



# A Statistical Learning View of Simple Kriging

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# Introduction

## *Geostatistical context*

Geo-databases: information from **location and value** of the data



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- data sets of **spatial** nature  
⇒ **dependence structure**:  
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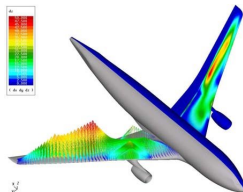


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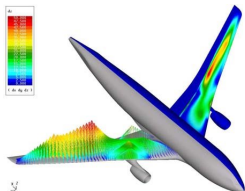
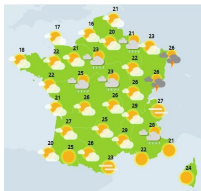


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Different from usual statistical learning theory:  
**non** independent observations



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## *Motivations*

**Machine Learning:**

**Spatial Analysis:**



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  - **Limits:** lack of nonasymptotic results

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- how **dependence structure** of spatial data affects learning rates?
- how spatial data can be processed by ML techniques with generalisation guarantees?
- connections between **Simple Kriging** and **Kernel Ridge Regression**?

Objective: develop framework for **kriging** based on (nonasymptotic) study of the performances of a (nonparametric) **covariance estimator**



# Preliminaries

1. Simple Kriging
2. Kernel Ridge Regression





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## *Notations*

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- $\Sigma(\mathbf{s}_n) = \text{Var}(\mathbf{X}(\mathbf{s}_n)) = (\text{Cov}(X_{s_j}, X_{s_i}))_{1 \leq i, j \leq n}$  covariance matrix



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 $\longrightarrow \checkmark$  allows to **control the spectrum** of the covariance matrix



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**Simple Kriging:** predict the value of  $X$  at some unobserved location  $s$ , based on  $n$  sampled observations  $(X_{s_i})_{i \leq n}$ , assuming a **linear combination** of the observations:  $f_\lambda(s) = \langle \lambda(s), \mathbf{X}(s_n) \rangle$ .

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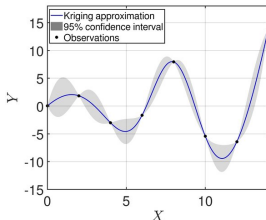
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### Remark (Exact Interpolation):

- at observed points: exact interpolator
- at unobserved points: linear combination of data





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- $\implies$  need to establish **rate bounds** that assess the **generalization capacity** of the resulting predictive map



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- **predict** the values of a random variable for unobserved input
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$$\hat{f} = \arg \min_{f \in \mathcal{H}} \left\{ \frac{1}{2} \sum_{i=1}^n (y_i - f(x_i))^2 + \frac{\eta}{2} \|f\|_{\mathcal{H}}^2 \right\}, \quad \text{where } (\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}}) \text{ RKHS}$$

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$$\implies \hat{f}(x) = {}^t \mathbf{Y}_n (\eta \mathbf{I}_n + \mathcal{K}_n)^{-1} \mathbf{K}_n(x)$$

Gram matrix  $\leftarrow$  $\leftarrow$  kernel vector



# Main Results

1. Connections between SK and KRR
2. Nonasymptotic bound for the Excess of Risk
3. Illustrative Numerical Experiments



## Main Results

*Connections: ML ↔ Geostat*

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$\implies$  kriging predictor **same** form as kernel ridge regressor:

- regularised Gram matrix  $\leftrightarrow$  covariance matrix
- kernel vector  $\leftrightarrow$  covariance vector



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## *Nonasymptotic theory*

What global gap between optimal **theoretical** predictor and **empirical** predictor **errors**?



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⇒ **Goal:** define **nonasymptotic** bound of global excess risk:

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## *Additional Assumptions*

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- Assumption 6:  $c$  is of class  $\mathcal{C}^1$  and its gradient is bounded by  $D$  (**regularity hypothesis**)  
→ ✓ taken into account when studying the **estimation error** of the covariance function for **all lags** (**smoothness** of the covariance function)



# Main Results

*Nonasymptotic bound for Excess of Risk*

## Theorem ([Siviero et al., 2022])

For any  $\delta \in (0, 1)$ , we have with probability at least  $1 - \delta$ :

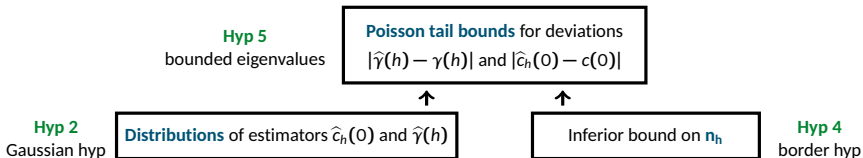
$$L_S(f_{\hat{\lambda}}) - L_S(f_{\lambda^*}) \leq C_6 \frac{\log(n/\delta)}{n} + \frac{2D^2}{n+1},$$

as soon as  $n \geq C'_6 \log(n/\delta)$ , where  $C_6$  and  $C'_6$  are nonnegative constants depending on  $j_1$ ,  $m$  and  $M$  solely.



# Sketch of Proof

## Poisson tail bounds

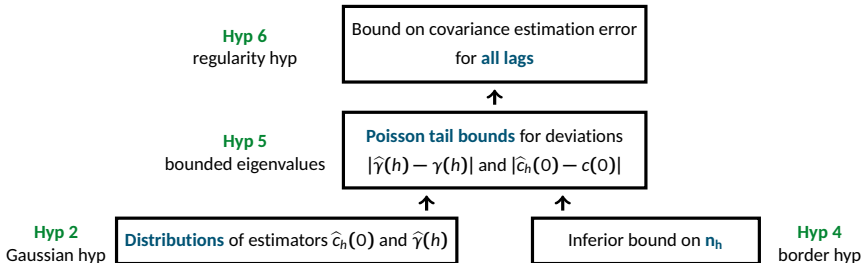






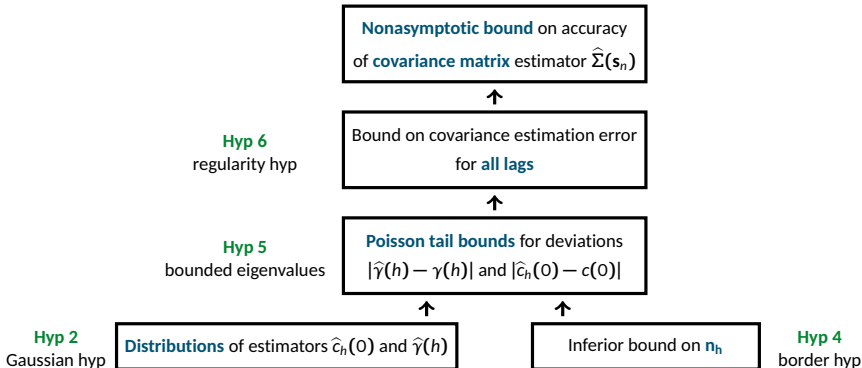
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## Bound on covariance estimation error



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Bound on accuracy of  $\hat{\Sigma}(s_n)$





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*Bound on accuracy of  $\hat{\Sigma}(s_n)$*

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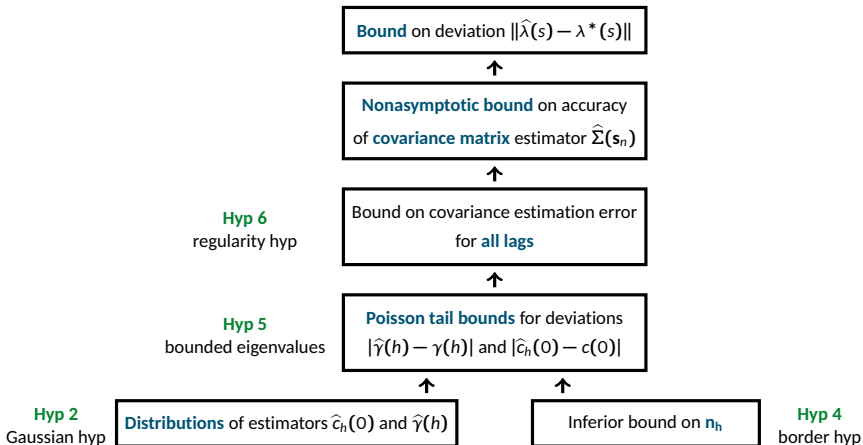
⇒ nonasymptotic bound on accuracy of covariance matrix estimator

$$\rho \left( \widehat{\Sigma}(s_n) - \Sigma(s_n) \right)$$



## Sketch of Proof

$$\forall s \in S, (f_{\hat{\lambda}}(s) - f_{\lambda^*}(s))^2 \leq \|\hat{\lambda}(s) - \lambda^*(s)\|^2 \times \|\mathbf{X}(s_n)\|^2$$





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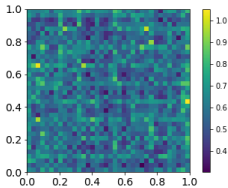


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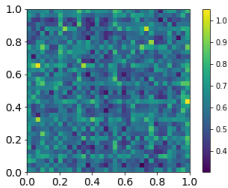


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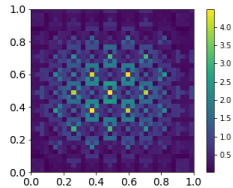


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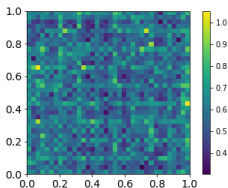


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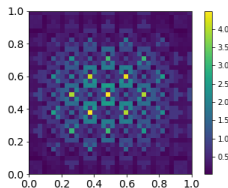


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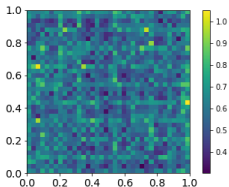


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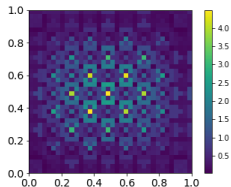


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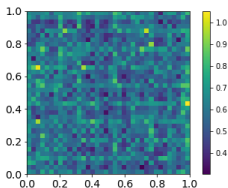


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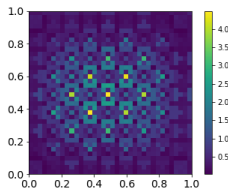


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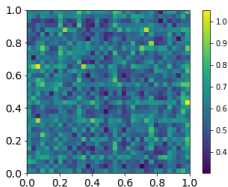


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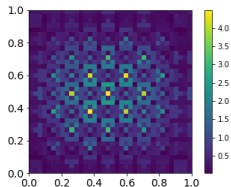


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⇒ results for Gaussian covariance encourages to relax **Hyp 4**



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  - Assumption 2: outside the *Gaussian* case
- **partitioning methods** (dyadic CART): divide spatial domain into clusters where the process is *locally stationary*



## Conclusion

- novel theoretical framework offering **guarantees** for empirical simple Kriging rules in the form of **non-asymptotic bounds**



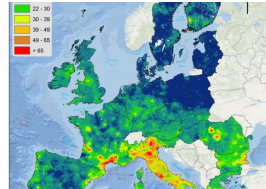
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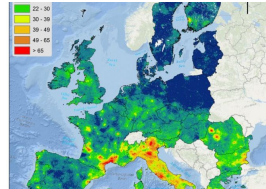
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     $\implies$  industrial assets and many possible **applications**
- **possible extensions** to a more general framework





**Thanks for your attention !**



# References I

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