# A general exponential kernel to handle mixed-categorical variables for Gaussian process

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***Toulouse, France***

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**Thierry Lefebvre (ONERA)**
**Joseph Morlier (ISAE-SUPAERO/ICA)**

P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, and J. Morlier. A mixed-categorical correlation kernel for gaussian process, 2022. Submitted to Neurocomputing. Available at SSRN: https://dx.doi.org/10.2139/ssrn.4296794

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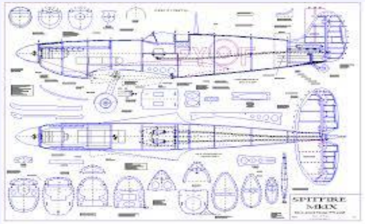

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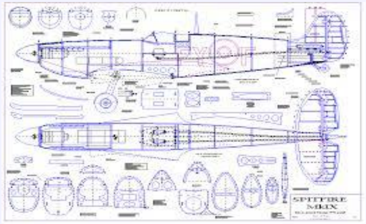

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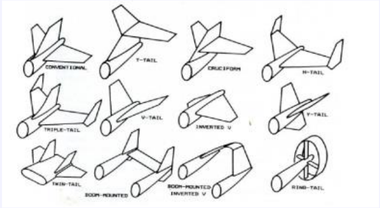

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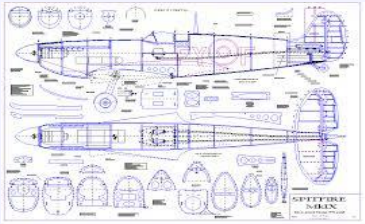

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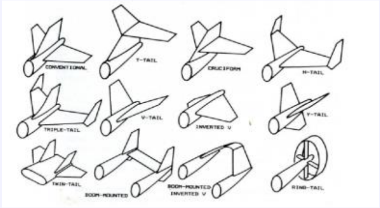

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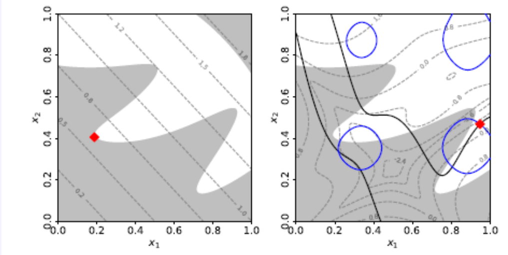

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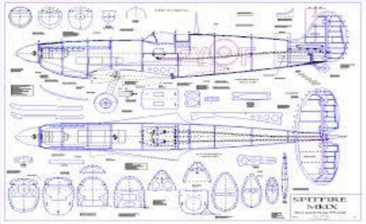

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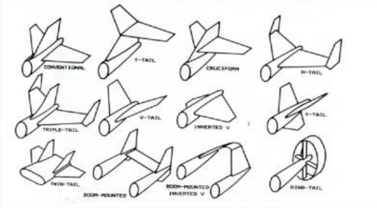

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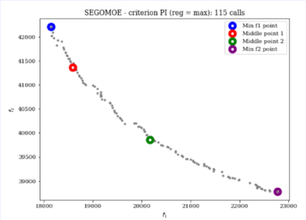


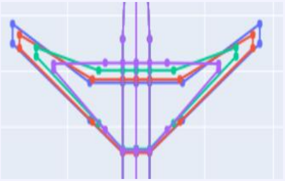

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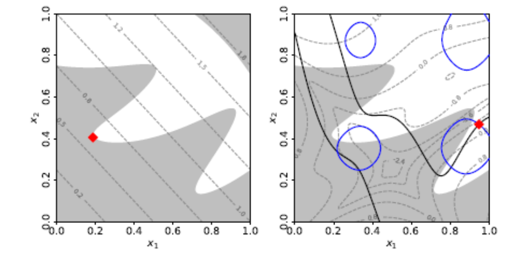

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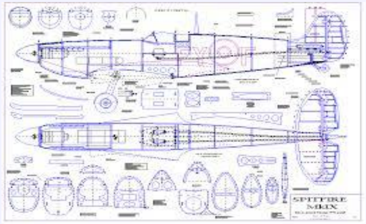

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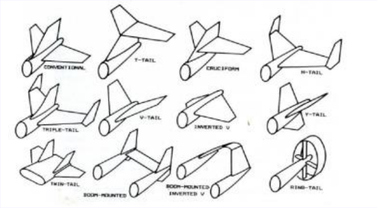
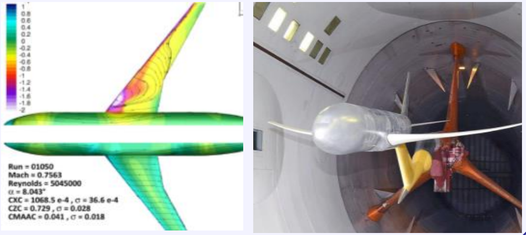


**Multifidelity database**

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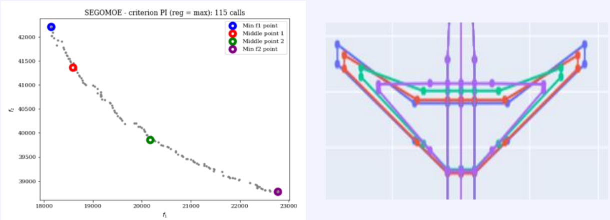


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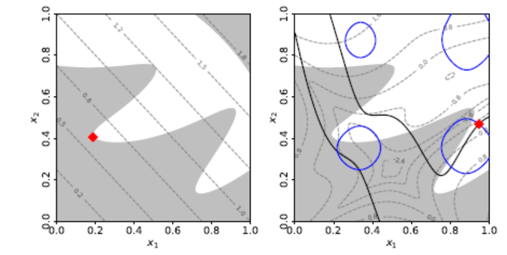

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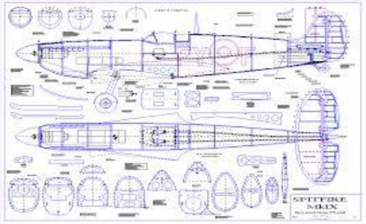

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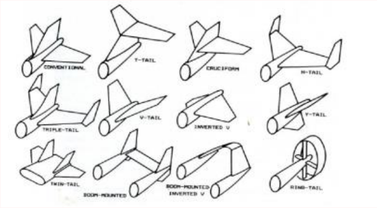

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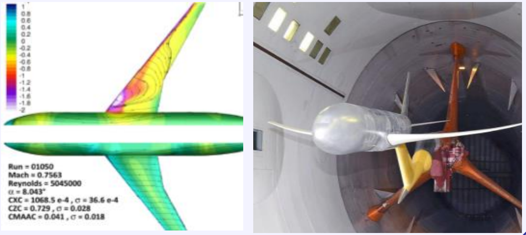


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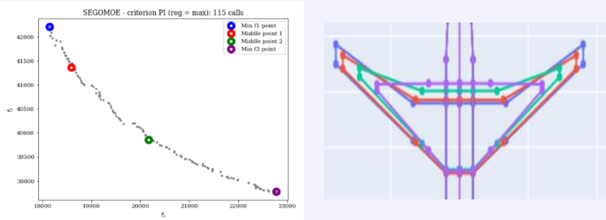


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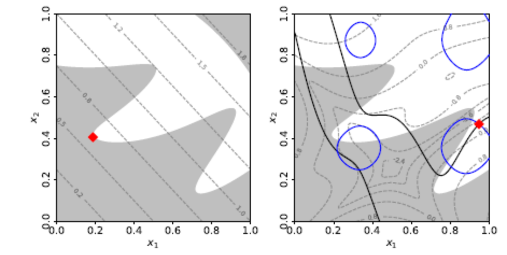
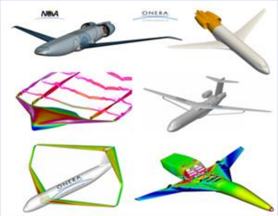


# Bayesian optimization applied to aircraft design

**New concepts**



$\Omega$

Kim, S. H., and Boukouvala, F., "Surrogate-Based Optimization for Mixed-Integer Nonlinear Problems," Computers & Chemical Engineering, Vol. 140, 2020, p. 106847.

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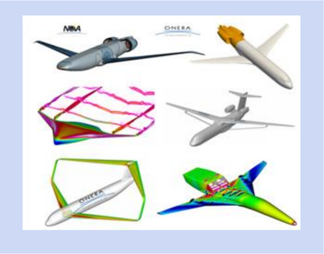
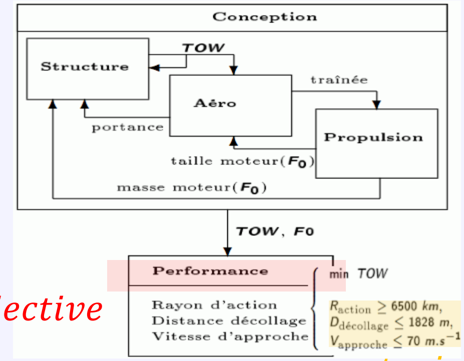


Ω

Analyze

## Multidisciplinary Design Analysis




*objective*

*constraints*

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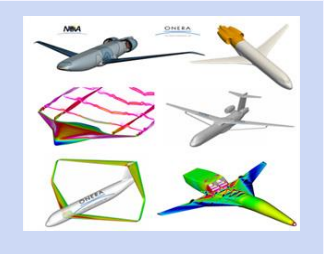


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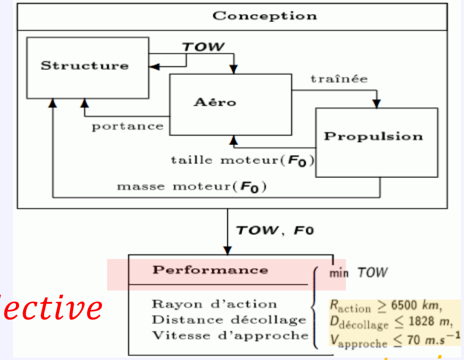


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**Improvements**

## Global optimization

## MDF Formulation

$$\min_{\text{inputs} \in \Omega} \ objective\,(\text{inputs})$$
$$s.t \quad constraints\,(\text{inputs})$$

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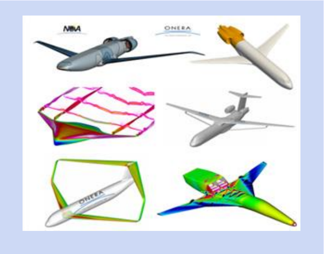


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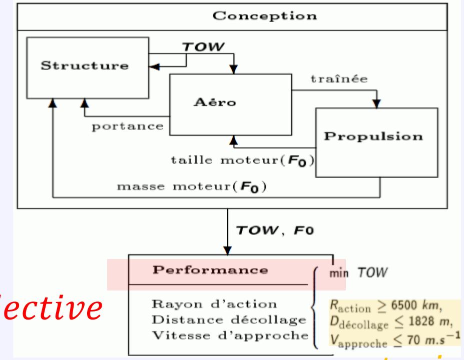


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**Expensive computations**

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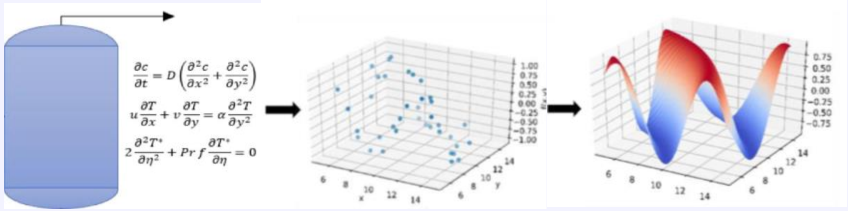


**Expensive black-box** **Design of Experiments** **Gaussian processes**

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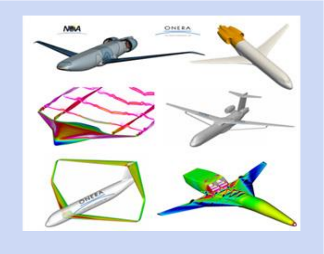

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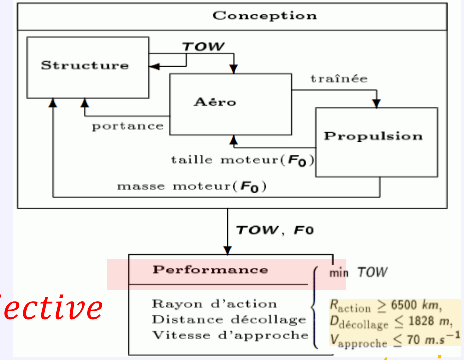


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**Expensive black-box optimization**

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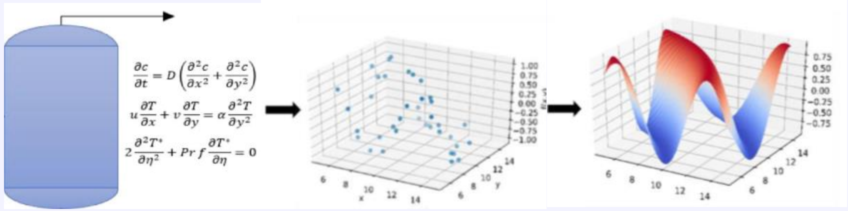


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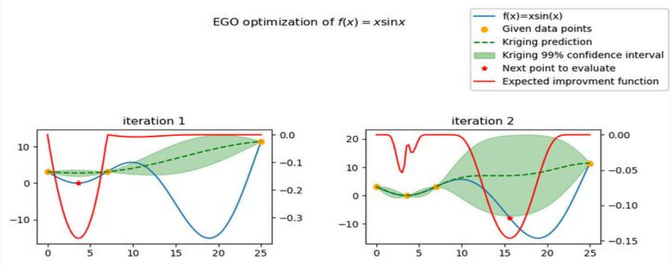
## Efficient Global Optimization

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# Two frameworks

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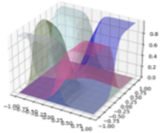
SMT: Surrogate Modeling Toolbox

github.com/SMTorg/smt

- Open source python toolbox: surrogate modeling methods, sampling techniques, and benchmarking functions
- Focus on derivatives (training derivatives used for gradient-enhanced modeling, prediction derivatives)
- New Kriging based surrogate models for higher dimension (KPLS and KPLS-K)
- Noisy Kriging to handle uncertainties on data
- Multifidelity Kriging with or without noise (MFK, MFKPLS)
- Mixture of experts technique for heterogeneous functions



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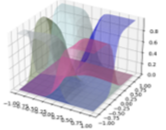

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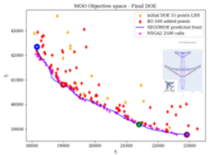
## SEGOMOE

- Mono & multi objective Bayesian optimizer
- Mono & Multi fidelity sources
- Handling non linear objectives & constraints (black box, no derivative available)
- Equality & inequality constraints (1 ~ 100 constraints)
- Intermediate dimension problem (1 ~ 100 variables)




- Heterogenous variables (continuous, discrete, categorical)
- Costly evaluation (CFD, FEM, objective and/or constraints)
- Based on SMT toolbox for surrogate models
- Remote access via a **web interface**

ONERA WhatsOpt

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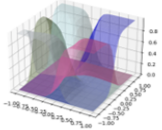

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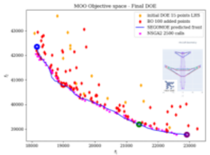

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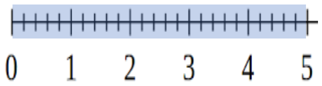
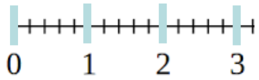
**Hybrid variables**

**Variables types:**

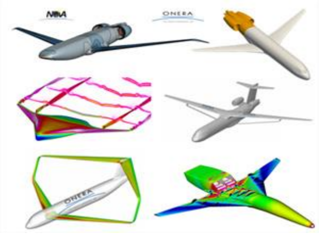
- **Continuous (x) Ex:** wing length




- **Integer (z) Ex:** winglet number




- **Categorical (u) Ex:** Plane shape / material properties



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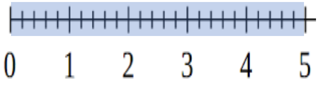


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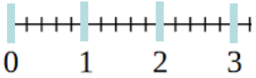


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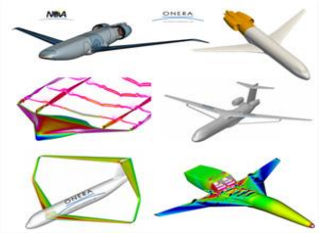

**Categorical variables: n variables, n=2**
u1= shape
u2= color

**Levels:** $L_i$ levels for I in 1,..n, $L_1$=3, $L_2$=2
Levels(u1)= square, circle, rhombus
Levels(u2)= blue, red

**Categories:** $\prod_{i=1}^{n} L_i$, 2*3=6
- Blue square
- Blue circle
- Blue rhombus
- Red square
- Red circle
- Red rhombus

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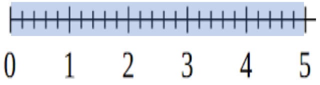


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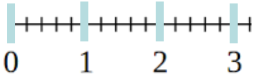


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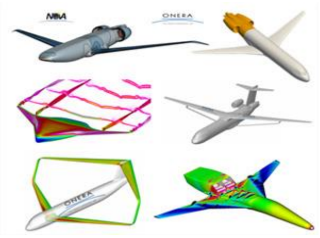

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**Categories:** $\prod_{i=1}^{n} L_i$, 2*3=6
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- Blue rhombus
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6 possibilities

# From continuous to mixed-integer Gaussian process

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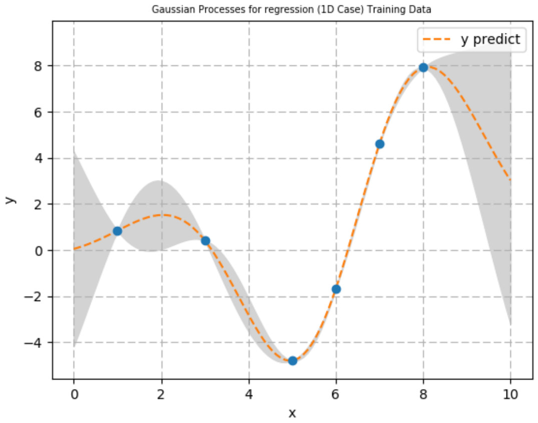


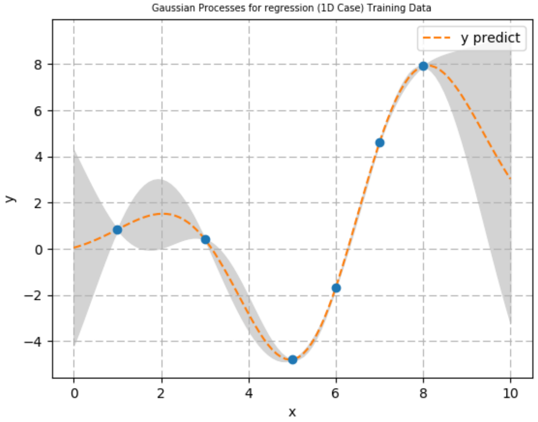

$x \in [0,10]$

## Exponential kernels

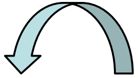
$$k(x^r, x^s) = \prod_{i=0}^{n} \exp[-\theta_i |x_i^r - x_i^s|]$$

$$k(x^r, x^s) = \prod_{i=0}^{n} \exp[-\theta_i |x_i^r - x_i^s|^2]$$

# From continuous to mixed-integer Gaussian process




$x \in [0,10]$



$c$: Blue color / Red color / Green color

## Exponential kernels

$$k(x^r, x^s) = \prod_{i=0}^{n} \exp[-\theta_i |x_i^r - x_i^s|]$$

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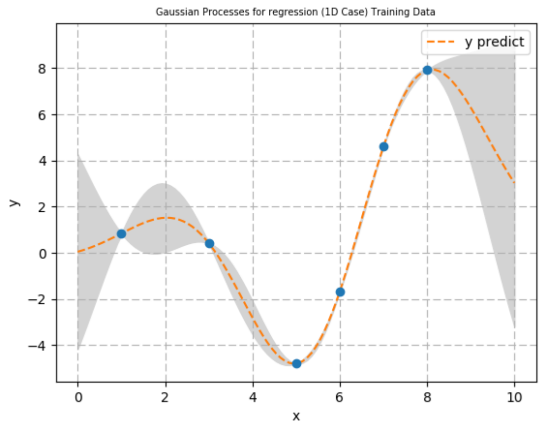
# From continuous to mixed-integer Gaussian process

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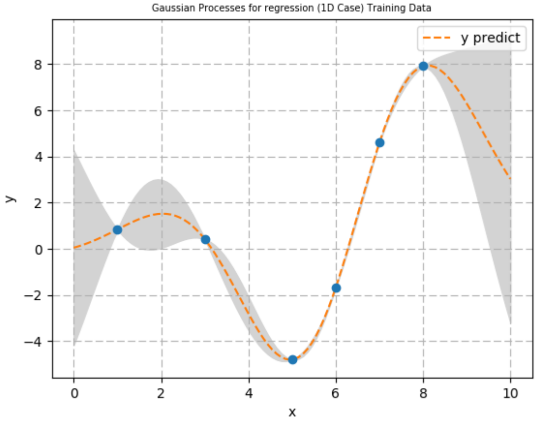
## ? kernel

$k(blue, red)$
$k(blue, green)$
$k(red, green)$

# From continuous to mixed-integer Gaussian process

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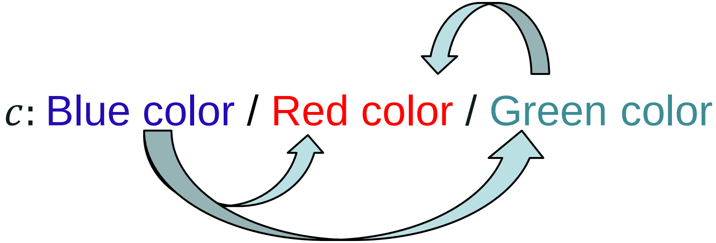


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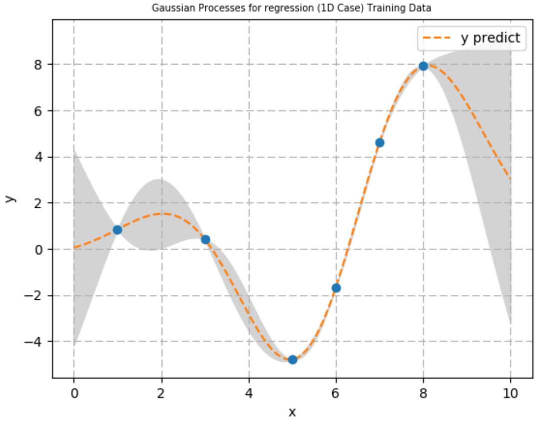
$$\Theta_{color} = \begin{pmatrix} 1 & \theta_{blue/red} & \theta_{blue/green} \\ & 1 & \theta_{red/green} \\ Sym & & 1 \end{pmatrix}$$

# From continuous to mixed-integer Gaussian process

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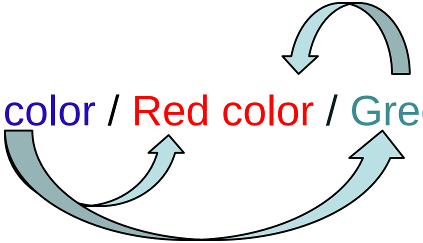

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To optimize

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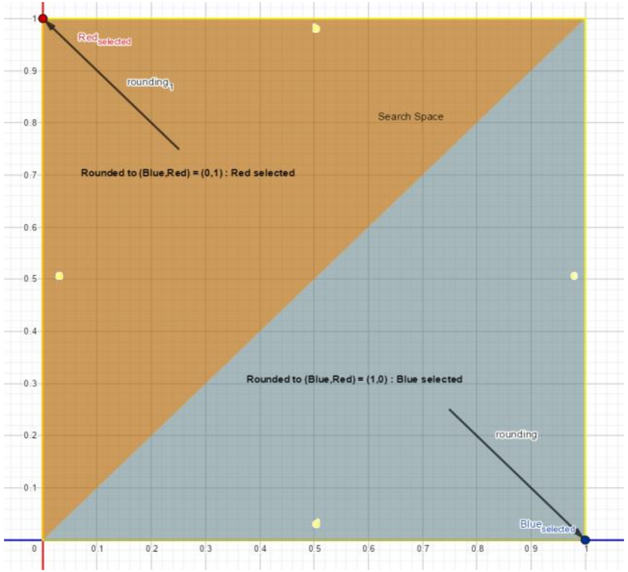
# State-of-the-art approaches

- *Continuous relaxation*

Example with 1 categorical variable and two levels
- Red color
- Blue color

➔ **One-hot encoding:** Categorical variable replaced by two continuous variables denoted by $X_1$ and $X_2$

- If $X_1 > X_2 \Rightarrow e_{c_1^b} = (1., 0.) \Rightarrow$ Blue color
- If $X_1 < X_2 \Rightarrow e_{c_1^r} = (0., 1.) \Rightarrow$ Red color




E. C. Garrido-Merchán, and D. Hernández-Lobato. "Dealing with categorical and integer-valued variables in Bayesian Optimization with Gaussian processes". Neurocomputing, vol. 380 (2020), pages 20-35

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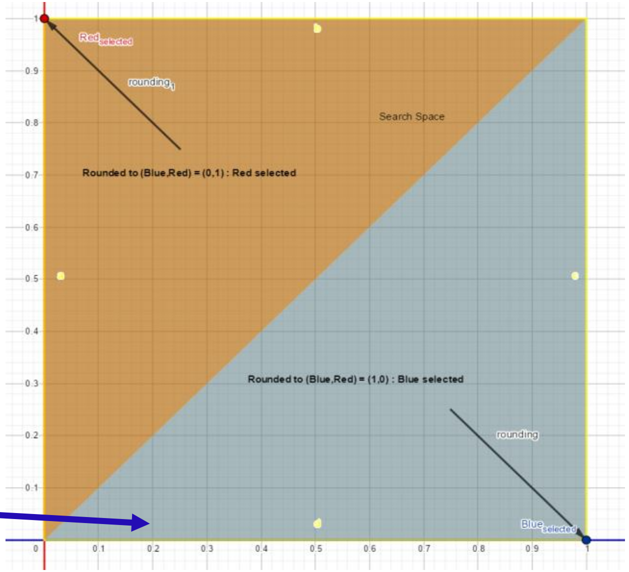


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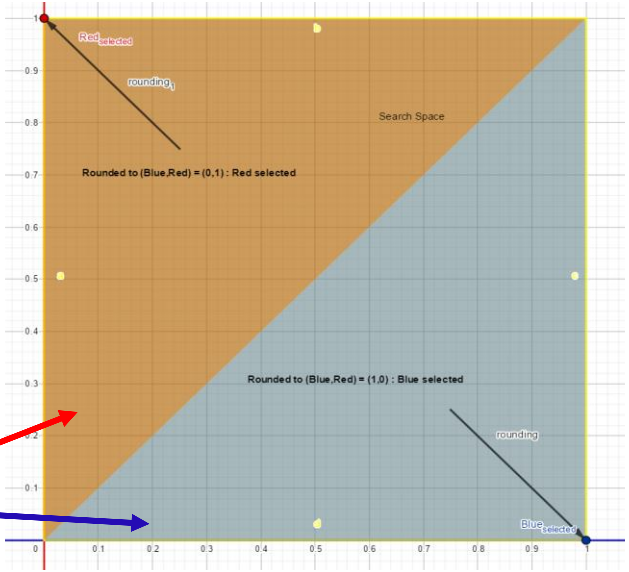


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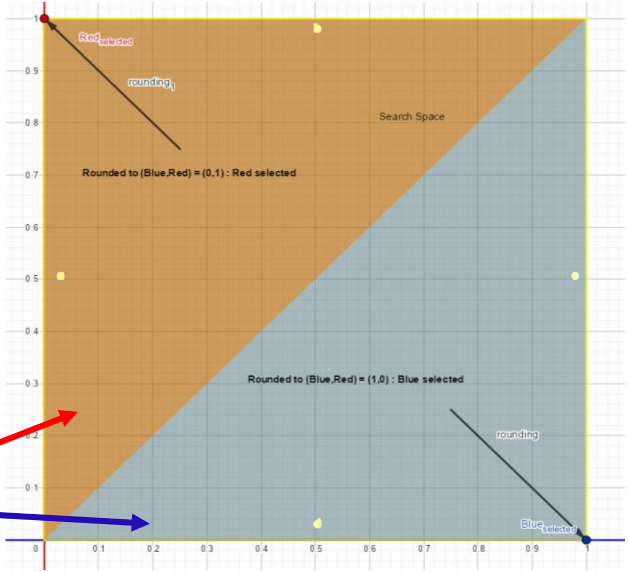


**$n$ relaxed dimension**

$$x^r, x^s \in \mathbb{R}^n$$

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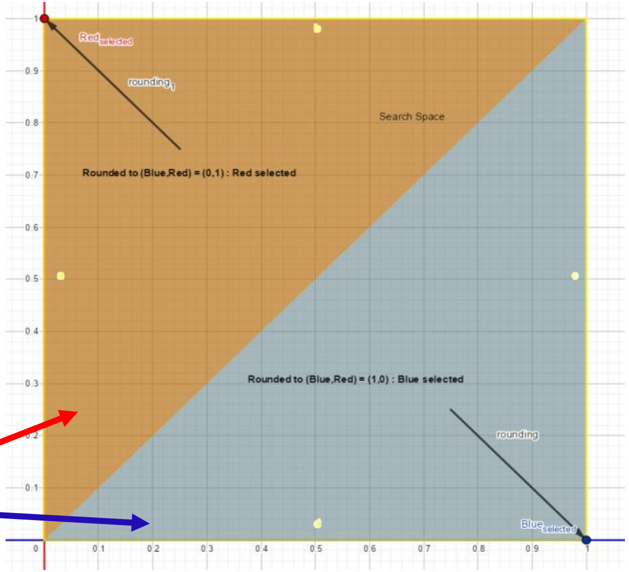


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# State-of-the-art approaches

- *Gower distance*

Example with 2 variables:

- $c_1$: Red color / Blue color,
- $x_1 \in [0,1]$

$$\Delta_{gow}\big((red, 0.2), (blue, 0.5)\big) = \boldsymbol{s}(\mathrm{red}, \mathrm{blue}) + |0.2 - 0.5| = 1.3$$
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$\boldsymbol{n}$ **continuous dimension**

$$\boldsymbol{x}^r, \boldsymbol{x}^s \in \mathbb{R}^n$$

$\boldsymbol{l}$ **categorical variables**

$$\boldsymbol{c}^r, \boldsymbol{c}^s \in \prod_{j=1}^{j=l} \{ \boldsymbol{L}_1, \dots, \boldsymbol{L}_j\}$$

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- *Homoscedastic hypersphere mixed kernel*

Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E.-G., and Guerin, Y., Overview and Comparison of Gaussian Process-Based Surrogate Models for Mixed Continuous and Discrete Variables: Application on Aerospace Design Problems, Springer International Publishing, 2020, pp. 189–224

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- $c_1$: Blue color / Red color / Green color,
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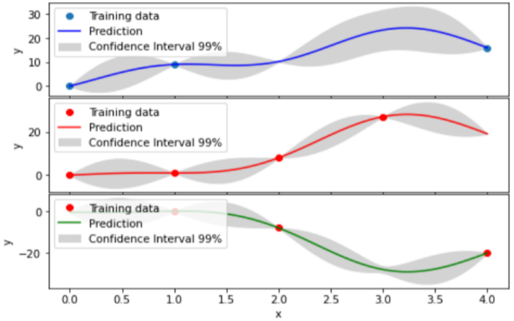


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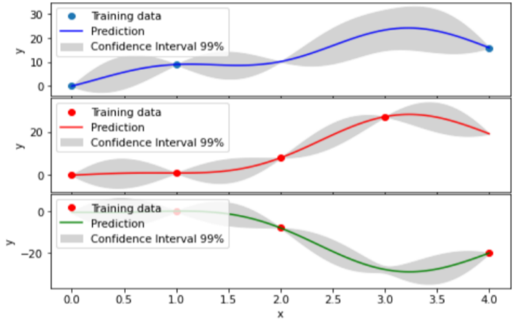


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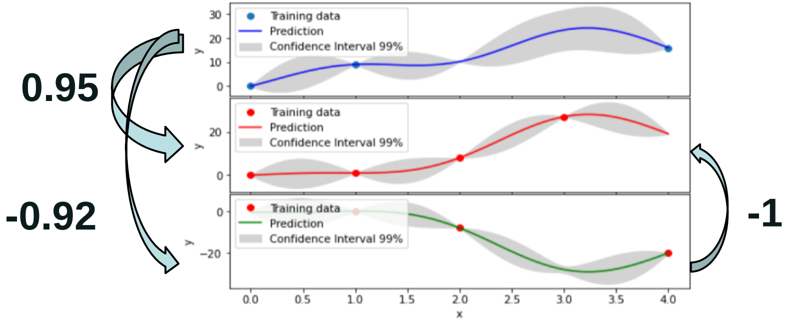


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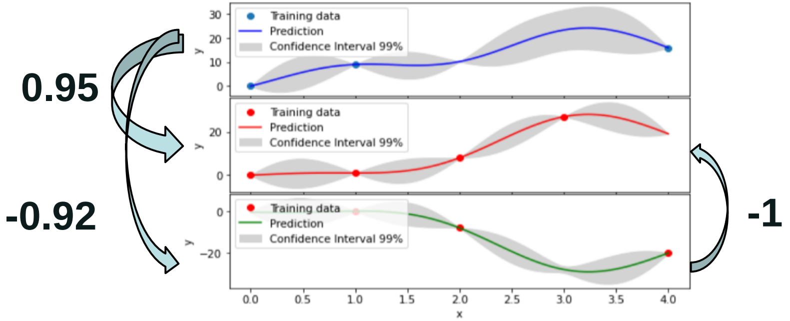


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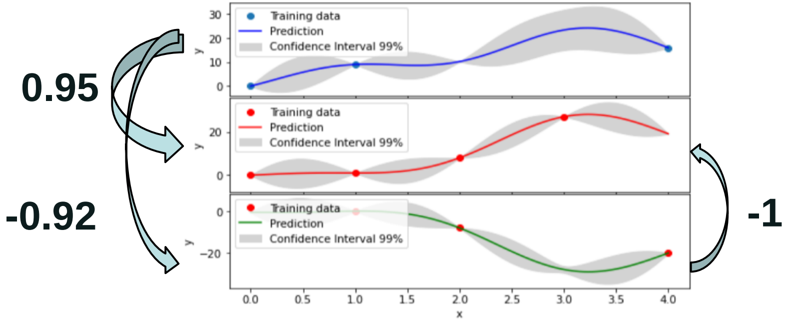


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**The matrix $\Theta_j$ should be SPD!**

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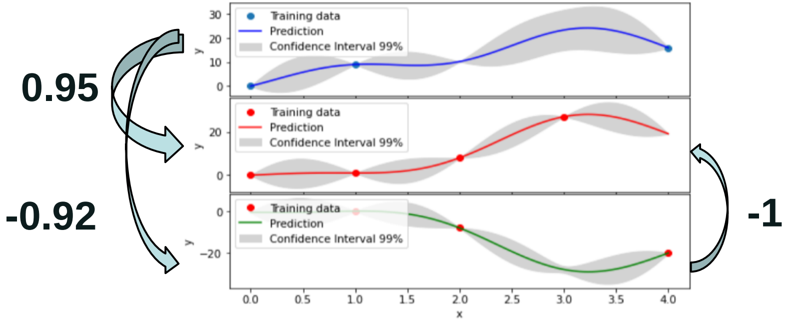


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**The input $c_j^r$ takes the level of index $l_r^j$**

- $c_1$: Blue color / Red color / Green color,

  1 2 3

**if** $c_1^r = \text{"}red\text{"},\ l_r^1 = 2\ \ (index)$

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SPD SPD

**The input $c^r_j$ takes the level of index $l^j_r$**

- $c_1$: Blue color / Red color / Green color,

 1 2 3

if $c^r_1 = \text{"red"}$, $l^1_r = 2\ (index)$

$$\begin{pmatrix} 1 & \theta_{blue/red} & \theta_{blue/green} \\ & 1 & \theta_{red/green} \\ Sym & & 1 \end{pmatrix} = \begin{pmatrix} 1 & \theta_{1,2} & \theta_{1,3} \\ & 1 & \theta_{2,3} \\ Sym & & 1 \end{pmatrix}$$

# Unification of the mixed models

- **Every model can be written as**

$$k(w^r, w^s, \theta) = \prod_{j=1}^{l} \theta^{cat}_{c_j^r, c_j^s} \prod_{j=1}^{n} \exp\left(-(x_j^r - x_j^s)\theta_j^{cont}(x_j^r - x_j^s)\right)$$

$$= \prod_{j=1}^{l} [R_j(\Theta_j)]_{\ell_r^j, \ell_s^j}$$

$$= \prod_{j=1}^{l} \kappa([\Phi(\Theta_j)]_{\ell_j^r, \ell_j^s})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s, \ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^r, \ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s, \ell_j^s})$$

**SPD** **SPD**

**The input $c_j^r$ takes the level of index $l_r^j$**

- $c_1$: Blue color / Red color / Green color,

**1** **2** **3**

**if $c_1^r = \text{"red"}, l_r^1 = 2\ (index)$**

$$\begin{pmatrix} 1 & \theta_{blue/red} & \theta_{blue/green} \\ & 1 & \theta_{red/green} \\ Sym & & 1 \end{pmatrix} = \begin{pmatrix} 1 & \theta_{1,2} & \theta_{1,3} \\ & 1 & \theta_{2,3} \\ Sym & & 1 \end{pmatrix}$$

*Example: Homoscedastic hypersphere mixed kernel*

- $[\Phi(\Theta_j)]_{r,s} = [C(\Theta_j)C(\Theta_j)^T]_{r,s}$ → Hypersphere Decomposition
- $\kappa = \mathbb{1}_{L_i}$

# The naïve Exponential kernel (Full model)

- *Extension of the Exponential kernel*

$$[R_i(\Phi(\Theta_i))]_{\ell^i_r,\ell^i_s} = \exp\left( - \sum_{j=1}^{L_i} \sum_{j'=1}^{L_i} \left| [e_{c^r_i} - e_{c^s_i}]_j \right|^{p/2} [\Phi(\Theta_i)]_{j,j'} \left| [e_{c^r_i} - e_{c^s_i}]_{j'} \right|^{p/2} \right)$$

$$[\boldsymbol{R_i}]_{\boldsymbol{r,s}}$$

# The naïve Exponential kernel (Full model)

- *Extension of the Exponential kernel*

$$[R_i(\Phi(\Theta_i))]_{\ell^i_r,\ell^i_s} = \exp\left(-\sum_{i=1}^{L_i}\sum_{i'=1}^{L_i} \left|[e_{c^r_i} - e_{c^s_i}]_j\right|^{p/2} [\Phi(\Theta_i)]_{j,j'} \left|[e_{c^r_i} - e_{c^s_i}]_{j'}\right|^{p/2}\right)$$

$$[\boldsymbol{R_i}]_{\boldsymbol{r,s}} = \exp\left(-\left([\Phi(\Theta_i)]_{\ell^i_r,\ell^i_r} + [\Phi(\Theta_i)]_{\ell^i_s,\ell^i_s} + [\Phi(\Theta_i)]_{\ell^i_r,\ell^i_s} + [\Phi(\Theta_i)]_{\ell^i_s,\ell^i_r}\right)\right)$$

# The naïve Exponential kernel (Full model)

- *Extension of the Exponential kernel*

$$[R_i(\Phi(\Theta_i))]_{\ell_r^i,\ell_s^i} = \exp\left(-\sum_{i=1}^{L_i}\sum_{i'=1}^{L_i} \left|[e_{c_i^r} - e_{c_i^s}]_j\right|^{p/2} [\Phi(\Theta_i)]_{j,j'} \left|[e_{c_i^r} - e_{c_i^s}]_{j'}\right|^{p/2}\right)$$

$$[\boldsymbol{R_i}]_{r,s} = \exp\left(-\left([\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_r^i}\right)\right)$$

$$= \exp\left(-[\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} - [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i}\right) \exp\left(-2[\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i}\right)$$

# The naïve Exponential kernel (Full model)

- *Extension of the Exponential kernel*

$$[R_i(\Phi(\Theta_i))]_{\ell_r^i,\ell_s^i} = \exp\left(-\sum_{i=1}^{L_i}\sum_{i'=1}^{L_i} \left|[e_{c_i^r} - e_{c_i^s}]_j\right|^{p/2} [\Phi(\Theta_i)]_{j,j'} \left|[e_{c_i^r} - e_{c_i^s}]_{j'}\right|^{p/2}\right)$$

$$[\boldsymbol{R}_i]_{r,s} = \exp\left(-\left([\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_r^i}\right)\right)$$

$$= \exp\left(-[\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} - [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i}\right) \exp\left(-2[\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i}\right)$$

**Continuous Relaxation (CR)** $[\boldsymbol{S}_i]_{r,s}$

**Exponential Homoscedastic Hypersphere (EHH)** $[\boldsymbol{T}_i]_{r,s}$

# The naïve Exponential kernel  (Full model)

- *Extension of the Exponential kernel*

$$[R_i(\Phi(\Theta_i))]_{\ell_r^i,\ell_s^i} = \exp\left(-\sum_{i=1}^{L_i}\sum_{i'=1}^{L_i} \left|[e_{c_i^r} - e_{c_i^s}]_j\right|^{p/2} [\Phi(\Theta_i)]_{j,j'} \left|[e_{c_i^r} - e_{c_i^s}]_{j'}\right|^{p/2}\right)$$

$$[\boldsymbol{R_i}]_{\boldsymbol{r,s}} = \exp\left(-\left([\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i} + [\Phi(\Theta_i)]_{\ell_s^i,\ell_r^i}\right)\right)$$

$$= \underbrace{\exp\left(-[\Phi(\Theta_i)]_{\ell_r^i,\ell_r^i} - [\Phi(\Theta_i)]_{\ell_s^i,\ell_s^i}\right)}_{\text{Continuous Relaxation (CR)}} \underbrace{\exp\left(-2[\Phi(\Theta_i)]_{\ell_r^i,\ell_s^i}\right)}_{\text{Exponential Homoscedastic Hypersphere (EHH)}}$$

**Continuous Relaxation (CR)** $[\boldsymbol{S_i}]_{\boldsymbol{r,s}}$

**Exponential Homoscedastic Hypersphere (EHH)** $[\boldsymbol{T_i}]_{\boldsymbol{r,s}}$

**Warning:** $\exp(\boldsymbol{x}) > \boldsymbol{0}$

# The naïve Exponential kernel (Full model)

- *Construction of the correlation matrix* $[R_i]$

Rebonato, R. and Jäckel, P. (1999) The Most General Methodology to Create a Valid Correlation Matrix for Risk Management and Option Pricing Purposes. Journal of Risk, 2, 17-28.

# The naïve Exponential kernel (Full model)

- *Construction of the correlation matrix* $[R_i]$

$$[R_i]_{r,s} = [S_i]_{r,s}[T_i]_{r,s} \quad \text{if } r \neq s$$
$$[R_i]_{r,r} = 1,$$

Rebonato, R. and Jäckel, P. (1999) The Most General Methodology to Create a Valid Correlation Matrix for Risk Management and Option Pricing Purposes. Journal of Risk, 2, 17-28.

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$$[R_i]_{r,r} = 1,$$

**Continuous Relaxation diagonal kernel**

$$[S_i]_{r,s} = \prod_{j=1}^{L_i} \exp\left(-[\Phi(\Theta_i)]_{j,j}\left((e_{c_i^r})_j - (e_{c_i^s})_j\right)^2\right)$$

**Exponential Homoscedastic Hypersphere**

$$[T_i]_{r,s} = \exp\left(-2[\Phi(\Theta_i)]_{r,s}\right)$$

$$[\Phi(\Theta_i)]_{j,j} := [\Theta_i]_{j,j} \geq 0$$
$$[\Phi(\Theta_i)]_{j,j'} := \frac{\log \epsilon}{2}([C(\Theta_i)C(\Theta_i)^\top]_{j,j'} - 1) \quad \text{if } j \neq j',$$

Rebonato, R. and Jäckel, P. (1999) The Most General Methodology to Create a Valid Correlation Matrix for Risk Management and Option Pricing Purposes. Journal of Risk, 2, 17-28.

# The naïve Exponential kernel (Full model)

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$$[R_i]_{r,s} = [S_i]_{r,s}[T_i]_{r,s} \quad \text{if } r \neq s$$
$$[R_i]_{r,r} = 1,$$

**Continuous Relaxation diagonal kernel**

$$[S_i]_{r,s} = \prod_{j=1}^{L_i} \exp\left(-[\Phi(\Theta_i)]_{j,j}\left((e_{c_i^r})_j - (e_{c_i^s})_j\right)^2\right)$$

$$[S_i]_{r,s} \geq 0$$
$$[S_i]_{r,s} \leq 1$$

**Exponential Homoscedastic Hypersphere**

$$[T_i]_{r,s} = \exp\left(-2[\Phi(\Theta_i)]_{r,s}\right)$$

$$[T_i]_{r,s} = \epsilon \exp\left(-(\log \epsilon)[C_i C_i^T]_{r,s}\right)$$
$$[T_i]_{r,s} = \epsilon \exp\left(-(\log \epsilon)[C_i C_i^T]_{r,s}\right) \geq \epsilon \exp 0 = \epsilon$$
$$[T_i]_{r,s} = \epsilon \exp\left(-(\log \epsilon)[C_i C_i^T]_{r,s}\right) \leq \frac{\epsilon}{\epsilon} = 1$$

$$[\Phi(\Theta_i)]_{j,j} := [\Theta_i]_{j,j} \geq 0$$
$$[\Phi(\Theta_i)]_{j,j'} := \frac{\log \epsilon}{2}([C(\Theta_i)C(\Theta_i)^\top]_{j,j'} - 1) \quad \text{if } j \neq j',$$

$1 \gg \epsilon > 0$

$C_i$: **Homoscedastic hypersphere**

Rebonato, R. and Jäckel, P. (1999) The Most General Methodology to Create a Valid Correlation Matrix for Risk Management and Option Pricing Purposes. Journal of Risk, 2, 17-28.

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
|---|---|---|---|
| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i (L_i - 1)$ |

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
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| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i(L_i - 1)$ |
| Our full model (FE) | $\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))\ \exp(-2\,[\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i + 1)$ |

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
|---|---|---|---|
| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i(L_i - 1)$ |
| Our full model (FE) | $\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))\ \exp(-2[\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i + 1)$ |
| Our model as Exponential Homoscedastic Hypersphere (EHH) | $\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2[\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i - 1)$ |

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
|---|---|---|---|
| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i(L_i - 1)$ |
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| Our model as Exponential Homoscedastic Hypersphere (EHH) | $\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2 [\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i - 1)$ |
| Our model as Continuous Relaxation (CR) | $\begin{pmatrix} [\Theta_i]_{11} & 0 & 0 \\ & [\Theta_i]_{22} & 0 \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))$ | $L_i$ |

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
|---|---|---|---|
| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i(L_i - 1)$ |
| Our full model (FE) | $\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))\ \exp(-2\,[\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i + 1)$ |
| Our model as Exponential Homoscedastic Hypersphere (EHH) | $\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2\,[\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i(L_i - 1)$ |
| Our model as Continuous Relaxation (CR) | $\begin{pmatrix} [\Theta_i]_{11} & 0 & 0 \\ & [\Theta_i]_{22} & 0 \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))$ | $L_i$ |
| Our model as Gower distance (GD) | $[\Theta_i]_{cov} \begin{pmatrix} 0 & 1 & 1 \\ & 0 & 1 \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2\,[\Theta_i]_{cov})$ | 1 |

# Modeling categorical kernels

| Model | $\Theta_i$ (example with 3 levels) | $K_i(c_i^r, c_i^s, \Theta_i)$ | # of parameters |
|---|---|---|---|
| Homoscedastic Hypersphere (HH) | $\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$ | $[\Theta_i]_{c_i^r, c_i^s}$ | $\frac{1}{2} L_i (L_i - 1)$ |
| Our full model (FE) | $\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s})) \exp(-2 [\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i (L_i + 1)$ |
| Our model as Exponential Homoscedastic Hypersphere (EHH) | $\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2 [\Theta_i]_{c_i^r, c_i^s})$ | $\frac{1}{2} L_i (L_i - 1)$ |
| Our model as Continuous Relaxation (CR) | $\begin{pmatrix} [\Theta_i]_{11} & 0 & 0 \\ & [\Theta_i]_{22} & 0 \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$ | $\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))$ | $L_i$ |
| Our model as Gower distance (GD) | $[\Theta_i]_{cov} \begin{pmatrix} 0 & 1 & 1 \\ & 0 & 1 \\ \text{Sym.} & & 0 \end{pmatrix}$ | $\exp(-2 [\Theta_i]_{cov})$ | 1 |

# Summary for $\kappa$ and $\Phi$

## Every model can be written as

$$[R_j(\Theta_j)]_{\ell_r^j,\ell_s^j} = \prod_{j=1}^{l} \kappa([\Phi(\Theta_j)]_{\ell_j^r,\ell_j^s})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s,\ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^r,\ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s,\ell_j^s})$$

| Name | $\kappa$ | $\Phi(\Theta_i)$ |
|---|---|---|
| GD | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := \frac{1}{2}\theta_i \quad ; \quad [\Phi(\Theta_i)]_{j\neq j'} := 0$ |
| CR | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := [\Theta_i]_{j,j} \quad ; \quad [\Phi(\Theta_i)]_{j\neq j'} := 0$ |
| EHH | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := 0 \quad ; \quad [\Phi(\Theta_i)]_{j\neq j'} := \frac{\log \epsilon}{2}([C(\Theta_i)C(\Theta_i)^\top]_{j,j'} - 1)$ |
| HH | $\mathbb{I}_{L_i}$ | $[\Phi(\Theta_i)]_{j,j} := 1 \quad ; \quad [\Phi(\Theta_i)]_{j\neq j'} := ([C(\Theta_i)C(\Theta_i)^\top]_{j,j'}$ |

Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E.-G., and Guerin, Y., Overview and Comparison of Gaussian Process-Based Surrogate Models for Mixed Continuous and Discrete Variables: Application on Aerospace Design Problems, Springer International Publishing, 2020, pp. 189–224

# Summary for $\kappa$ and $\Phi$

## Every model can be written as

$$[R_j(\Theta_j)]_{\ell_r^j,\ell_s^j} = \prod_{j=1}^{l} \kappa([\Phi(\Theta_j)]_{\ell_j^r,\ell_j^s})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s,\ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^r,\ell_j^r})\ \kappa([\Phi(\Theta_j)]_{\ell_j^s,\ell_j^s})$$

| Name | $\kappa$ | $\Phi(\Theta_i)$ |
|---|---|---|
| GD | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := \frac{1}{2}\theta_i$ ; $[\Phi(\Theta_i)]_{j\neq j'} := 0$ |
| CR | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := [\Theta_i]_{j,j}$ ; $[\Phi(\Theta_i)]_{j\neq j'} := 0$ |
| EHH | $\exp(.)$ | $[\Phi(\Theta_i)]_{j,j} := 0$ ; $[\Phi(\Theta_i)]_{j\neq j'} := \frac{\log \epsilon}{2}([C(\Theta_i)C(\Theta_i)^\top]_{j,j'} - 1)$ |
| HH | $\mathbb{I}_{L_i}$ | $[\Phi(\Theta_i)]_{j,j} := 1$ ; $[\Phi(\Theta_i)]_{j\neq j'} := ([C(\Theta_i)C(\Theta_i)^\top]_{j,j'}$ |

**Our new kernel EHH is Gaussian and categorical!**

Pelamatti, J., Brevault, L., Balesdent, M., Talbi, E.-G., and Guerin, Y., Overview and Comparison of Gaussian Process-Based Surrogate Models for Mixed Continuous and Discrete Variables: Application on Aerospace Design Problems, Springer International Publishing, 2020, pp. 189–224

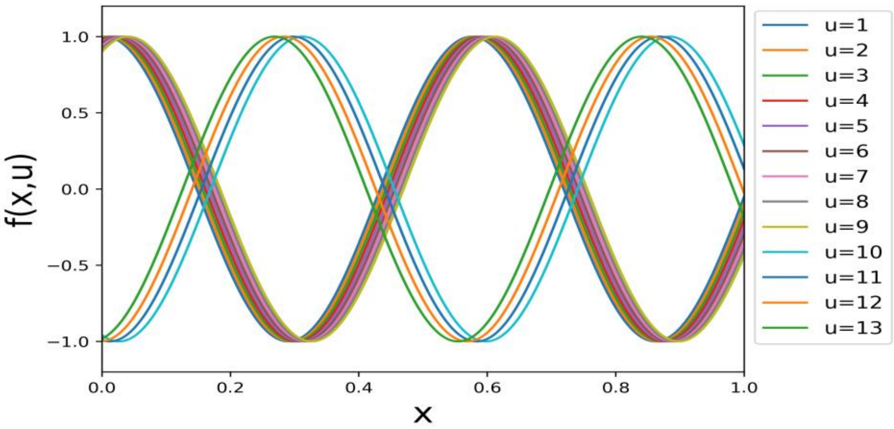
# Results

- *An illustration case*

2 design variables

- 1 continuous variable
- 1 categorical variable: 13 levels
- 14 dimensions

- DoE: LHS with 98 points (7 per dimension)




Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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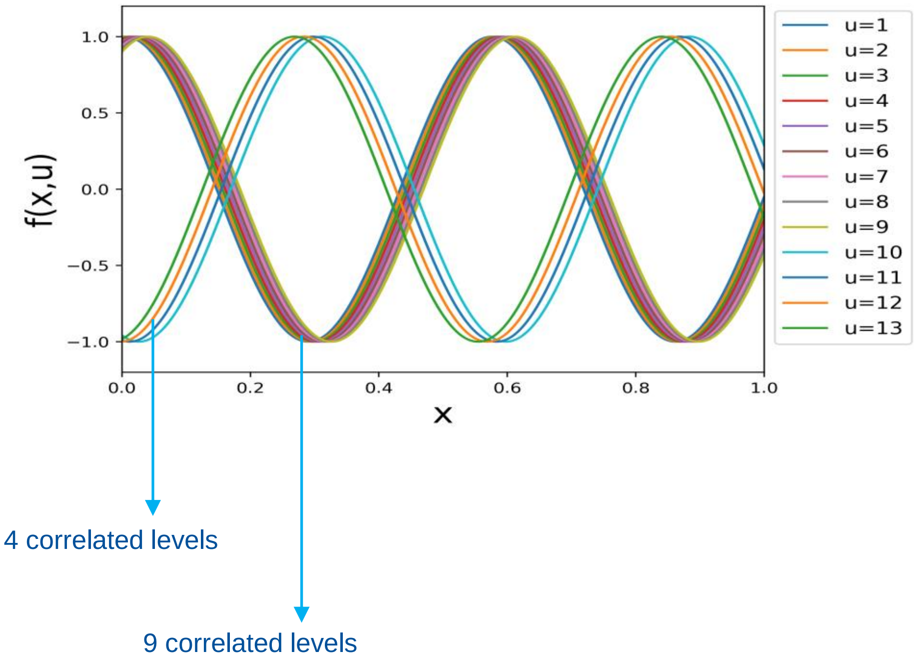


Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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- *An illustration case*

2 design variables
- 1 continuous variable
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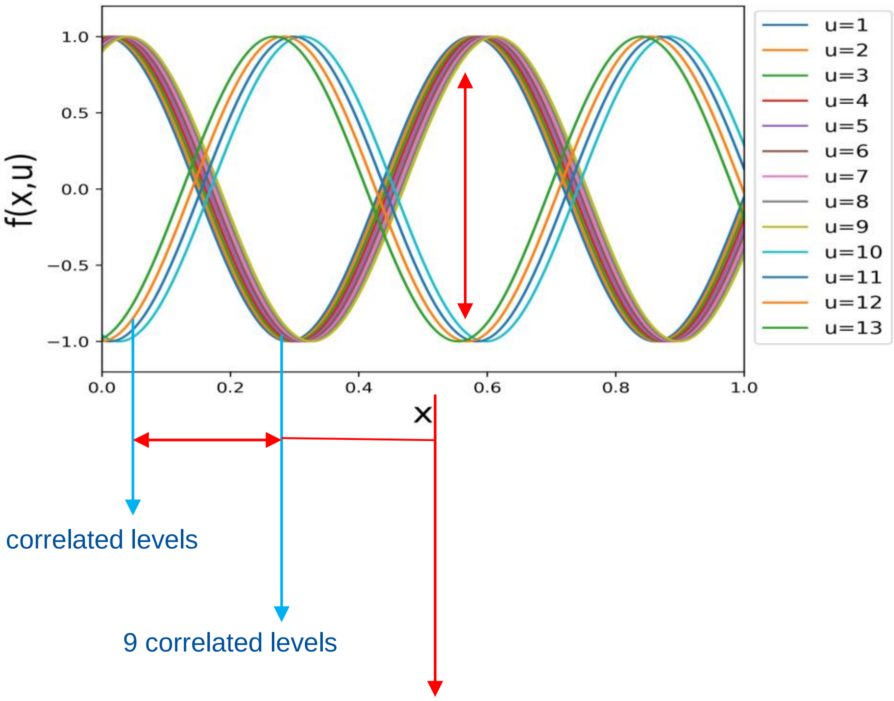


4 correlated levels

9 correlated levels

Anticorrelated groups

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

# Results

- *An illustration case*

2 design variables
- 1 continuous variable
- 1 categorical variable: 13 levels
- 14 dimensions

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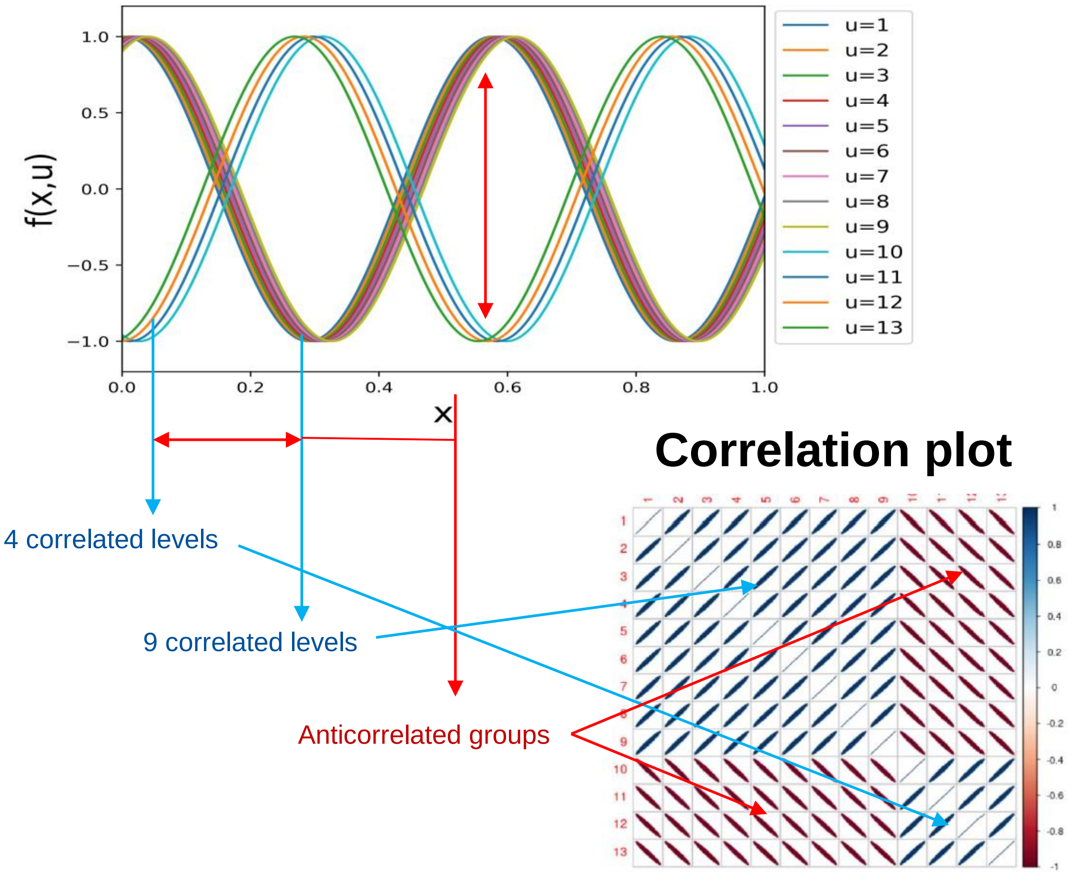
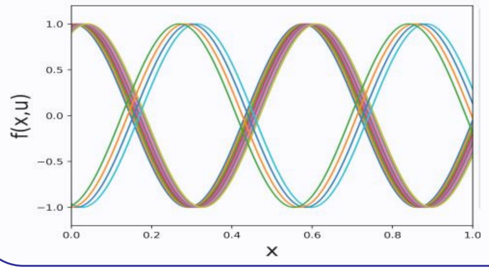



Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

# Results




**2 variables**
- **One continuous variable**
- **One categorical variable: 13 levels**

⇒ **14 dimensions**

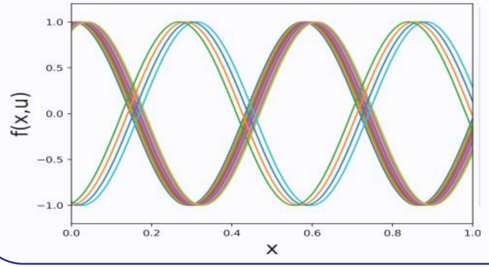
**DoE : LHS (n = 98)**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

# Results

**Full model**

- 92 hyperparameters
- Time = 642 seconds
- RMSE = 22.6




**2 variables**
- **One continuous variable**
- **One categorical variable: 13 levels**

⇒ **14 dimensions**

**DoE : LHS (n = 98)**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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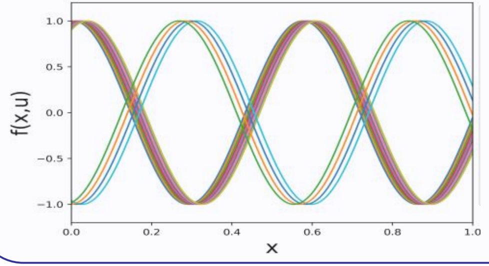


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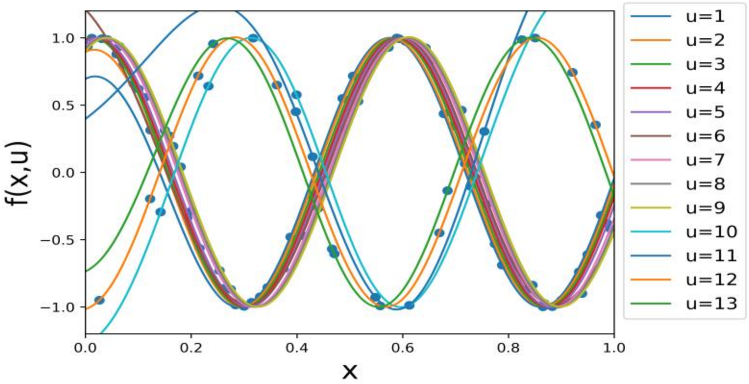


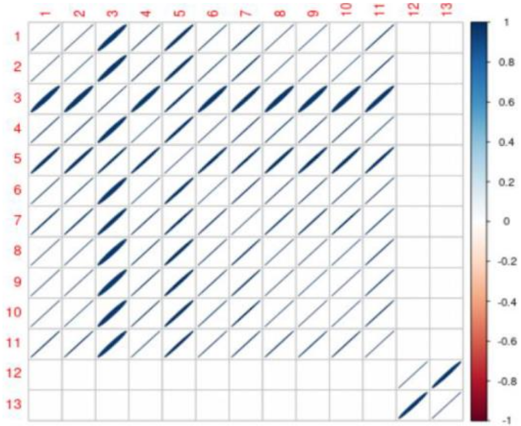

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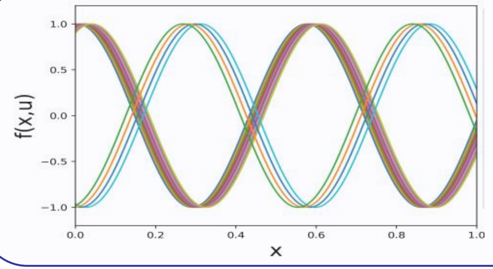


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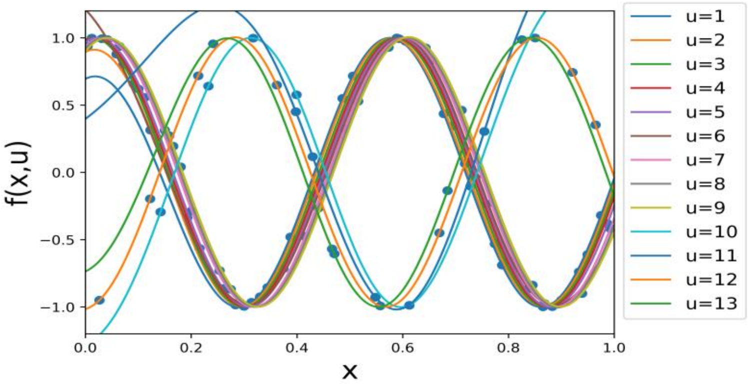


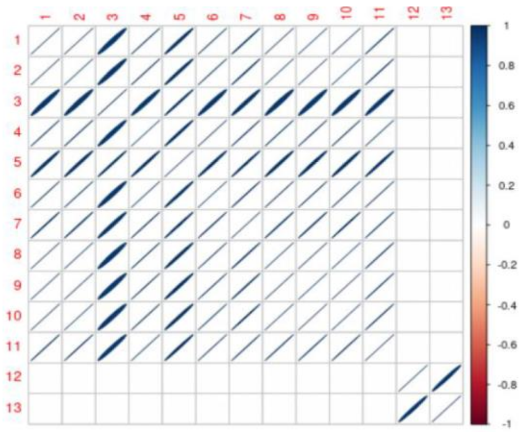

**Many hyperparameters are useless! Expensive with many numerical issues.**


Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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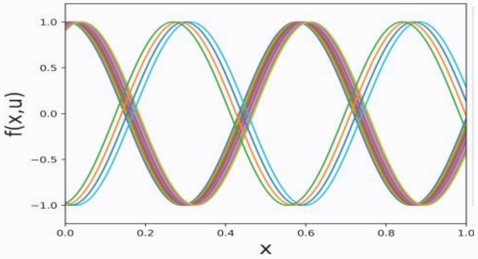


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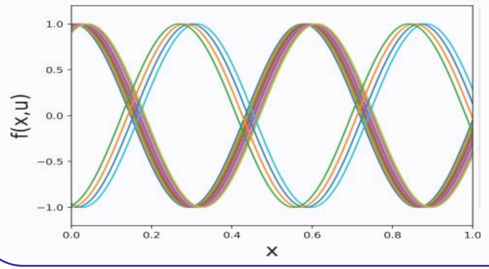
# Results

**Gower case**

- 2 hyperparameters
- Time = 1.4 seconds
- RMSE = 30.1

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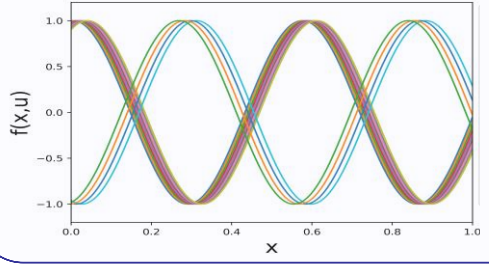


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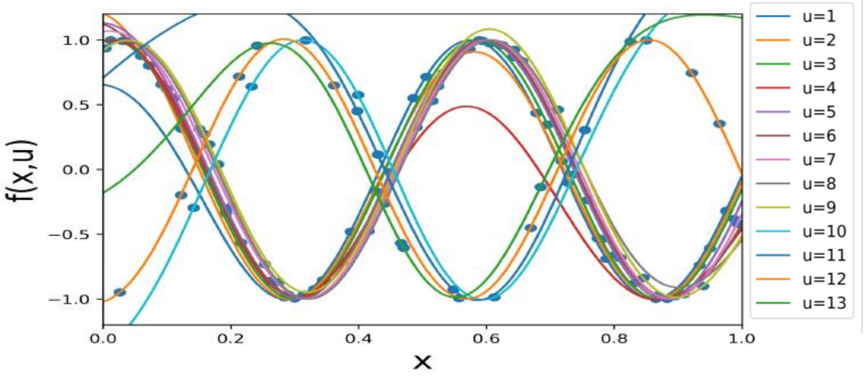


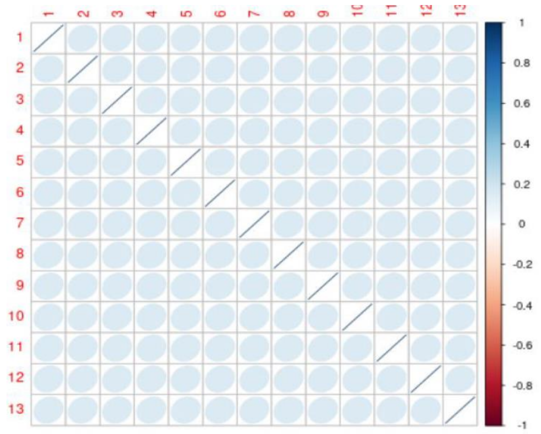

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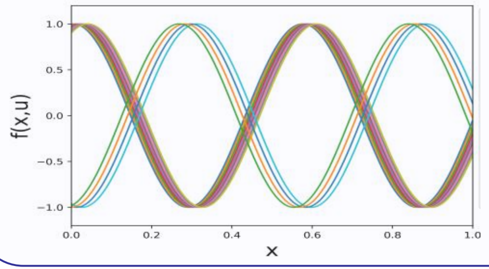


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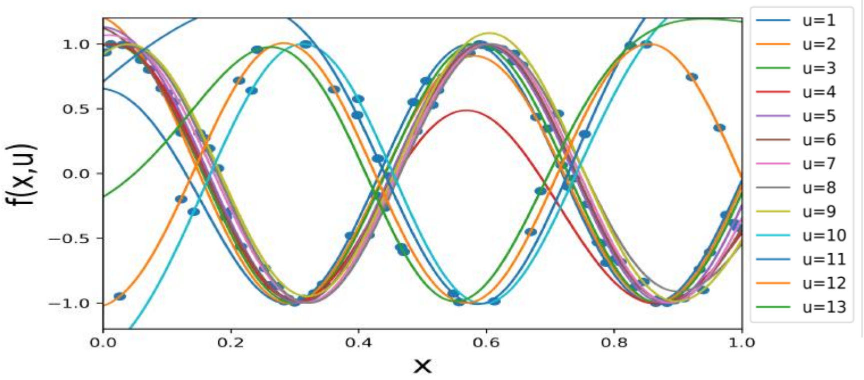


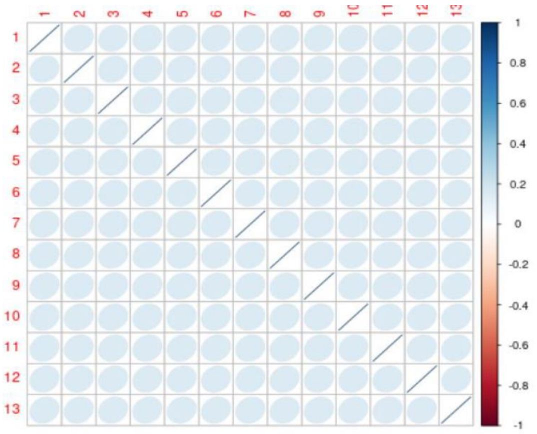


**Only few hyperpameters are used which may not be enough.**


Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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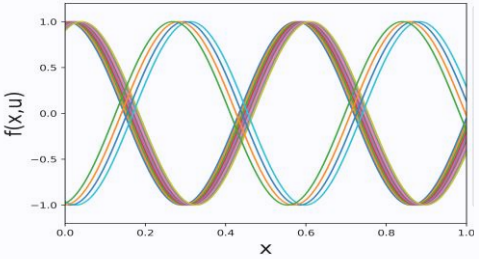


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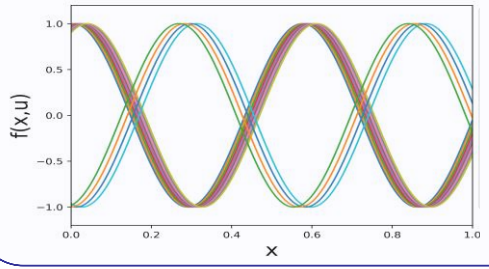
# Results

**Continuous relaxation case**

- 14 hyperparameters
- Time = 24.5 seconds
- RMSE = 22.3

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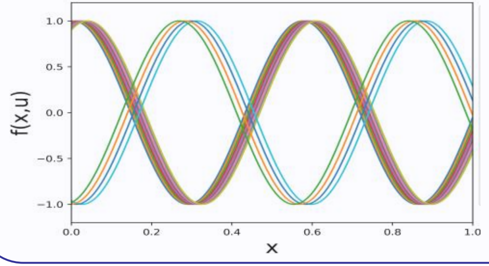


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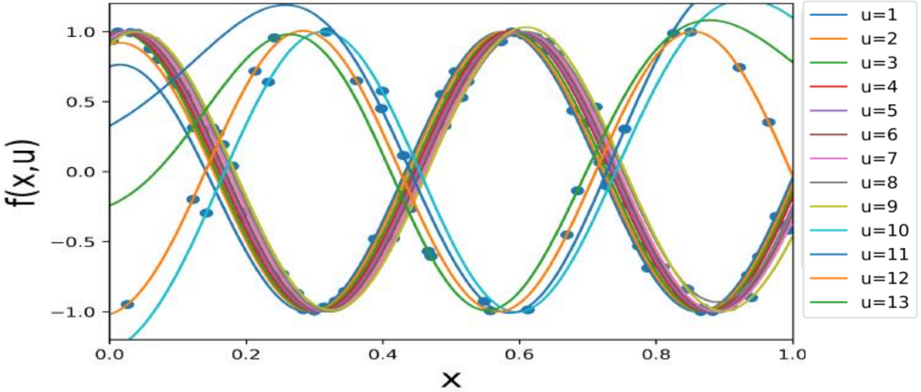


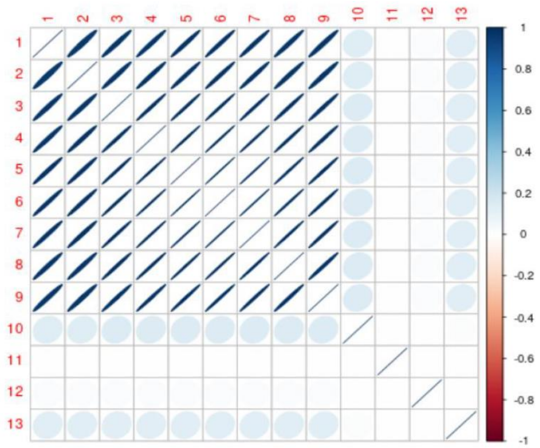


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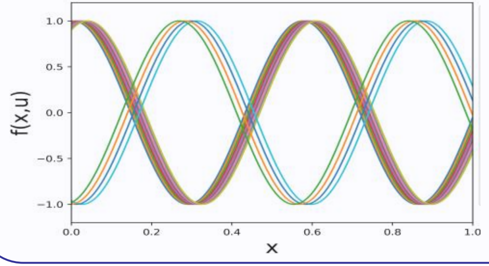


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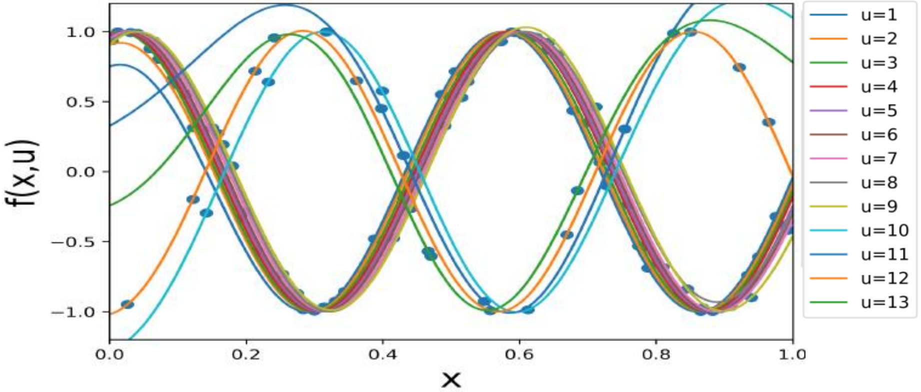


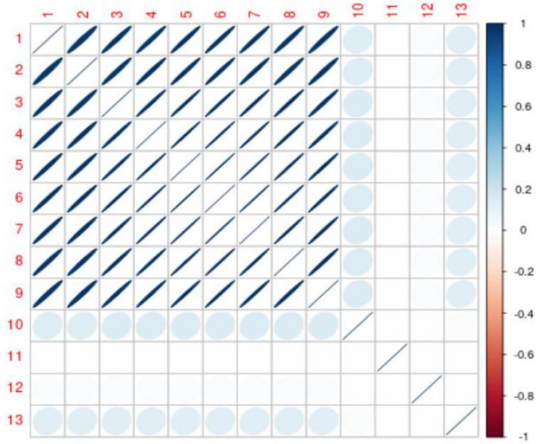

**Best trade-off: number of hyperparameters vs model accuracy!**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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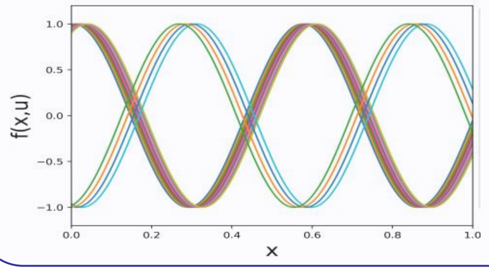


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$\Rightarrow$ **14 dimensions**

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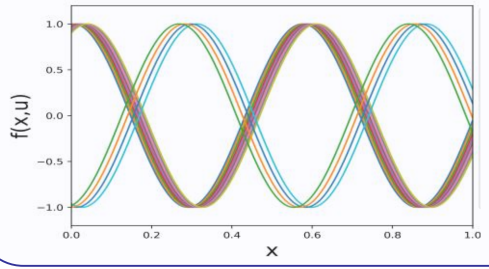
# Results

**Exponential Homoscedastic hypersphere case**

- 79 hyperparameters
- 514.5 seconds
- RMSE = 1.8

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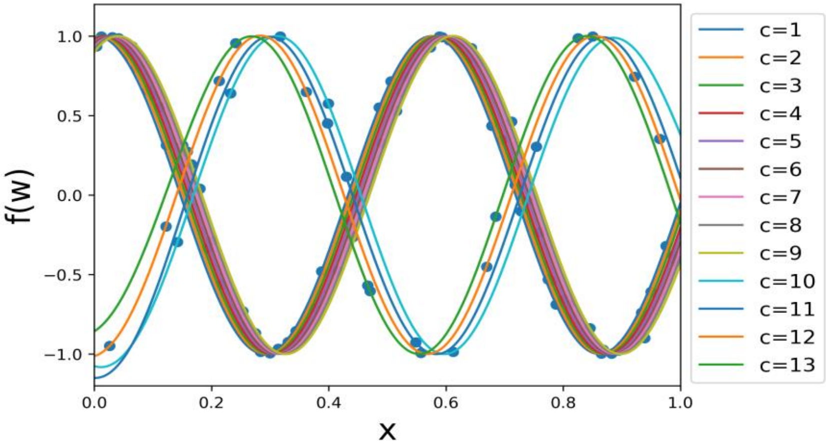


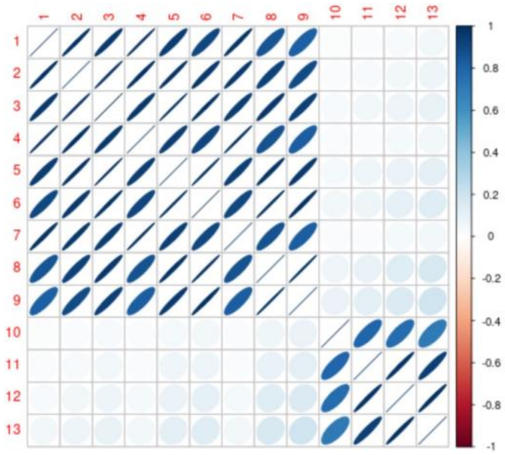

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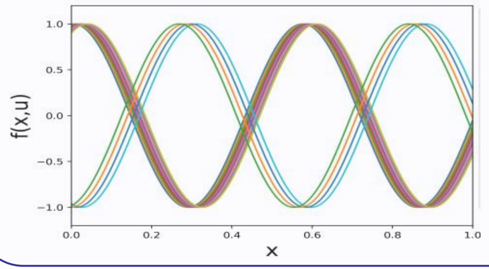


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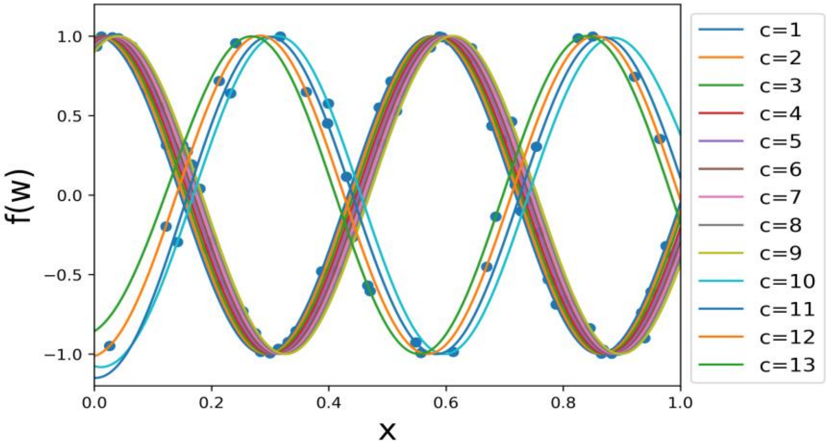
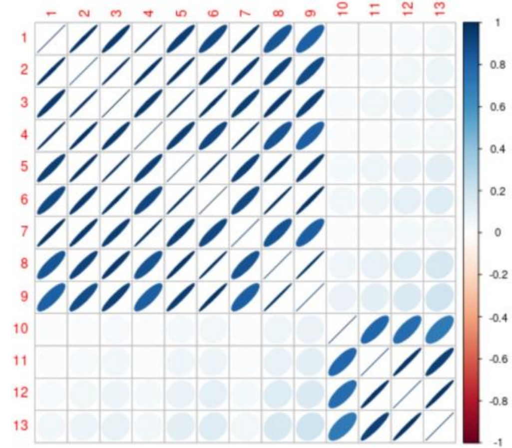



> 0

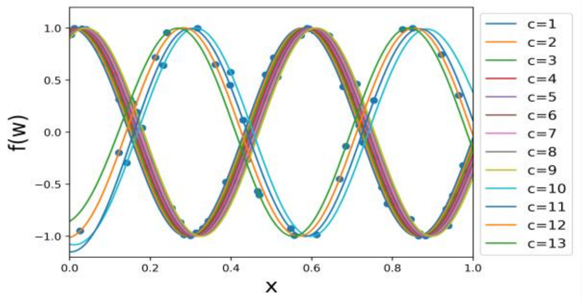


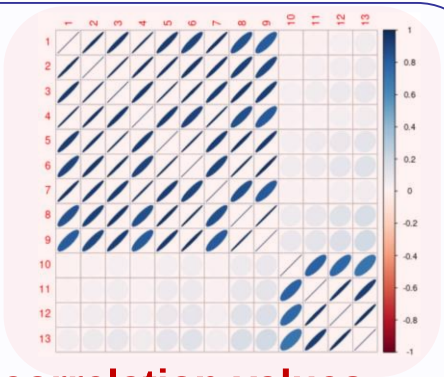
**Accurate model but expensive. Only positive correlations can be handled.**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

# Results

**Our Exponential homoscedastic hypersphere kernel**



$\in [0, 1]$

**Efficient method with positive correlation values**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

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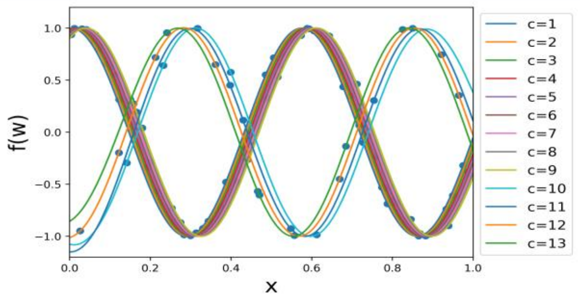
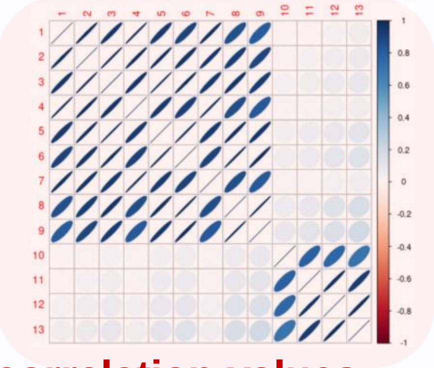
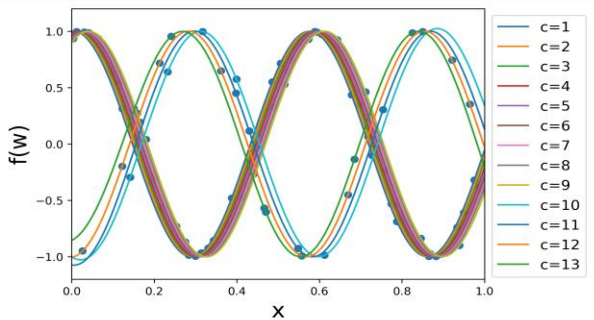


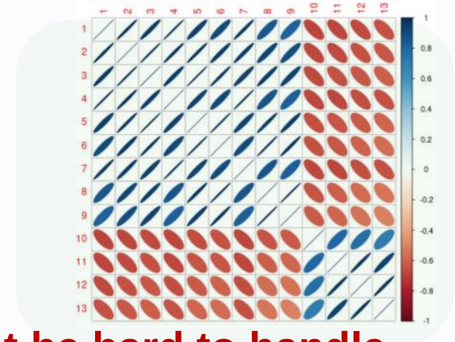



$\in [0,1]$

**Efficient method with positive correlation values**

**Homoscedastic hypersphere kernel** *(Pelamatti et al., 2020)*



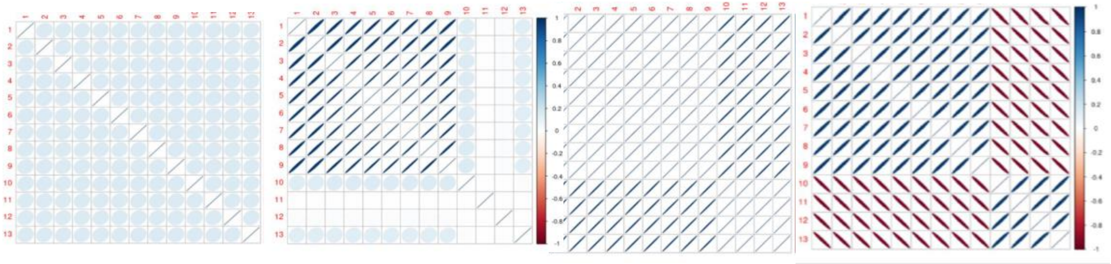
$\in [-1,1]$ **but hard to optimize**

**Include general correlation values but might be hard to handle**

Roustant, O., E. Padonou, Y. Deville, A. Clément, G. Perrin, J. Giorla, and H. Wynn (2020). Group kernels for Gaussian process metamodels with categorical inputs. SIAM J.Uncertain. 8, 775–806.

# Results

- *An illustration case*



2 design variables
- 1 continuous variable
- 1 categorical variable: 13 levels
- 14 dimensions

- DoE: LHS with 98 points (7 per dimension)

Validation set of 30603 points

$$RMSE = \left( \frac{1}{30603} \sum_{i=1}^{30603} \left( \hat{f}(w_i) - f(w_i) \right)^2 \right)^{1/2}$$

$$PVA = \log \left( \frac{1}{30603} \sum_{i=1}^{30603} \frac{\left( \hat{f}(w_i) - f(w_i) \right)^2}{\sigma^f(w_i)^2} \right)$$

Table 4: Kernel comparison for the cosine test case

| Kernel | # of Hyperparam. | RMSE | PVA | CPU time (s) |
|---|---|---|---|---|
| GD | 2 | 30.079 | 21.99 | 1.4 |
| CR | 14 | 22.347 | 23.04 | 24.5 |
| EHH | 79 | 1.882 | 23.74 | 514.5 |
| HH | 79 | 1.280 | 24.31 | 514.5 |

C.Demay, Iooss, B., Gratiet, L. L., and Marrel, A., "Model selection based on validation criteria for Gaussian process regression: An application with highlights on the predictive variance," Quality and Reliability Engineering International, Vol. 38, 2022, pp. 1482–1500.

# Exemple of application: Bayesian optimization

SMT

Table of Contents



Previous topic

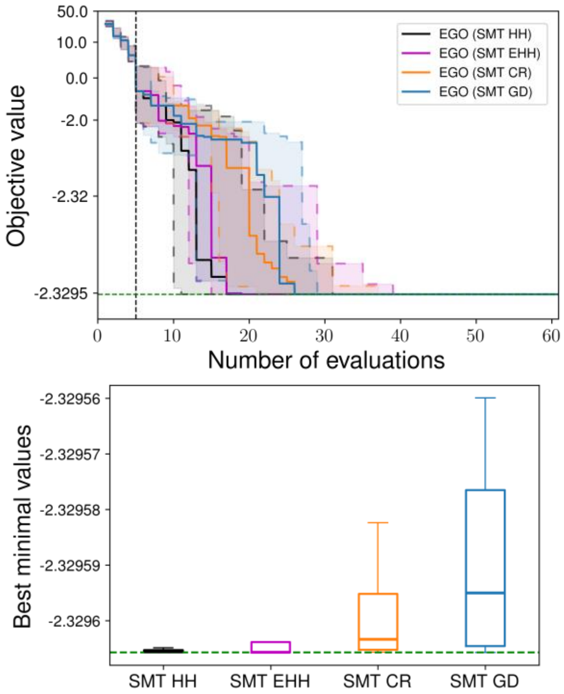

Mixed Integer and Hierarchical usage (Variables, Sampling and Context)


## Branin

```
#Import the Mixed Integer API
from smt.surrogate_models import (KRG,XSpecs,XType,
  XRole,MixIntKernelType)
from smt.applications.mixed_integer import(
MixedIntegerSamplingMethod as misamp,
MixedIntegerContext)
#Define the function
from smt.problems import Branin
fun = Branin(ndim=2)
#Define the mixed variables
xtypes = [XType.ORD,XType.FLOAT]
xlimits = fun.xlimits
xspecs = XSpecs(xtypes=xtypes, xlimits=xlimits)
#Perform a mixed integer sampling with LHS
from smt.sampling_methods import LHS
smp = misamp(LHS,xspecs,random_state=42)
xdoe = smp(10)
# Call the Bayesian optimizer
from smt.applications import EGO
criterion = "EI"  #'EI' or 'SBO' or 'LCB'
ego = EGO(xdoe=xdoe,
  n_iter=20,
  criterion="EI",
  random_state=42,
  surrogate=KRG(xspecs=xspecs,
   categorical_kernel=MixIntKernelType.GOWER))
x_opt, y_opt, _, _, _ = ego.optimize(fun=fun)
# Check if the result is correct
self.assertAlmostEqual(0.494, float(y_opt), delta=1)
```

Figure 7: Example of usage of mixed integer surrogates for Bayesian optimization

## Toy problem





M. M. Zuniga and D. Sinoquet. Global optimization for mixed categorical-continuous variables based on gaussian process models with a randomized categorical space exploration step. INFOR: Information Systems and Operational Research, 58:310–341, 2020

# Conclusion & perspectives

# Conclusion & perspectives

- *Contributions*

- Extended continuous Gaussian kernels to handle mixed-categorical variables.
- Proposed a unified framework for continuous relaxation and Gower distance based kernels.
- Validated the efficiency of the proposed method on a challenging mixed-categorical problem.

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- Extended continuous Gaussian kernels to handle mixed-categorical variables.
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- Validated the efficiency of the proposed method on a challenging mixed-categorical problem.

- *Current works*

Apply dimension reduction (*e.g.*, PLS) using the proposed Gaussian kernel to model large-scale mixed-categorical problems. “Mixed categorical Gaussian process for high-dimensional Bayesian optimization” in Structural and Multidisciplinary Optimization.

Couple mixed-discrete variables with hierarchical variables. SMT 2.0: A Surrogate Modeling Toolbox with a focus on Hierarchical and Mixed Variables Gaussian Processes” in Advances in Engineering Software.

# The End

## Thank you for your attention !

P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, and J. Morlier. A mixed-categorical correlation kernel for gaussian process, 2022. Submitted to Neurocomputing. Available at SSRN: https://dx.doi.org/10.2139/ssrn.4296794