathcal{C}$ is either a face of both s_1 and s_2, or empty.

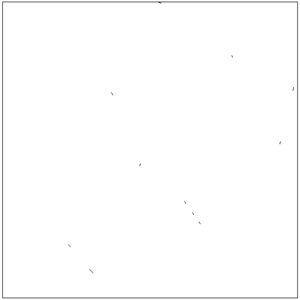


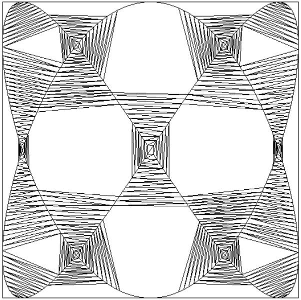
- Ex : Delauney, Rips complex, α-shape, witness complex ...
- s.c. are used for:
  - dimension estimation,
  - topological inference,
  - reconstruction.
- Initial idea of this work : fit a s.c. on the data.

General framework of the talk

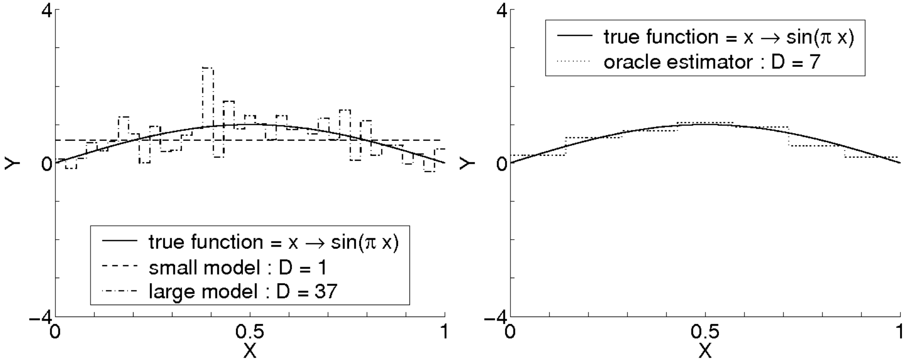
- Observations $X_1, \dots, X_n$.
- Choose some landmarks points.
- Several possible s.c. can be defined on the landmarks :
  $\longrightarrow$ a collection of s.c. $(\mathcal{C}_{\alpha \in \mathcal{A}})$ indexed by a scale parameter α.
- Which s.c should be chosen ?

Framework of the talk

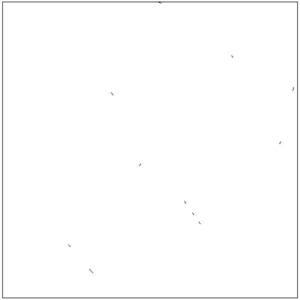


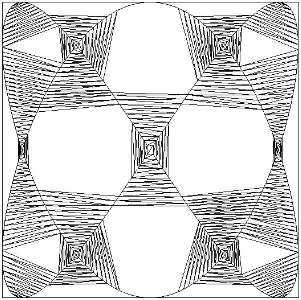


bias-variance tradeoff



Framework of the talk





Aims of this work :

- Define a statistical framework for the simplicial approximation.
- Use some model selection tools to find a “convenient” s.c. in the collection.

Outline

Geometric model

- $\mathcal{G}$ is an unknown geometric object embedded in $\mathbb{R}^D$,

$$\forall i = 1, \ldots, n, \quad X_i = \bar{x}_i + \sigma \xi_i \quad \text{with} \quad \bar{x}_i \in \mathcal{G}$$

  where the original points $\bar{x}_i$ are unknown. The r.v. ξ_i are independent standard Gaussian vectors.

- equivalent statement :

$$\mathbf{X} = \bar{\mathbf{x}} + \sigma \boldsymbol{\xi} \quad \text{with} \quad \bar{\mathbf{x}} \in \mathcal{G}^n,$$

- Best approximating point of $\bar{\mathbf{x}}$ belonging to $\mathcal{C}^n$ is the least square estimator (LSE) of $\bar{\mathbf{x}}$ associated to $\mathcal{C}^n$:

$$\hat{\mathbf{x}}_{\mathcal{C}} := \operatorname{argmin}_{\mathbf{t} \in \mathcal{C}^n} \|\mathbf{X} - \mathbf{t}\|^2.$$

  Notation : $\forall u \in \mathbb{R}^{nD}$, $\|u\|^2 := \frac{1}{nD} \sum_{i=1}^{nD} u_i^2$.

- A collection of s.c. $(\mathcal{C}_{\alpha \in \mathcal{A}}) \longrightarrow$ a collection of LSE : $(\hat{\mathbf{x}}_\alpha)_{\alpha \in \mathcal{A}}$

Asymptotic model selection criterion

- Model selection via penalization :

$$\mathrm{crit}(m) = \gamma_n(\hat{\mathbf{x}}_m) + \mathrm{pen}(m)$$

  γ_n : empirical contrast: least squares or log likelihood.
  pen : $\mathcal{A} \to \mathbb{R}^+$: penalty function.

- C_p Mallows : penalized least square regression, pen $= 2D\sigma^2/n$.
- AIC : density estimation, pen $= D/n$
- BIC : density estimation pen $= D \log n/n$

- All these criterion are based on asymptomatic results.
- In our context : can be hardly applied since
  - no theoretical justifications,
  - what is D ?

Non asymptotic Gaussian model selection

- Birgé and Massart : non asymptotic model selection theory.
- Gaussian model selection (in our context)

$$\mathbf{X} = \bar{\mathbf{x}} + \sigma \boldsymbol{\xi} \quad \text{with } \bar{\mathbf{x}} \in \mathbb{R}^{Q}$$

- Collection of models $(C_\alpha)_{\alpha \in \mathcal{A}}$, where $C_\alpha \subset \mathbb{R}^Q$
  $\rightarrow$ LSE estimators $(\hat{\mathbf{x}}_\alpha)_{\alpha \in \mathcal{A}}$.
- Risk of $\hat{\mathbf{x}}_\alpha$: $\mathbb{E}_{\bar{\mathbf{x}}}\left(\|\bar{\mathbf{x}} - \hat{\mathbf{x}}_\alpha\|^2\right)$.
- Oracle (unknown): $\alpha_{or} := \underset{\alpha \in \mathcal{A}}{\operatorname{argmin}} \mathbb{E}_{\bar{\mathbf{x}}}\left(\|\bar{\mathbf{x}} - \hat{\mathbf{x}}_\alpha\|^2\right)$.
- Aim : find a penalty function pen such that the risk of $\hat{\mathbf{x}}_{\hat{\alpha}}$ where

$$\hat{\alpha} := \underset{\alpha \in \mathcal{A}}{\operatorname{argmin}} \left\{\|\mathbf{X} - \hat{\mathbf{x}}_\alpha\|^2 + \operatorname{pen}(\alpha)\right\},$$

is close to the benchmark $\min_{\alpha \in \mathcal{A}} \mathbb{E}_{\bar{\mathbf{x}}}\left(\|\bar{\mathbf{x}} - \hat{\mathbf{x}}_\alpha\|^2\right)$.

Non asymptotic Gaussian model selection

- The penalty function depends on (see the theorem hereafter)
  1. the "size" of the model collection,
  2. the complexity of the models.
- Hypothesis on the model collection "size" : some weights w_α fulfills

$$\sum_{\alpha \in \mathcal{A}} e^{-w_\alpha} = \Sigma < \infty.$$

- Complexity of each model : entropy measure. For all $\alpha \in \mathcal{A}$, the auxiliary entropic function Φ_α is defined by

$$\Phi_\alpha(u) = \kappa \int_0^u \sqrt{\mathrm{H}(C_\alpha, \|\cdot\|, r)}\, dr.$$

For all $\alpha \in \mathcal{A}$ let d_α defined by the equation (if it exits)

$$\Phi_\alpha\left(\frac{2\sigma\sqrt{Q}}{\sqrt{d_\alpha}}\right) = \frac{\sigma d_\alpha}{\sqrt{Q}}.$$

Non asymptotic Gaussian model selection

Theorem 1 - Birgé Massart 01 [2]

Let $\eta > 1$. For a penalty such that

$$\mathrm{pen}(\alpha) \geq \eta\, \sigma^2 \left(\sqrt{d_\alpha} + \sqrt{2 w_\alpha} \right)^2$$

Then, almost surely, there exists a minimizer $\hat{\alpha}$ of the penalized criterion

$$\mathrm{crit}(\alpha) = \|\mathbf{X} - \hat{\mathbf{x}}_\alpha\|^2 + \mathrm{pen}(\alpha).$$

Furthermore, the following risk bound holds for all $\bar{\mathbf{x}} \in \mathbb{R}^Q$

$$\mathbb{E}_{\bar{\mathbf{x}}} \|\hat{\mathbf{x}}_{\hat{\alpha}} - \bar{\mathbf{x}}\|^2 \leq c_\eta \left[\inf_{\alpha \in \mathcal{A}} \left\{ d(\bar{\mathbf{x}}, C_\alpha)^2 + \mathrm{pen}(\alpha) \right\} + \sigma^2 (\Sigma + 1) \right]$$

where c_η depends only on η and $d(\bar{\mathbf{x}}, C_\alpha) := \inf_{\mathbf{y} \in C_\alpha} \|\bar{\mathbf{x}} - \mathbf{y}\|$.

Non asymptotic linear Gaussian model selection

- The models C_α are linear subspaces of $\mathbb{R}^{nD}$.
- d_α is equal to the dimension of C_α.
- Risk bound : true oracle inequality :

$$\mathbb{E}_{\bar{\mathbf{x}}} \|\hat{\mathbf{x}}_{\hat{\alpha}} - \bar{\mathbf{x}}\|^2 \leq c'_\eta \left[\inf_{\alpha \in \mathcal{A}} \left\{ \mathbb{E}_{\bar{\mathbf{x}}} \left(\|\bar{\mathbf{x}} - \hat{\mathbf{x}}_\alpha\|^2 \right) \right\} + \sigma^2 (\Sigma + 1) \right]$$

- But if $\mathcal{C}_\alpha$ is a simplicial complex, of course $C_\alpha = \mathcal{C}_\alpha^n$ is not a linear subspace.

Model selection on simplicial complexes

- $(\mathcal{C}_\alpha)_{\alpha\in\mathcal{A}}$ a collection of k-homogeneous s.c. in $\mathbb{R}^D$
- Hypothesis on the collection "size". Weights : $w_\alpha = L \ln |\mathcal{C}_\alpha|_k$ with

$$\sum_{\alpha\in\mathcal{A}} \frac{1}{x_\alpha^L} = \Sigma < \infty$$

- Notation :
  Δ_s : diameter of the smallest including ball of the simplex s.
  $|\mathcal{C}|_k := (\sum_{s\in\mathcal{C}^+} \Delta_s^k)^{1/k}$ and $\delta_\mathcal{C} := \inf_{s\in\mathcal{C}_\alpha^+} \Delta_s$ where $\mathcal{C}_\alpha^+$ is the subset of simplices of $\mathcal{C}_\alpha$ of maximal dimension k.
- Hypothesis on the s.c. complexity. For all $\alpha \in \mathcal{A}$,

$$\sigma \leq \delta_{\mathcal{C}_\alpha} \sqrt{\frac{D}{k}} \left[4\kappa \left(\sqrt{\ln \frac{4|\mathcal{C}_\alpha|_k}{\delta_{\mathcal{C}_\alpha}}} + \sqrt{\pi} \right) \right]^{-1}.$$

Model selection on simplicial complexes

Theorem 2 - Caillerie and M. (2009) [4]

There exists some absolute constants c_1 and c_2 such that for all $\eta > 1$, if

$$\mathrm{pen}(\alpha) \geq \eta\, \sigma^2 \left(c_1\, nk \left[\ln \frac{|\mathcal{C}_\alpha|_k \sqrt{D}}{\sigma\sqrt{k}} + c_2 \right] \right),$$

then, almost surely, there exists a minimizer $\hat{\alpha}$ of the penalized criterion

$$\mathrm{crit}(\alpha) = \|\mathbf{X} - \hat{\boldsymbol{x}}_\alpha\|^2 + \mathrm{pen}(\alpha)$$

and the penalized estimator $\hat{\boldsymbol{x}}_{\hat{\alpha}}$ satisfies the following risk bound

$$\mathbb{E}_{\bar{\boldsymbol{x}}} \|\hat{\boldsymbol{x}}_{\hat{\alpha}} - \bar{\boldsymbol{x}}\|^2 \leq c_\eta \left[\inf_{\alpha \in \mathcal{A}} \left\{ d(\bar{\boldsymbol{x}}, \mathcal{C}^n_\alpha)^2 + \mathrm{pen}(\alpha) \right\} + \sigma^2 (\Sigma + 1) \right].$$

Remarks

- A quite general result.
- A qualitative result.
- Roughly speaking : pen is proportional to $\ln |\mathcal{C}_\alpha|_k$.
  For a collection of graph : $|\mathcal{C}_\alpha|_1$ is the graph length.
- Not exactly an oracle inequality ... additional work necessary to control the shape of the risk.
- If the true positions $\bar{\mathbf{x}}$ are sampled on $\mathcal{G}$ according to μ, for the integrated risk :

$$\int_{\bar{x}\in\mathcal{G}} \mathbb{E}_{\bar{x}} \|\hat{x}_{\hat{\alpha}} - \bar{x}\|^2 \, d\mu(\bar{x}) \leq c_\eta \left[\inf_{\alpha\in\mathcal{A}} \left\{ \int_{\bar{x}\in\mathcal{G}} d(\bar{x}, \mathcal{C}_\alpha)^2 \, d\mu(\bar{x}) + \mathrm{pen}(\alpha) \right\} + \sigma^2(\Sigma + 1) \right]$$

Sketch of the proof

- $C_\alpha = \mathcal{C}_\alpha^n$
- $Q = nD$
- Based on the following entropic result :

Proposition

For all k-homogeneous simplicial complex $\mathcal{C}$ of $\mathbb{R}^D$ and all $r \leq \delta_{\mathcal{C}}$

$$\mathrm{N}\left(\mathcal{C}^n, \|\cdot\|, r\right) \leq \left(\frac{4|\mathcal{C}|_k}{r}\right)^{nk}.$$

Outline

Slope heuristics

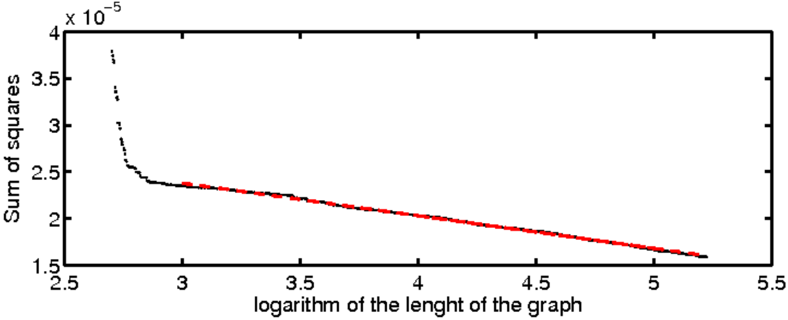
- The penalty type is known : $\text{pen}(\alpha) = c \log |\mathcal{C}_\alpha|_k$, but c is unknown.
- Slope heuristics method :
  1. For each simplicial complex, compute the sum of squares $SS(\alpha) := \|\hat{\mathbf{x}}_\alpha - \mathbf{X}\|^2$.
  2. Plot the point cloud $\{\ln |\mathcal{C}_\alpha|_k, SS(\alpha)\}_{\alpha \in \mathcal{A}}$ and check that a linear trend is observed for large α.
  3. Compute the slope $\hat{\beta}$ of the linear regression of $SS(\alpha)$ on $\ln |\mathcal{C}_\alpha|_k$ for large α.
  4. Select the simplicial complex in the collection minimizing

$$\text{crit}(\alpha) = \|\bar{\mathbf{x}} - \hat{\mathbf{x}}_\alpha\|^2 - 2\hat{\beta} \ln |\mathcal{C}_\alpha|_k \ .$$

- Theoretical results on the slope heuristics [3, 1].

Slope heuristics for graphs

"the optimal penalty is twice the minimal penalty"

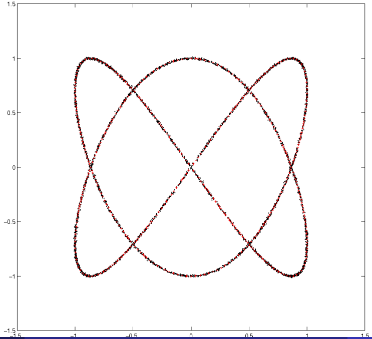


Selection of α-graphs : framework

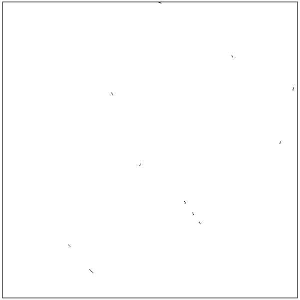
- An observed sample $X_1, \ldots, X_n$.
- Define a set of landmarks from the X_i.
- Define a collection of α-graphs (α-shape of dim 1).
- For each graph, compute the length $l(\alpha)$ and $SS(\alpha) := \|\hat{\mathbf{x}}_\alpha - \mathbf{X}\|^2$.
- Proceed the slope heuristics method to select a graph.

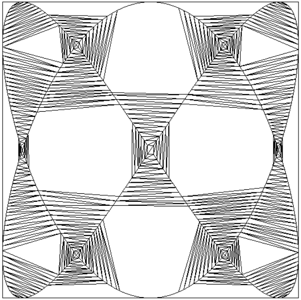
Lissajous curve (1)

- True points : $\bar{x}_1, \ldots, \bar{x}_n$ ($n = 5000$) sampled on the Lissajous curve.
- Observed points : $\forall i = 1, \ldots, n, \quad X_i = \bar{x}_i + \sigma\xi_i$, $\sigma = 0.005$.
- Landmarks points : Furthest point strategy on a set of true points (located on the Lissajous curve) $\rightarrow$ 500 landmark points.
- Compute the α-graphs on the landmark points.
- Compute the same experience 500 times to estimate the oracle graph (with fixed landmarks).

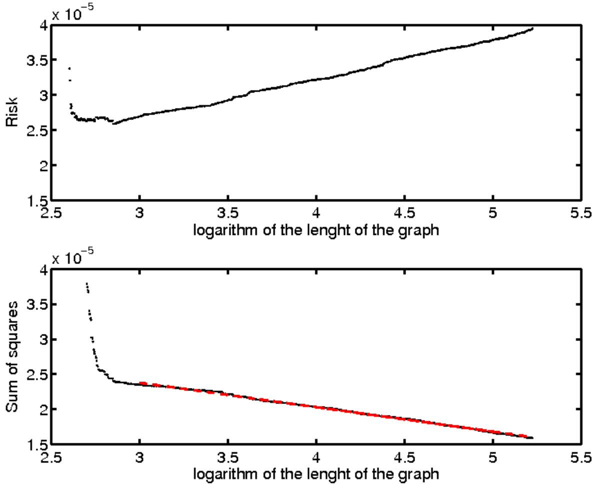


Lissajous curve (1) - extremal graphs



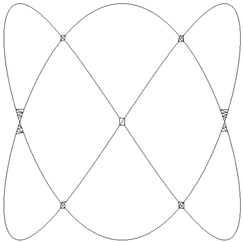


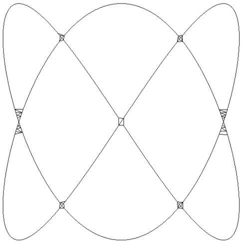
Lissajous curve (1) - risk and $SS(\alpha)$



$\Rightarrow$ the slope heuristics can be applied.

Lissajous curve (1) oracle and selected graphs





Lissajous curve (1) - 500 experiences

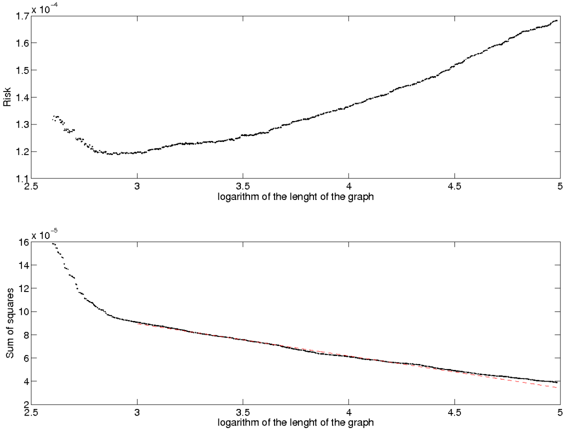
$\alpha \times 10^{-3}$	$\alpha_{\min}\ldots$	1.129	1.255	1.256	1.283	1.286	1.298	1.344
$N(\alpha)$	0	1	369	6	19	77	3	10
Selection perc.	0	0.2	73.8	1.2	3.8	15.4	0.6	2
Length	0.0394	16.86	17.30	17.37	17.45	17.50	17.57	17.64
Risk $\times 10^{-5}$	29841	2.627	2.589	2.588	2.591	2.594	2.594	2.596

$\alpha \times 10^{-3}$	1.493	1.603	1.643	1.669	1.672	1.748	$\ldots\alpha_{\max}$
$N(\alpha)$	6	4	1	2	1	1	0
Selection perc.	1.2	0.8	0.2	0.4	0.2	0.2	0
Length	17.71	17.97	18.10	18.31	18.46	18.61	185.8
Risk $\times 10^{-5}$	2.606	2.618	2.623	2.639	2.641	2.642	3.946

Lissajous curve (2)

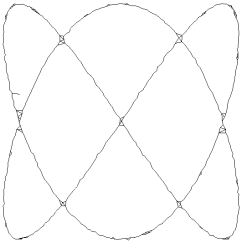
- Initial point set $\mathcal{P}$: $X_i = \bar{x}_i + \sigma\xi_i$, ($\sigma = 0.005$) where the $\bar{x}_i$ are sampled on the Lissajous curve.
- $\mathcal{P}$ is randomly separated into $\mathcal{P}_o$ (5000 points) and $\mathcal{P}_l$ (5000 points)
- Observed points : $\mathcal{P}_o$
- Landmark points : 500 landmarks points defined from $\mathcal{P}_l$ thanks to the neural-gas algorithm.
- Compute the α-graphs on the landmark points.
- Simulate $\mathcal{P}_o$ 500 times to estimate the oracle graph (with fixed landmarks).

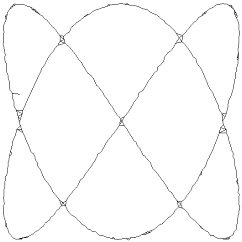
Lissajous curve (2) - risk and $SS(\alpha)$



$\Rightarrow$ the slope heuristics can be applied.

Lissajous curve (2) oracle and selected graphs



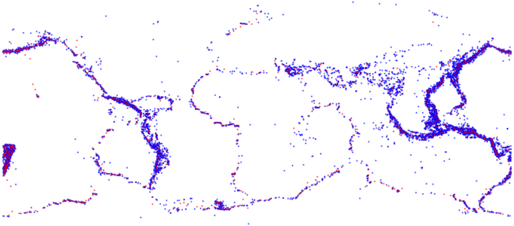


Lissajous curve (2) - 500 experiences

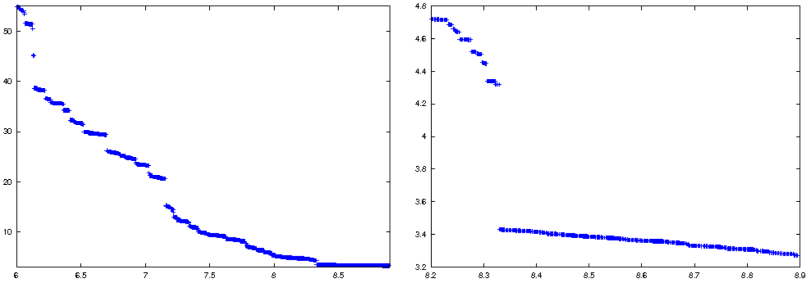
$\alpha \times 10^{-3}$	$\alpha_{min}\ldots$	0.9537	0.9891	1.051	1.076	1.078	1.084
$N(\alpha)$	0	38	3	107	36	281	2
Selection perc.	0	7.6	0.6	21.4	7.2	56.2	0.4
Length	0.03083	17.45	17.64	17.87	17.97	18.02	18.09
Risk $\times 10^{-4}$	308	1.1910	1.1899	1.1897	1.1942	1.1939	1.1937

$\alpha \times 10^{-3}$	1.126	1.183	1.187	1.200	1.205	1.271	$\ldots\alpha_{max}$
$N(\alpha)$	13	12	0	4	1	3	0
Selection perc.	2.6	2.4	0	0.8	0.2	0.6	0
Length	18.29	18.34	18.38	18.49	18.55	18.82	146.1
Risk $\times 10^{-4}$	1.1898	1.1886	1.1885	1.1899	1.1932	1.1944	1.6823

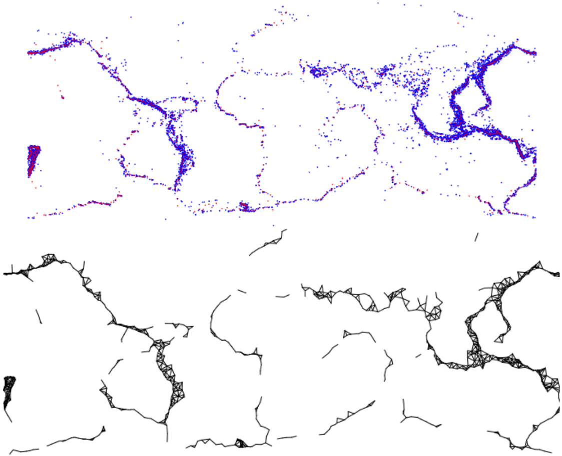
Real data : locations of earthquakes



Earthquakes : $SS(\alpha)$



Real data : selected graph



Outline

Discussion

- A first attempt to use modern model selection tools for geometric inference.
- Model selection via penalization : a general result gives the penalty form.
- For application : the slope heuristics does not work all the times (α -Rips)
- Future works :
  - theoretical aspects : a theory on s.c. approximation to control the bias.
  - heterogeneous s.c. ?
  - application : the same procedure in higher dimensions, other s.c families...

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