# A discussion of the current and potential uses of Gaussian Processes in mechanics

#### Rodolphe Le Riche

CNRS LIMOS at Mines Saint-Etienne and UCA, France

in collaboration with David Gaudrie, Jhouben Cuesta-Ramirez, Sami Ben Elhaj Salah, Olivier Roustant, Victor Picheny, Nicolas Durrande, Xavier Bay, Julien Bruchon, Nicolas Moulin

> March 10 2022 SF2M journée scientifique matériau - numérique

#### Co-authors acknowledgement

This talk is based on the following works:

- Kriging courses in collaboration with Nicolas Durrande, [Le Riche and Durrande, 2019] and Xavier Bay.
- Bayesian optimization for shapes, with David Gaudrie, Victor Picheny, Benoît Enaux, Vincent Herbert, [Gaudrie et al., 2020].
- Mixed Bayesian optimization, with Jhouben Cuesta-Ramirez, Olivier Roustant, Guillaume Perrin, Cédric Durantin, Alain Glière, [Cuesta-Ramirez et al., 2021].
- Random permeability field generation, with Sami Ben Elhaj Salah, Julien Bruchon and Nicolas Moulin (to appear).

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#### Context: small data

- Deep neural nets need typically a lot of data ( $\sim$ 1000 per class in classification)
- But many problems in mechanics come with a limited number of samples: real experiments, 3D or nonlinear finite element simulations.



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# Context (cont.): small data and explanability

• Kriging is a machine learning technique that applies to small data, is expressive and somewhat explainable

as we will argue here.

# Kriging

 Kriging (a.k.a. conditional Gaussian Processes – GPs –) is often used in the context of expensive (numerical) experiments



trajectories, samples mean  $\pm$  std. deviation •  $x \in \mathcal{X}$ : index of the GP. Ex: position in space, design variable (discrete, continuous, mixed), ...

• x: costly data. Ex: displacement / stress / permeability at x, ... cost, performance.

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# Kriging's language: kernels



• 
$$Y(x) \sim \mathcal{N}(\mu(x), k(x, x))$$

 $\mu(x)$ , the mean of the trajectories.

k(x, x') = Cov(Y(x), Y(x')), the covariance function a.k.a. the kernel, k(x, x) the variance.

Ex: 
$$\mu(x) = 10x^2$$
,  $k(x, x') = \sigma^2 \left(1 + \sqrt{3} \frac{|x-x'|}{\theta}\right) \exp\left(-\frac{|x-x'|}{\theta}\right)$ ,  
 $\sigma^2 = 1, \ \theta = 0.2$ 

(plots from https://durrande.shinyapps.io/gp\_playground/)

# From kernel to trajectory

Mathematically,

• 
$$X = \{x^1, ..., x^n\}, K_{ij} = k(X, X)_{ij} = k(x^i, x^j)$$

• eigendecomposition :  $K = VD^2V^{\top}$ 

• 
$$y(X) = \mu(X) + VDE$$
 where  $E \sim \mathcal{N}(0, I_n)$ 

In pseudo-R,

- choose mean function mu() and kernel function k(,)
- build a fine grid X and the covariance matrix, K[i,j]=k(X[i],X[j])
- eigendecomposition, Keig = eigen(K)
- sample,

diag(sqrt(Keig\$values)) %\*% matrix(rnorm(n))

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#### Kernels change a lot of things (I)

 $Y(x) \sim \mathcal{N}(\mu(x), k(x, x)), \ \mu(x) = 10x^2, \ \sigma^2 = 1, \ \theta = 0.2$ 



#### Kernels change a lot of things (II)

#### Parameterize k(,): length-scales $\theta$ 's and variance $\sigma^2$ , $k(x, x') = \sigma^2 \times r(x, x'; \theta)$ , r(,) correlation

$$k(x, x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{\theta^2}\right)$$

trajectories 
$$y(x)$$



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#### Conditioning with data

Kriging = conditional GP = GP regression = (Y(x)|Y(X) = F)



 $\begin{aligned} Y(x)|Y(X) &= F \text{ is } \mathcal{N}(m(.),c(.,.)) \text{ with} \\ m(x) &= \mu(x) + k(x,X)k(X,X)^{-1}(F - \mu(X)) \\ c(x,x') &= k(x,x') - k(x,X)k(X,X)^{-1}k(X,x') \end{aligned}$ 

⇒ the kernel k(,) is the main modeling choice ⇒ Kriging is interpolating by construction

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The likelihood of the model for one observation of the vector F is

Likelihood 
$$= p_{Y(X)}(F) = \frac{1}{(2\pi)^{n/2} \det(k(X,X))^{1/2}} \times \exp\left(-\frac{1}{2}(F - \mu(X))^{\top}k(X,X)^{-1}(F - \mu(X))\right)$$

Maximize *L* with respect to the kernel ( $\sigma$ ,  $\theta$ ) and other model parameters (e.g., those of  $\mu$ ()) to tune kriging

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## Kernel design I

So, one would like to design the kernel to fit a given task.

- A valid kernel is
  - any symmetric function, k(x, x') = k(x', x)
  - which is positive semi-definite

$$\forall X \in \mathcal{X}^n, \forall \alpha \in \mathbb{R}^n, \ \alpha^{\top} k(X, X) \alpha \geq 0$$

Usually, kernels are taken off the shelf. Expl: Matérn, squared exponential kernels, mentioned earlier. Other expl:
k(x, x') = σ<sup>2</sup>xx' (linear), = σ<sup>2</sup>δ<sub>x,x'</sub> (white noise),
= σ<sup>2</sup> min(x, x') (Brownian), cf. [Le Riche and Durrande, 2019].

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- To create new kernels, increase their dimension, the following transformations can be combined:
  - Sum
    - on the same space  $k(x,x') = k_1(x,x') + k_2(x,x')$
    - on the tensor space  $k(x, x') = k_1(x_1, x'_1) + k_2(x_2, x'_2)$
  - Multiplication
    - on the same space  $k(x,x') = k_1(x,x') imes k_2(x,x')$
    - on the tensor space  $k(x,x') = k_1(x_1,x_1') imes k_2(x_2,x_2')$
  - Composition with a function  $k(x, x') = k_1(h(x), h(x'))$

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## Costly shape optimization: airfoil

Predict and minimize the drag of an airfoil, from [Gaudrie et al., 2020].



 $\begin{array}{c} {\rm CAD \ shape \ } \phi \ {\rm generation}, \\ {\rm not \ costly} \end{array}$ 



Contours of Pressure Coefficient

Feb 20, 2017 ANSYS Fluent 14.5 (2d, pbns, rke)

# Navier-Stokes resolution, $f(\phi)$ the drag, costly

#### An infinite dimensional problem



Not really infinite: an airfoil is not any shape ....

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### Eigenshape decomposition I

From a database of possible shapes  $[\phi^{(1)}, \ldots, \phi^{(5000)}]$ ,



extract a basis of most impor-  ${}_{\text{\sc s}}$  tant shapes by principal component analysis,  $\{V^1,\ldots,V^d\}$ 

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#### Eigenshape decomposition II

Shapes are now described with their eigencomponents  $\alpha$ 's,  $\phi\approx\overline{\phi}+\sum_{i=1}^d\alpha_iV^i$ 



#### Dimension reduction in GP I

We build a GP to infer the drag from a shape,  $Y(\alpha)$  and reduce dimension.

Anisotropic kernel has 1  $\theta_i$  per dimension, isotropic has 1 for all dimensions.

Expl: 
$$k_{ani}(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^d \frac{(x_i - x'_i)^2}{\theta_i^2}\right)$$
  
 $k_{iso}(x, x') = \sigma^2 \exp\left(-\frac{(x_i - x'_i)^2}{\theta^2}\right)$ 

#### Dimension reduction in GP II

• Likelihood that favors sparsity [Yi et al., 2011]:

$$max_{\theta}$$
 Likelihood( $\theta$ ;  $F$ ) –  $\lambda \|\theta^{-1}\|_1$ 

 $\Rightarrow$  active and non-active dimensions,  $\alpha_{\rm a}$  and  $\alpha_{\rm \bar{a}}.$ 

• GP as the sum of an anisotropic and isotropic GPs [Allard et al., 2016]:

$$\mathbf{k}(\alpha, \alpha') = \mathbf{k}_{\mathsf{ani}}(\alpha_{\mathbf{a}}, \alpha'_{\mathbf{a}}) + \mathbf{k}_{\mathsf{iso}}(\alpha_{\bar{\mathbf{a}}}, \alpha'_{\bar{\mathbf{a}}})$$

Expl NACA22 :  $\alpha_a = (\alpha_1, \alpha_2, \alpha_3) , d = 20$  $\Rightarrow 21 \text{ to } 6 \text{ kernel parameters}$ 



## GPs allow global optimization

Red curve : Expected Improvement =  $\mathbb{E} \max(0, f_{\min} - Y(x))$ 



Its iterative maximization defines a global optimizer based on a GP (Bayesian Optimization) An effective optimizer in low to medium dimensions [Le Riche and Picheny, 2021]

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# Example: NACA 22 airfoil drag minimization



(important optimization features not covered here: how to optimize in reduced dimension, replication strategy to stay on the manifold of feasible  $\alpha$ 's, cf. article). In the reduced eigenshape basis,

- faster decrease of the objective function,
- smoother airfoils.

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#### Design with mixed variables I

Many design problems are mixed = with continuous (x) and discrete (u) optimization variables.

$$\min_{x\in\mathbb{R}^{d_c},u\in\mathbb{R}^{d_d}}f(x,u)$$

f() costly (experiments, nonlinear simulations), cannot solve the problem for all u combinations.

# Design with mixed variables II

Example: structural design, material is discrete, dimensions are continuous, at micro (architectured materials) or macro scale

solar cell design



from [Zhang et al., 2020]

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#### Design with mixed variables III

Example: structural design, shape taken out of a catalogue (discrete), some dimensions continuous.

Design of a cantilever beam



from [Cuesta-Ramirez et al., 2021]

Usual trick: learn a metamodel from observations. Here, GP. How to correlate discrete variables?

Kernel design rules used:

multiplication and composition with a function,

$$k((x, u), (x', u')) = \sigma^2 \prod_{i=1}^{d_c} r(x_i, x'_i) \times \prod_{i=1}^{d_d} r(h(u_i), h(u'_i))$$

Image: A Image: A

#### Latent variables I

The discrete variables are the expression of hidden quantities, the latent variables.

The distances between these variables can be summarized by the transformation h() (link with explainability).

 $h(): \mathbb{D} \mapsto \mathbb{R}^2$  is sufficient in practice, [Zhang et al., 2020]

underlying (physical) latent variable space

2D (numerical) latent variable space



#### Latent variables II

Identification of the latent variables

$$r(u_i, u'_i) = \langle h(u_i), h(u'_i) \rangle$$
,  $h(u_i = l'_j) = h'_j$ 

and the  $h_j^i$  are the  $2 \times \sum_{i=1}^{n_d} (\text{nb\_levels}(u_i) - 1)$  parameters estimated from the data by maximization of the likelihood (with the  $\theta$ 's of the continuous variables and  $\sigma^2$ ).

 $\Rightarrow$  the GP Y(x, h(u)) can be built.

The correlation between the discrete variables is learnt from data through the latent variables h.

#### Latent variables III

Beam example:  $d_d = 1$  discrete variable with 12 levels (the shapes below) with a physical latent variable, the normalized inertia  $\tilde{l} = l/S^2$ ;  $d_c = 2$  continuous variables, the length and the cross-section. Correlations learned from 96 samples:



#### Latent variables IV

Example: latent variables of an Anti-Reflective Coating, from [Zhang et al., 2020].



The order found is consistent with the refractive indices of the material. ( $z \equiv h$  in our notation)

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#### From latent variables to problem relaxation I

Choice of the next experiment/simulation :

 $\max_{(x, u) \in \mathbb{R}^{d_c} \times \mathbb{D}^{d_d}} \mathsf{Expected\_Improvement}(x, u)$ 

but discrete optimization is not trivial in general.

Facilitate it by relaxation into a continuous set of latent variables,  $\tilde{h} \in \mathbb{R}^2$ 



#### From latent variables to problem relaxation II

Only the correlation of the discrete variables changes :  $r(h(u), h(u')) \rightarrow r(\tilde{h}, \tilde{h}')$ 

The relaxed optimization problem is:

$$\begin{array}{ll} \min & \mathsf{Expected\_Improvement}(x,\tilde{h})\\ (x,\tilde{h}) \in \mathbb{R}^{d_c+2d_d}\\ \text{such that} & \min_{u\in \mathbb{D}^{d_d}} \|h(u) - \tilde{h}\| \leq \varepsilon \end{array}$$

Encouraging experimental results found in [Cuesta-Ramirez et al., 2021].

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# Permeability is a random (tensor) field



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#### Principle



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## A kernel based on Darcy's law I

Assumption: the standard deviation of the permeability (written Y(x) here!) is proportional to the pressure gradient. Since  $V(x) = -Y(x)/\mu \nabla P(x)$ , for a scalar (isotropic) permeability,

$$k(x, x') = \|V(x)\| \|V(x')\| \tilde{\sigma}^2 r(x, x')$$

where  $r(x, x') = \exp(-||x - x'||^2/\theta^2)$  and V(x) calculated with a constant nominal permeability.

A valid kernel by multiplication and composition with a function of a linear kernel.

$$Var(Y(x)) = ||V(x)||^2 \tilde{\sigma}^2$$
,  $Corr(Y(x), Y(x')) = r(x, x')$ 

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#### A kernel based on Darcy's law II

(white lines = resin fronts at t = 23s)



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#### Kernels for macroscopic folds I

Not enough experiments to train a neural net, yet we know how the folds look like.

 $\boldsymbol{\alpha}$  rotation angle of the permeability tensor.



#### Kernels for macroscopic folds II

The rotation angle  $\alpha(x, y)$  is modeled as a GP whose kernel is

$$k\left(\begin{pmatrix}x\\y\end{pmatrix},\begin{pmatrix}x'\\y'\end{pmatrix}\right) = a(x,y)a(x',y')k\left(\begin{pmatrix}R(x,y)\\\theta(x,y)\end{pmatrix},\begin{pmatrix}R(x',y')\\\theta(x',y')\end{pmatrix}\right)$$

where a(x, y) is an activation (of the randomness) function and  $(R, \theta)$  polar coordinates. It is a valid kernel.



#### Kernels for macroscopic folds III



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#### Conclusions

- Kriging is a machine learning technique
- fitted to small data because it is interpolating and sparsely parameterized
- yet, thanks to kernel design, it is flexible and partly explainable.

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