Domain selection for Gaussian Processes

An application to electrocardiogram signals

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This work...

Gabriel Martos, PhD. Associate Professor at the Department of Mathematics and Statistics of Universidad Torcuato Di Tella, Buenos Aires, Argentina.

Hernández, N., & Martos, G. (2023). Domain Selection for Gaussian Process Data: An application to electrocardiogram signals. arXiv preprint arXiv:2306.00538.

(some) issues in the High-dimensional setting...

what is the deal with having too much data?

Overfitting

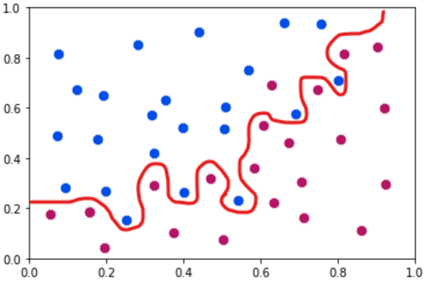
Estimation precision

Computational complexity

Interpretability

what is the deal with having too much data?

- **Overfitting**



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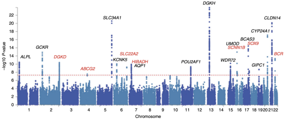
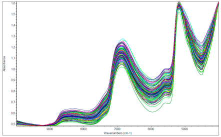


➡ Genetic Data



➡ Spectral Data (Chemometrics)

➡ Health records, e.g. electrocardiograms

(some) solution to these problems...

How can we tackle these issues?

- Dimension reduction methods (e.g. PCA)

Regularisation (e.g. LASSO)

Variable selection

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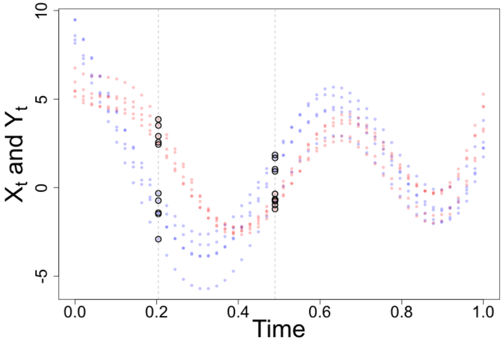
- Dimension reduction methods (e.g. PCA)
- Regularisation (e.g. LASSO)
- **Variable selection**

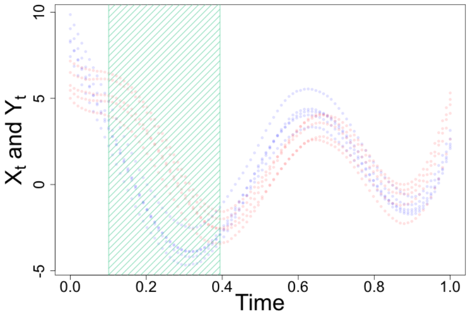
Focus on variable selection...



Select isolated variables

- find models with good prediction power,
- estimate the true "sparsity pattern".

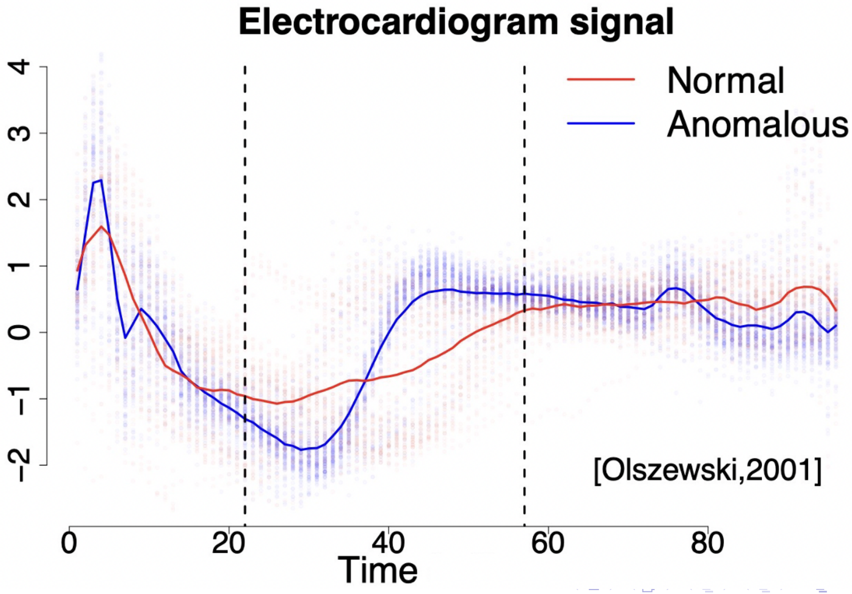
... but adding some restrictions: Domain Selection



Domain (interval) selection

- Select set of variables (intervals).
- Take advantage of the covariance structure.
- Variables are recorded almost continuously.

Motivation


Electrocardiogram signal
Normal
Anomalous
[Olszewski,2001]
Time
0
20
40
60
80
−2
−1
0
1
2
3
4

Objective: Domain Selection

For a pair of random processes, what is the region (domain) where they statistically differ the most?

- **Inference:**
  - Characterise and quantify the uncertainty around the estimation of the domain bounds.
  - Improve the power of a hypothesis test, i.e: two-sample test.
- **Prediction:** improve a classification model outcome, i.e: the misclassification error rate.
- **Computational burden:** reduce time and memory storage in the big data context. Future collection Strategy.

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Domain Selection: How?

compute differences with a local approach

↓

Kullback-Leibler divergence

↓

Let P and Q be two distributions of a continuous random variable x. Then the KL is:

$$\text{KL}(P||Q) = \int_{-\infty}^{\infty} p(x) log(\frac{p(x)}{q(x)}) dx$$

Domain Selection: How?

compute differences with a local approach

Kullback-Leibler divergence + **Gaussian** framework

$$\mathrm{KL}(X||Y) = \frac{1}{2}\left(\frac{\sigma_X^2}{\sigma_Y^2} - 1 + \frac{(\mu_X - \mu_Y)^2}{\sigma_Y^2} + \ln\left(\frac{\sigma_Y^2}{\sigma_X^2}\right)\right).$$

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Learning problem and local features

- Let $X(t) \sim GP(\mu_X(t), \sigma_X(t,s))$ be a GP **indexed on the compact set** $T \subset \mathbb{R}$, with:
  - $\mu_X(t) = E\{X(t)\}$ and $\sigma_X(t,s) = E\{(X(t) - \mu_X(t))(X(s) - \mu_X(s))\}$.
  - Likewise for $Y(t)$

Learn the interval where $X(t)$ and $Y(t)$ statistically differ the most.

- Estimate a compact subset $A \subset T$ with $\lambda(A) > 0$:

(A) **Differences in Mean.** $t \in A$: $|\mu_X(t) - \mu_Y(t)| > \nu$, and $t' \notin A : |\mu_X(t') - \mu_Y(t')| \leq \nu$.

Differences in Variance. $(t,s) \in A \times A$: $|\sigma_X(t,s) - \sigma_Y(t,s)| > \nu$, and $(t',s') \notin A \times A : |\sigma_X(t',s') - \sigma_Y(t',s')| \leq \nu$.

(A) and (B) simultaneously, possibly on different subsets A_μ and A_σ and for different ν_μ and ν_σ.

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The KL divergence in the GP context

- In practice GP data is recorded over a finite grid $\mathcal{T} = (t_1, \dots, t_p)$.
- In this case it corresponds to realisations of p-variate Gaussian random vectors and the KL has the following closed form:

$$\mathrm{KL}_{\mathcal{T}}(\mathbf{X}||\mathbf{Y}) \equiv \frac{1}{2}\left(\mathrm{tr}\left(\boldsymbol{\Sigma}_{\mathcal{T},Y}^{-1}\boldsymbol{\Sigma}_{\mathcal{T},X} - \mathbf{I}_p\right) + \Delta_{\mathcal{T}}^{\mathsf{T}}\boldsymbol{\Sigma}_{\mathcal{T},Y}^{-1}\Delta_{\mathcal{T}} + \ln\left(\frac{\det \boldsymbol{\Sigma}_{\mathcal{T},Y}}{\det \boldsymbol{\Sigma}_{\mathcal{T},X}}\right)\right),$$

where:

- $\Delta_{\mathcal{T}} = \left(\boldsymbol{\mu}_{\mathcal{T},Y} - \boldsymbol{\mu}_{\mathcal{T},X}\right)$,
- $\mathrm{tr}(\boldsymbol{\Sigma})$ denote the trace of $\boldsymbol{\Sigma}$, and
- $\det(\boldsymbol{\Sigma})$ the determinant of $\boldsymbol{\Sigma}$.

Domain Selection using the local-KL divergence

- For any subset $\mathcal{A} \subseteq \mathcal{T}$, we can also define the local–KL divergence as follows:

$$\mathrm{KL}_{\mathcal{A}}(X||Y) \equiv \frac{1}{2}\left(\mathrm{tr}\left(\mathbf{\Sigma}_{\mathcal{A},Y}^{-1}\mathbf{\Sigma}_{\mathcal{A},X} - \mathbf{I}_{|\mathcal{A}|}\right) + \Delta_{\mathcal{A}}^{\mathsf{T}}\mathbf{\Sigma}_{\mathcal{A},Y}^{-1}\Delta_{\mathcal{A}} + \ln\left(\frac{\det \mathbf{\Sigma}_{\mathcal{A},Y}}{\det \mathbf{\Sigma}_{\mathcal{A},X}}\right)\right)$$

- Consider $\mathcal{A} \in \mathcal{C}_{\mathcal{T}}$, collection of all contiguous subsets from $\mathcal{T}$

- $\mathcal{A}^*(c)$, with $c \in (0,1)$, is the domain with **maximum divergence**

$$\max_{\mathcal{A}\in\mathcal{C}_{\mathcal{T}}} \mathrm{KL}_{\mathcal{A}}(X||Y), \text{ s.t. } \mathrm{len}(\mathcal{A}) \leq c\lambda(\mathcal{T}).$$

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Local-KL Divergence properties

The $\mathrm{KL}_{\mathcal{A}}(X||Y)$ is a set function that satisfies the following properties:

(a) **Non-negative:** For fixed GPs X and Y, it holds: $\mathrm{KL}_{\mathcal{A}}(X||Y) : \mathcal{P}_{\mathcal{T}} \to \mathbb{R}_0^+$ and $\mathrm{KL}_{\mathcal{A}}(X||Y) = 0$ if and only if $\mu_X(t) = \mu_Y(t)$ for all $t \in \mathcal{A}$ and $\sigma_X(t,s) = \sigma_Y(t,s)$ for all $(t,s) \in \mathcal{A} \times \mathcal{A}$.

(b) The local KL divergence is **upper bounded** (i.e. $\mathrm{KL}_{\mathcal{T}}(X||Y) < \infty$) and a **monotone** set function (i.e. for $\mathcal{A}' \subseteq \mathcal{A}$ it holds: $\mathrm{KL}_{\mathcal{A}'}(X||Y) \leq \mathrm{KL}_{\mathcal{A}}(X||Y)$)

(c) The local divergence $\mathrm{KL}_{\mathcal{A}}(X||Y)$ is a **continuous** set function in $\mathcal{C}_{\mathcal{T}}$, the collection of all contiguous subsets from the ground set $\mathcal{T}$.

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Local-KL divergence estimation

- Samples recorded over the same discrete grid $\mathcal{T}$: $\mathcal{D}_X = \{\mathbf{x}_i\}_{i=1}^{n}$ and $\mathcal{D}_Y = \{\mathbf{y}_j\}_{j=1}^{m}$ drawn from $GP(\mu_X(t), \sigma_X(t,s))$ and $GP(\mu_Y(t), \sigma_Y(t,s))$.
- The **Maximum Likelihood** estimates are given by:

$$\widehat{\mu}_{\mathcal{T},X} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i; \quad \widehat{\boldsymbol{\Sigma}}_{\mathcal{T},X} = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \widehat{\mu}_{\mathcal{T},X})(\mathbf{x}_i - \widehat{\mu}_{\mathcal{T},X})^T,$$

(analogous expression holds for $\mu_{\mathcal{T},Y}, \boldsymbol{\Sigma}_{\mathcal{T},Y}$).

- The trace and determinant are continuous functions in the space of real symmetric matrices, then $\widehat{\mathrm{KL}}_{\mathcal{A}}(X||Y)$ inherits (fixed p), consistency, asymptotic normality and efficiency,

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Some notes on the estimation...

- **Symmetrised** KL divergence: $\dfrac{\text{KL}(X||Y) + \text{KL}(Y||X)}{2}$

- **Regularised** covariance matrix:
  $\widehat{\boldsymbol{\Sigma}}_\eta = \eta\,\widehat{\boldsymbol{\Sigma}} + (1-\eta)\,\text{diag}(\widehat{\boldsymbol{\Sigma}}), \text{ for } \eta \in [0,1].$

- Sampling designs and misalignment: data **asynchrony** may act as a **confounding** factor when the aim is the estimation of the interval of local maximum KL divergence

- Smoothing: **low signal to noise ratio** leading to problems in the estimation of the interval of local maximum KL divergence

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One-shot experiment

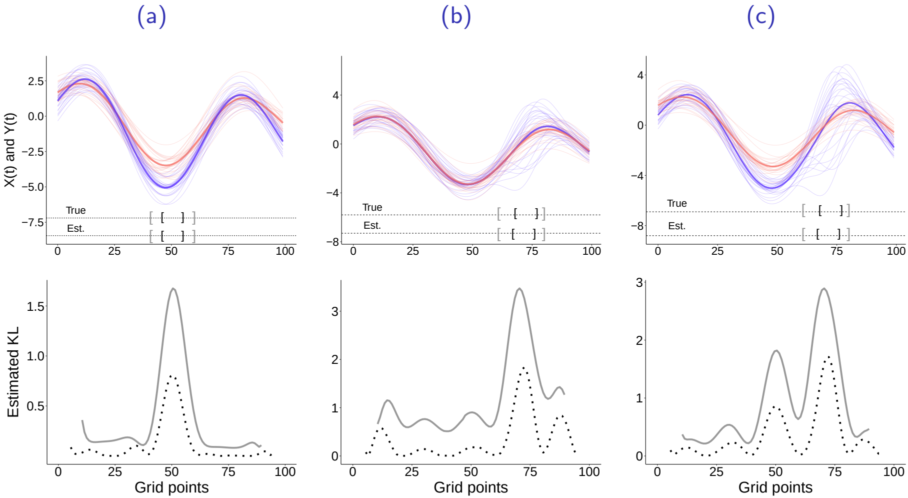


Figure: **One shot experiment:** Lower panels show the estimated local KL divergence for different interval lengths: $c = 0.1$ $(\cdots\cdots)$ and $c = 0.2$ (——)

Monte Carlo experiment

- MC replicates $= 1000$
- Sample size: $n = \{50, 100, 500, 1000\}$.
- Grid points: $p = \{50, 100, 200, 500\}$.
- c possible lengths: $(1\% - 99\%)$.
- Av. Jaccard Distance: $\text{AJD} = E\left\{ \int_0^1 \left[1 - \frac{|\mathcal{A}^*(c) \cap \widehat{\mathcal{A}}^*(c)|}{|\mathcal{A}^*(c) \cup \widehat{\mathcal{A}}^*(c)|}\right] \mathrm{d}c \right\}$

Monte Carlo results

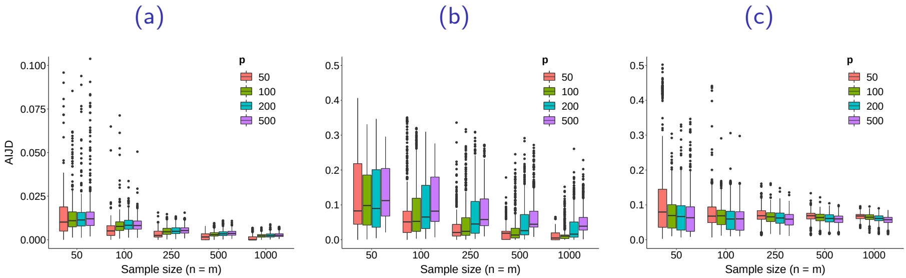
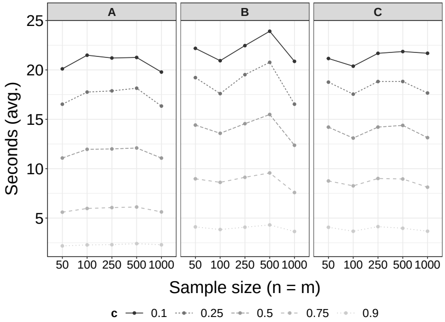


Figure: Empirical distribution of AIJD for different sample sizes n, m and grid resolution levels p.

Computational complexity



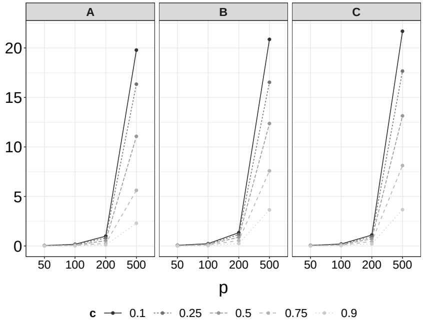


Figure: Average computational time required to estimate intervals of local maximum divergence.

Monitoring Electrocardiogram signals

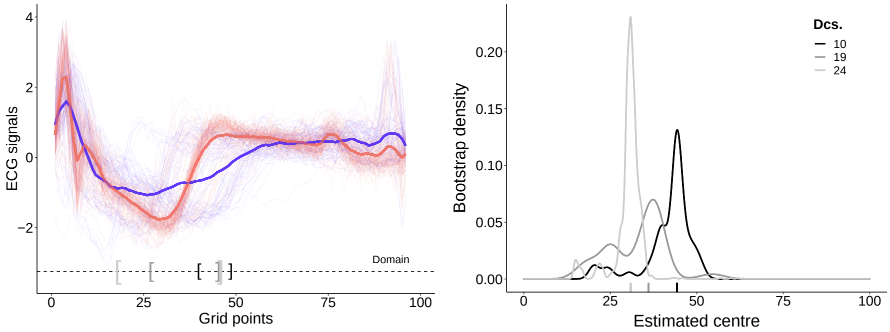


Figure: Left: ECG signals and selected domain for interval lengths 10, 19 and 24 dcs. Right: Bootstrap densities for the interval centre (same lengths)

ECG Classification

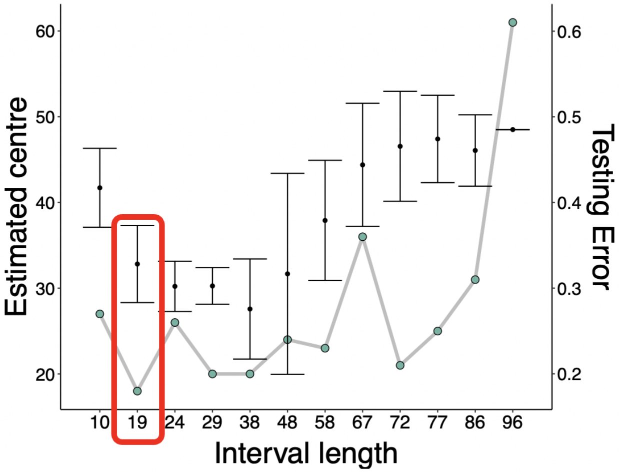


Figure: Estimated centre and classification error using a Discriminant model for different selected domains.

Summary and future work

✓ Tackle the problem of domain selection for electrocardiogram signals.

✓ Parameter of interest: interval ⇒ Covariance structure + almost continuously recorded data.

✓ Use the KL divergence and GP to develop an easy to implement algorithm for domain selection.

✓ Propose an estimator for $\mathcal{A}^*(c)$, and a nonparametric approach to assess the estimation uncertainty

⇒ Consider other model frameworks (non Gaussian), e.g.: *Wasserstein* divergence.

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Some references

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Thank you for listening! Comments are very welcome.

(flash for arXiv pre-print)