Combination of Optimization-free Kriging Models for High-Dimensional Problems

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1) **Introduction**
   - Design optimization and Kriging surrogate models
   - Challenges in high dimension

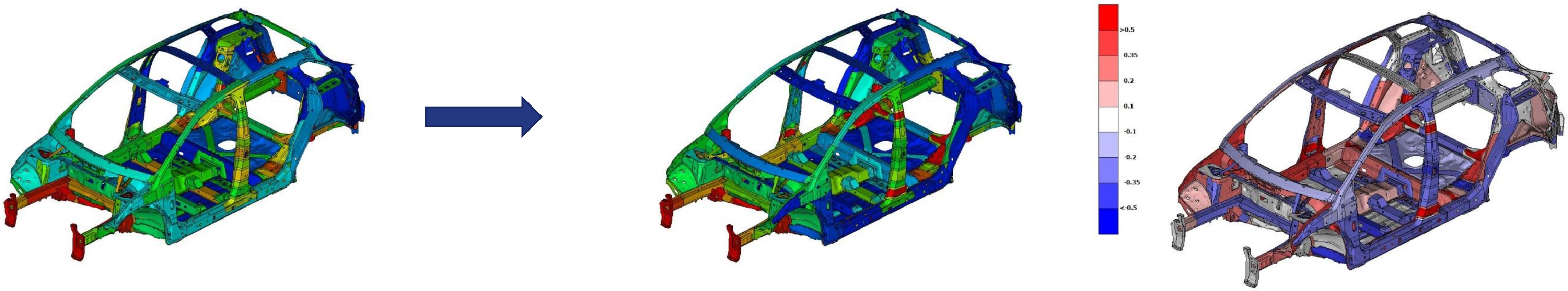
2) **High-dimensional surrogate via a combination of Kriging sub-models**

3) **Numerical results**

4) **Perspectives**

- Design optimization is used to improve the performances of an engineering design.

Initial model **Optimised model** **Thickness difference**



Example : optimization of the Peugeot 3008 to minimize the vehicle weight while satisfying the norms for chock resistance.

- Formally, we are interested in the optimization of a black-box function :

$$y : \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^d \rightarrow y(\boldsymbol{x}) \in \mathbb{R}.$$

→ We want to find the best design :

$$\boldsymbol{x}^* \in \arg\min_{\boldsymbol{x} \in \mathcal{X}} y(\boldsymbol{x}) \,.$$

- We are in the context where **the black-box function y is expensive to evaluate** :

→ Evaluating the function for a single design can take hours.

└→ **We can only afford of few observations**.

└→ We cannot use the usual optimization methods which require a large number of these evaluations.

Build a surrogate model

$$y(x) \approx \hat{y}(x)$$

Expensive true objective function

Cheap analytical approximation

- We dispose of n observations $\boldsymbol{Y} = \left(y(\boldsymbol{x_1}), \dots, y(\boldsymbol{x_n})\right)^T$ at the sample locations $\boldsymbol{X} = (\boldsymbol{x_1}, \dots, \boldsymbol{x_n})^T$.

→ The ordinary Kriging method approximates y as the realization of a Gaussian Process :

$$Y(.) \sim GP\left(\mu, k_{\sigma,\boldsymbol{\theta}}(.,.)\right).$$

- $k_{\sigma,\boldsymbol{\theta}}(.,.)$ is the covariance function (kernel) with σ^2 the variance of the GP and $\boldsymbol{\theta} \in \mathbb{R}^d$ the covariance length-scales.

- We obtain the Kriging predictors for the mean and predictive variance by conditioning the GP Y over $\mathcal{D} = (\boldsymbol{X}, \boldsymbol{Y})$:

$$\hat{y}(\boldsymbol{x}) = E(Y(\boldsymbol{x})|\mathcal{D}) = \mu + k(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}(\boldsymbol{Y} - \boldsymbol{1}\mu),$$

$$\hat{s}^2(\boldsymbol{x}) = Var(Y(\boldsymbol{x})|\mathcal{D}) = k(\boldsymbol{x}, \boldsymbol{x}) - k(\boldsymbol{x}, \boldsymbol{X})\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X})^{-1}k(\boldsymbol{X}, \boldsymbol{x}).$$

COVARIANCE FUNCTION

The choice of the covariance function is very important to obtain a good prediction.

Popular choices of 1D stationary covariance are :

- Exponential : $k_{\sigma,\theta}(x,x') = \sigma^2 \exp\left(-\frac{|x-x'|}{\theta}\right)$,
- Gaussian : $k_{\sigma,\theta}\,(x,x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{2\theta^2}\right)$,
- Matérn 5/2 : $k_{\sigma,\theta}\,(x,x') = \sigma^2 \left(1 + \sqrt{5}\frac{|x-x'|}{\theta} + \frac{5(x-x')^2}{3\theta^2}\right) \exp\left(-\sqrt{5}\frac{|x-x'|}{\theta}\right)$,

Typically, the hyperparameters are optimized to maximize the log-likelihood of the model :

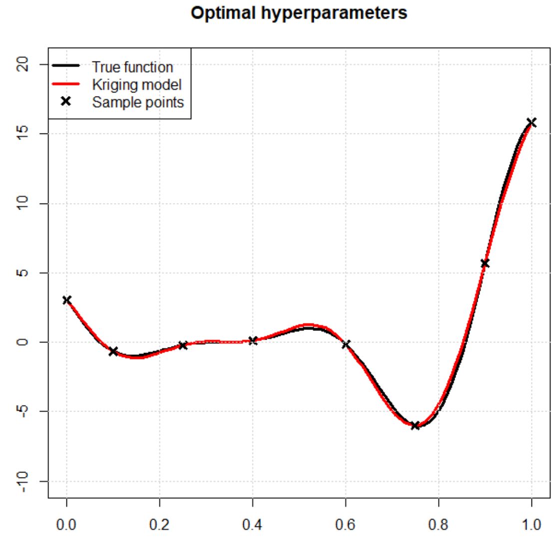
$$\mathcal{L}(\sigma, \boldsymbol{\theta}) = -\frac{1}{2}\boldsymbol{Y}^T \boldsymbol{K}_{\sigma,\boldsymbol{\theta}}^{-1}\boldsymbol{Y} - \frac{1}{2}\log|\boldsymbol{K}_{\sigma,\boldsymbol{\theta}}| - \frac{n}{2}\log(2\pi)\,.$$

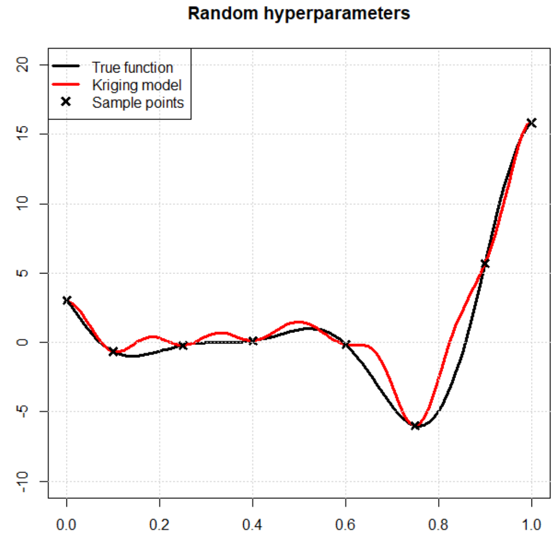
Denoting $\boldsymbol{R}$ the correlation matrix such that $\boldsymbol{K}_{\sigma,\boldsymbol{\theta}} = \sigma^2 \boldsymbol{R}_{\boldsymbol{\theta}}$, the MLE estimator for σ^2 is :

$$\hat{\sigma}^2_{MLE} = \frac{1}{n}\boldsymbol{Y}^T \boldsymbol{R}_{\boldsymbol{\theta}}^{-1}\boldsymbol{Y}.$$

And we obtain the length-scales by solving the minimization problem :

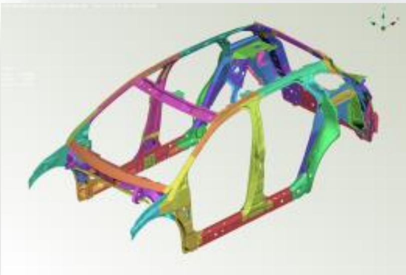
$$\theta_{MLE} = \arg\min_{\boldsymbol{\theta}} \; -\frac{1}{2}\log(\,\hat{\sigma}^2_{MLE}) \; -\frac{1}{2}\log(|\boldsymbol{R}_{\boldsymbol{\theta}}|)\,.$$



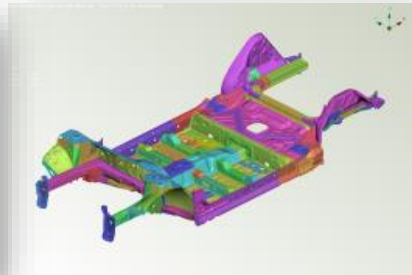


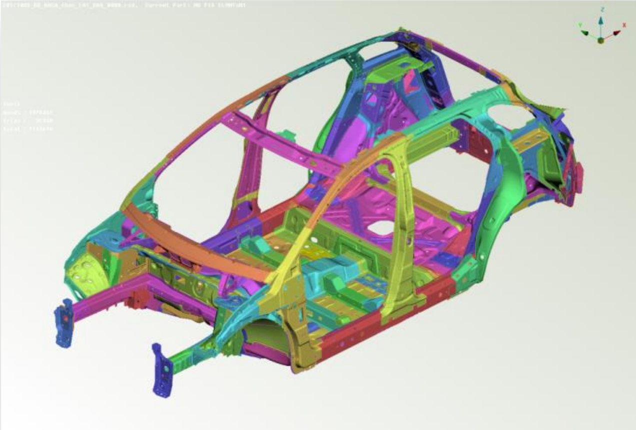
WHAT IS HIGH DIMENSION ?

53 sur périmètre superstructure



77 sur périmètre base





A total of 130 parameters for this example !

The dimension of the problem is the dimension of the design space.

→ That is, **the number of design variables in the problem**.

Typically, for a number of design variables superior to ≈ 20, the ordinary Kriging method begins to show its limits.

- The main issue is the **optimization of the hyperparameters**.

There is one length-scale hyperparameter per dimension, and all these hyperparameters need to be optimized.
→ The optimization of the hyperparameters is difficult :

- d-dimensional problem (with $d > 20$ up to $\approx 100 - 150$).
- **The optimization can be costly** due to the cost of the cost for the evaluation of the objective (log-likelihood) and its gradient is in $O(n^3)$.
- When the training data is sparse (which is often the case for high dimensional problems since we cannot afford to compute too many observations), **the likelihood criterion over-fit the data which lead to a bad estimation of the hyperparameters.**

ISSUES OF KRIGING IN HIGH DIMENSION

- Several methods have been proposed to solve this issue :

- Reduction of the problem's dimension by embedding the design space into a lower-dimension space (see for example Constantine et al., 2015, Bouhlel et al., 2016).
- Additive Kriging where the function is assumed to be a sum of one-dimensional components (see for example Durrande et al., 2012).
- Penalized version of the likelihood to improve the robustness of the hyperparameter optimization (see for example RobustGaSP in Gu et al., 2018).

→ In the following, we present a method to **bypass the hyperparameter optimization** by combining Kriging sub-models with fixed length-scales.

This method is both:

- **Fast** since it avoids the expensive hyperparameter optimization,
- **Easily generalized** since it does not assume a particular form of the underlying function.

→ We propose a model which is a combination of Kriging models with fixed length-scale (see preprint Appriou et al., 2022) :

$$M_{tot}(\boldsymbol{x}) = \sum_{i=1}^{p} w_i(\boldsymbol{x}) M_i(\boldsymbol{x}) \, , \qquad \text{with } M_i(x) = k_{\boldsymbol{\theta}_i}(\boldsymbol{x}, \boldsymbol{X}_i) K_{\boldsymbol{\theta}_i}^{-1}(\boldsymbol{Y}_i - \mu_i)$$ Kriging model with fixed length−scale vector $\boldsymbol{\theta}_i$.

- The weights of the combination can be obtained in **closed-form** and does not require a numerical optimization.

- The complexity of the combination is $O(pn^3)$ (one inversion of the $n \times n$ covariance matrix for each of the p sub-models). For a reasonable number of sub-models, this is less than the cost of ordinary Kriging in $O(\alpha_{iter} n^3)$ where α_{iter} is the number of matrix inversion for the hyperparameter optimization.

An appropriate method to select the length-scales of each sub-model is essential for this method to work.

- **We want to have variety in the sub-models**, so that the combined model can select well-suited behaviors through the weights in the combination.

→ To have variety among the sub-models, we need **variety among the length-scales** as they are the main source of difference between the sub-models.

- We want to avoid too small or too large values of the length-scales:

- For too small values:

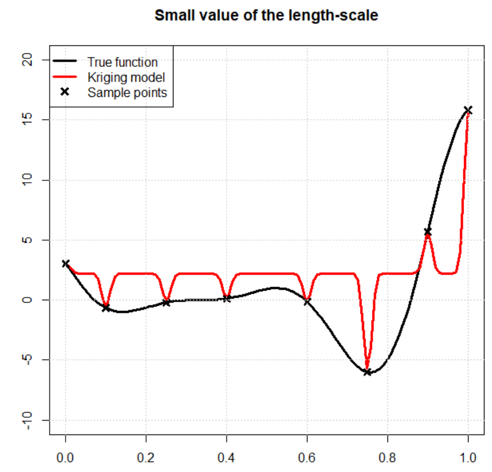
$$k_\theta(x_i, x_j) \longrightarrow 0 \text{ for all } i \neq j, \text{ and } \boldsymbol{K}_\theta \longrightarrow \sigma^2 \boldsymbol{I}_n.$$

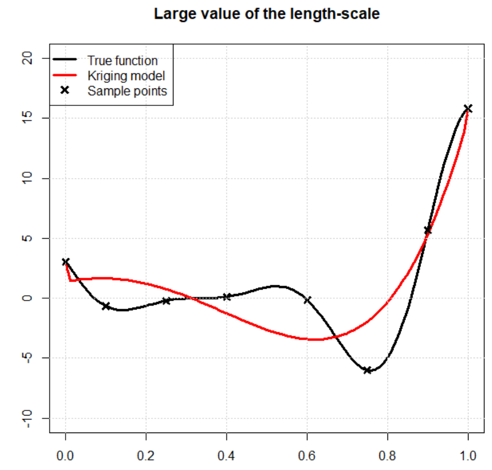
In this case, the Kriging model will return to its mean outside the observations.

- For too large values:

$$k_\theta(x_i, x_j) \longrightarrow 1, \text{ and } \boldsymbol{K}_\theta \longrightarrow \boldsymbol{1}_{n \times n}.$$

In this case, the covariance matrix is ill-defined and its inversion will pose numerical issues.





- To choose the length−scales, we use a criterion based on the entropy of the covariance.

How to use the knowledge about this entropy ?

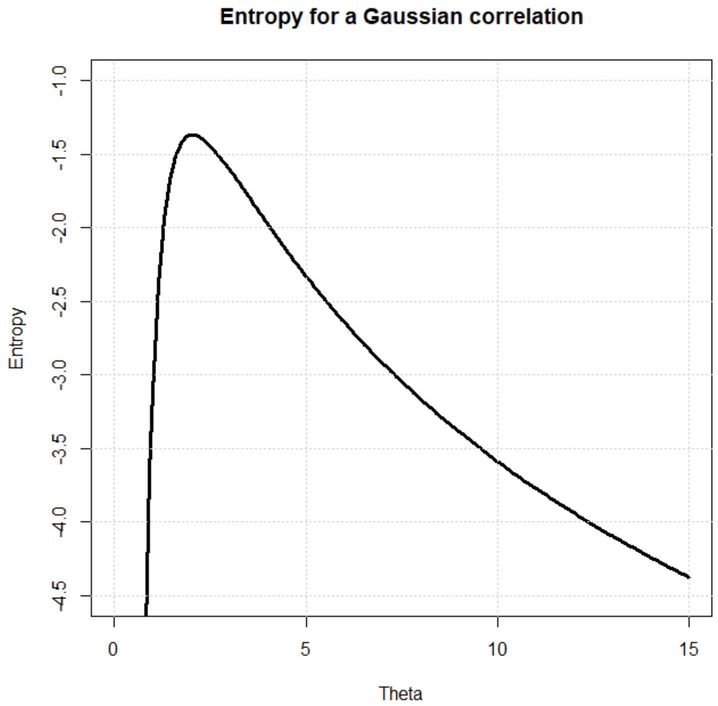
- When sampling the length-scales, **we want to favor θ corresponding to high entropy** values, which result in a high variability in the correlation.

- In the two degenerated cases of small and large length-scales: $R_{\theta_{small}} \longrightarrow \delta_0$ and $R_{\theta_{large}} \longrightarrow \delta_1$, which gives:

$$H\left(R_{\theta_{small}}\right) \longrightarrow -\infty \text{ and } H\left(R_{\theta_{large}}\right) \longrightarrow -\infty.$$

- Finally, we will sample the length-scales using a positive transformation of the entropy:

$$f(\theta) \propto \exp\left(H(R_\theta)\right).$$



Entropy of a Gaussian correlation in 50D for a uniform design.

WEIGHTS OF THE COMBINATION

Now, we present the method used to obtain the weights in the combination: $M_{tot}(\boldsymbol{x}) = \sum_{i=1}^{p} w_i M_i(\boldsymbol{x})$.

- One method (see for example Viana et al., 2009) relies on minimizing the LOOCV error of the combination:

$$e_{LOOCV}(M_{tot}) = \frac{1}{n}\sum_{k=1}^{n}\left(\sum_{i=1}^{p} w_i M_{i_{-k}}(x_k) - y(x_k)\right)^2 = \boldsymbol{w}^T\boldsymbol{C}\boldsymbol{w}.$$

→ The components of the matrix $\boldsymbol{C}$ are : $c_{ij} = \frac{1}{N} {e_{CV}}_i^T {e_{CV}}_j$, with $e_i^{(k)} = \left[K_i^{-1}Y\right]_k / \left[K_i^{-1}\right]_{k,k}$, $k = 1, \ldots, n$.

The weights are then obtained by :

$$\boldsymbol{w}_{LOOCV} = \arg\min_{w} \boldsymbol{w}^T\boldsymbol{C}\boldsymbol{w}\,, \qquad \text{subject to } \boldsymbol{1}^T\boldsymbol{w} = 1 \qquad \Longrightarrow \boldsymbol{w}_{LOOCV} = \frac{\boldsymbol{1}^T\boldsymbol{C}^{-1}}{\boldsymbol{1}^T\boldsymbol{C}^{-1}\boldsymbol{1}}\,.$$

- One of the main advantage of the Kriging method is that it naturally provides a measure of the model error. For a Kriging model $Y(.) \sim GP\left(\mu, k_{\sigma,\boldsymbol{\theta}}(.,.)\right)$:

$$\mathbb{E}\left(\left(M(x) - Y(x)\right)^2\right) = Var(Y(\boldsymbol{x})|Y(X)) = k(\boldsymbol{x},\boldsymbol{x}) - k(\boldsymbol{x},\boldsymbol{X})\boldsymbol{K}(\boldsymbol{X},\boldsymbol{X})^{-1}k(\boldsymbol{X},\boldsymbol{x})$$

→ **This prediction error is essential** to assess the model uncertainty when performing Bayesian optimization for example.

- For our combination of Kriging sub-models: $M_{tot}(\boldsymbol{x}) = \sum_{i=1}^{p} w_i M_i(\boldsymbol{x})$.

We can obtain the error prediction for every individual sub-model, but **the covariance structure between the sub-models is unknown**.

→ We cannot directly access the prediction error of the combination.

VARIANCE OF THE COMBINATION

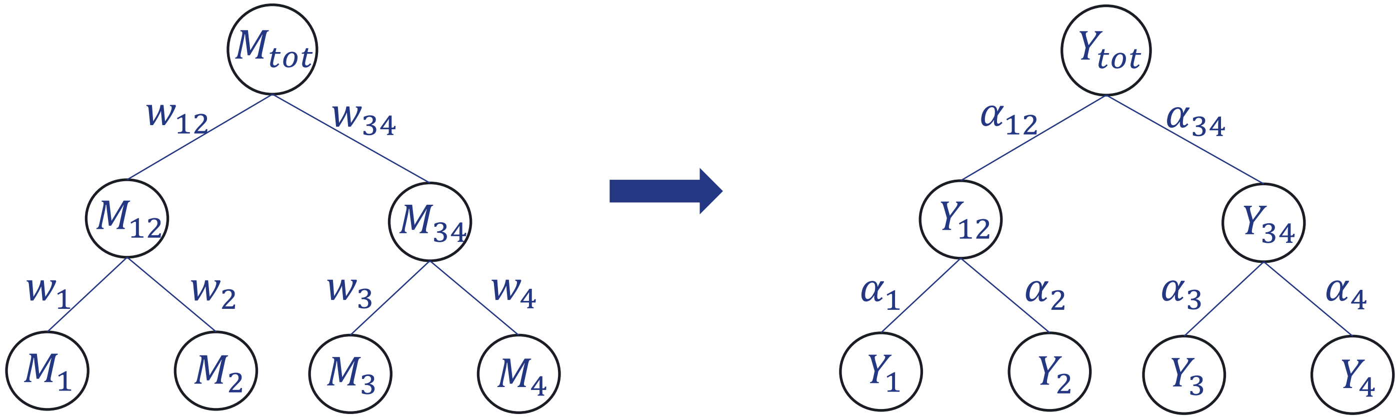
- To obtain the variance of the combination, we add the hypothesis that **the underlying Gaussian Process $\boldsymbol{Y}$ is a combination (with different weights) of independent Gaussian Processes**:

$$Y = \sigma_{tot}^2 \sum_{i=1}^{p} \alpha_p Y_p \,, \qquad \text{with } Y_p \sim GP\left(\mu_p, r_{\theta_p}(.,.)\right), \qquad \sum_{i=1}^{p} \alpha_p = 1, \qquad \text{and } \sigma_{tot}^2 \text{ the variance of the GP.}$$

Thus, the covariance of this GP is:

$$k_{tot}(.,.) = \sigma_{tot}^2 \sum_{i=1}^{p} \alpha_i^2 r_{\theta_i}(.,.)\,.$$

- To simplify the upcoming expressions, we will also assume that the sub-models (and the associated GPs) are combined following a binary tree structure:



- The weights α in the combination of GPs are chosen to minimize the expected mean-square error of the combined model under the corresponding hypothesis:

$$\alpha^* = \arg\min_{\alpha} \mathbb{E}\left[\int_{\mathcal{X}} (wM_1(\boldsymbol{x}) + (1-w)M_2(\boldsymbol{x}) \; - \alpha Y_1(\boldsymbol{x}) + (1-\alpha)Y_2(\boldsymbol{x}))^2 d\boldsymbol{x}\right].$$

By approximation the global MSE using the LOOCV error, we obtain:

$$\alpha^* = \arg\min_{\alpha} \mathbb{E}_{Y=\alpha Y_1+(1-\alpha)Y_2}\, e_{LOOCV}(M_{tot}) = \frac{a_1(w)}{a_1(w)+a_2(w)}, \qquad \text{with:}$$

$$a_1(w) = w^2\mathbb{E}_{Y=Y_2}\big(e_{LOOCV}(M_1)\big) + (1-w^2)\mathbb{E}_{Y=Y_2}\big(e_{LOOCV}(M_2)\big),$$

$$a_2(w) = (1-w)^2\mathbb{E}_{Y=Y_1}\big(e_{LOOCV}(M_2)\big) + (1-(1-w)^2)\mathbb{E}_{Y=Y_1}\big(e_{LOOCV}(M_1)\big).$$

- Once we obtain the weights α, the model uncertainty can be obtained as:

$$\begin{aligned}\mathbb{E}\left(\left(M_{comb}(\boldsymbol{x}) - Y(\boldsymbol{x})\right)^2\right) &= \mathbb{E}\left(M_{comb}(\boldsymbol{x})^2 + Y(\boldsymbol{x})^2 - 2M_{comb}(\boldsymbol{x})Y(\boldsymbol{x})\right) \\ &= Var\left(Y(\boldsymbol{x})\right) + Var\left(M_{comb}(\boldsymbol{x})\right) - 2cov\left(M_{comb}(\boldsymbol{x}), Y(\boldsymbol{x})\right) \\ &= Var\left(Y(\boldsymbol{x})\right) + \boldsymbol{w}^T\boldsymbol{K_M}(\boldsymbol{x})\boldsymbol{w} - 2\boldsymbol{w}^T\boldsymbol{k_M}(\boldsymbol{x}),\end{aligned}$$

With:

$$\left(K_M(\boldsymbol{x})\right)_{i,j} = Cov\left(M_i(\boldsymbol{x}), M_j(\boldsymbol{x})\right) = k_i(\boldsymbol{x},\boldsymbol{X})\boldsymbol{K}_i(\boldsymbol{X},\boldsymbol{X})^{-1}\, Cov\left(Y(\boldsymbol{X}), Y(\boldsymbol{X})\right)\, \boldsymbol{K}_j(\boldsymbol{X},\boldsymbol{X})^{-1}k_j(\boldsymbol{X},\boldsymbol{x}),$$

$$\left(k_M(x)\right)_i = Cov\left(M_i(\boldsymbol{x}), Y(\boldsymbol{x})\right) = k_i(\boldsymbol{x},\boldsymbol{X})\boldsymbol{K}_i(\boldsymbol{X},\boldsymbol{X})^{-1}Cov\left(Y(\boldsymbol{X}), Y(\boldsymbol{x})\right).$$

And:

$$Cov\left(Y(.), Y(.)\right) = k_{tot}(.,.) = \sigma_{tot}^2 \sum_{i=1}^{p} \alpha_i^2 r_{\theta_i}(.,.)\,.$$

- Finally, the last step is to calibrate the amplitude of the variance using the amplitude hyperparameter σ_{tot}^2.

Generally, this can be done by observing that **the normalized LOO errors should be normally distributed**:

$$\frac{e_{LOO}}{\sqrt{Var_{LOO}}} \sim \mathcal{N}(0, \sigma_{tot}^2).$$

→ Thus, one way to obtain the amplitude is:

$$\sigma_{tot}^2 = Var\left(\frac{e_{LOO}}{\sqrt{Var_{LOO}}}\right) = \frac{1}{n}\sum_{i=1}^{n} \frac{{e_{LOO}}_i^2}{{Var_{LOO}}_i}.$$

However, this definition tends to give too large amplitudes due to the presence of many outliers in the LOO error.

To have an expression for the amplitude **more robust to outliers** and which overall give prediction interval that are better calibrated, we fit the empirical inter-quartile distance of the LOO error to that of a Gaussian distribution:

$$IQ\left(\frac{e_{LOO}}{\sigma_{tot}\sqrt{Var_{LOO}}}\right) = IQ_{norm} \iff \sigma_{tot} = \frac{IQ\left(\frac{e_{LOO}}{\sqrt{Var_{LOO}}}\right)}{IQ_{norm}} = \frac{q_{0,75}\left(\frac{e_{LOO}}{\sqrt{Var_{LOO}}}\right) - q_{0,25}\left(\frac{e_{LOO}}{\sqrt{Var_{LOO}}}\right)}{IQ_{norm}}.$$

1) **Introduction**
   - Kriging surrogate models and Bayesian optimization
   - Challenges in high dimension

2) **High-dimensional surrogate via a combination of Kriging sub-models**

3) **Numerical results**
   - Analytical test function
   - Real-world applications

4) **Perspectives**

We tested the method for the approximation of a GP trajectory in 50D (with isotropic length-scale $\theta_{true} = 2$ or $\theta_{true} = 3$) :

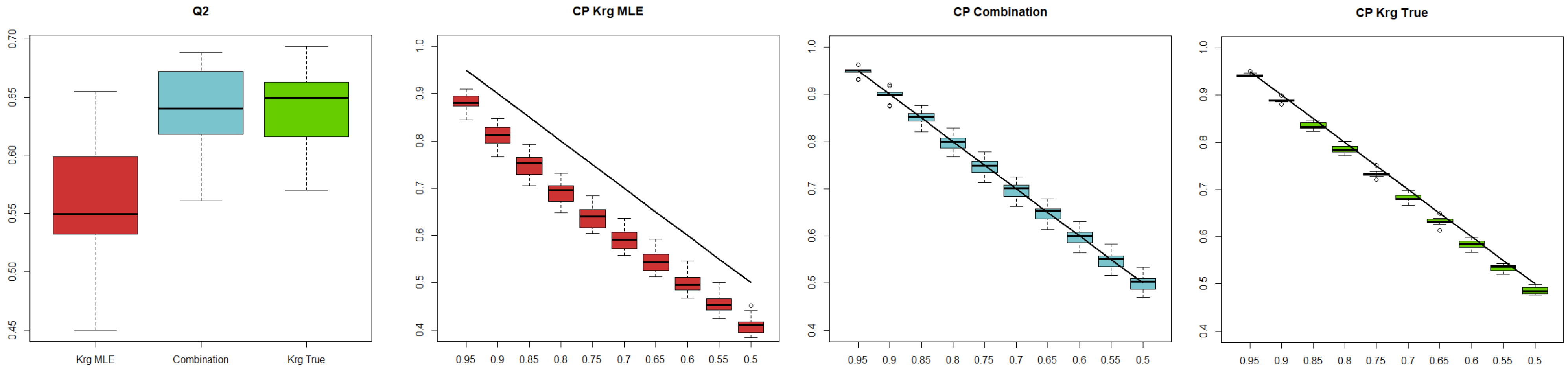
1. Sample a GP trajectory (known length-scale) in **dimension 50**.
2. Select **500 training points** on the trajectory and **5000 test points** to evaluate the precision.
3. Build 32 non-isotropic sub-models with different random length-scales each.
4. Build an ordinary Kriging model with hyperparameters estimated by MLE to compare the performances (300 maximum iterations).
5. Build an ordinary Kriging model with the true length-scales (same as the trajectory). This model is the ideal model whose precision we want to approach.
6. Repeat the experiment 10 times.

To measure the precisions for the 3 models, we compute the Q^2: $Q^2 = 1 - \frac{\sum_{i=1}^{n_{test}} \left(y_{test}(x_i) - \hat{y}(x_i)\right)^2}{\sum_{i=1}^{n_{test}} \left(y_{test}(x_i) - \frac{1}{n_{test}} \sum_{k=1}^{n_{test}} y_{test}(x_k)\right)^2}$

We also access the quality of the error prediction by computing the coverage probabilities for different levels.

NUMERICAL RESULTS – ANALYTICAL TEST FUNCTION

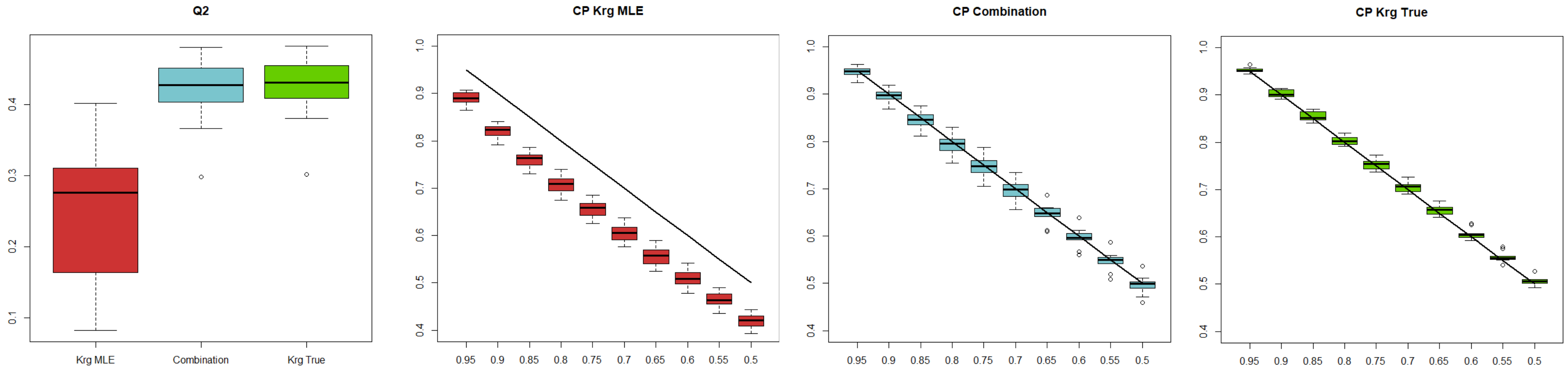
$$\theta_{true} = 3$$



Average computational time:

- Krg MLE: 2,9 mins
- Combination : 0,33 mins

$$\theta_{true} = 2$$

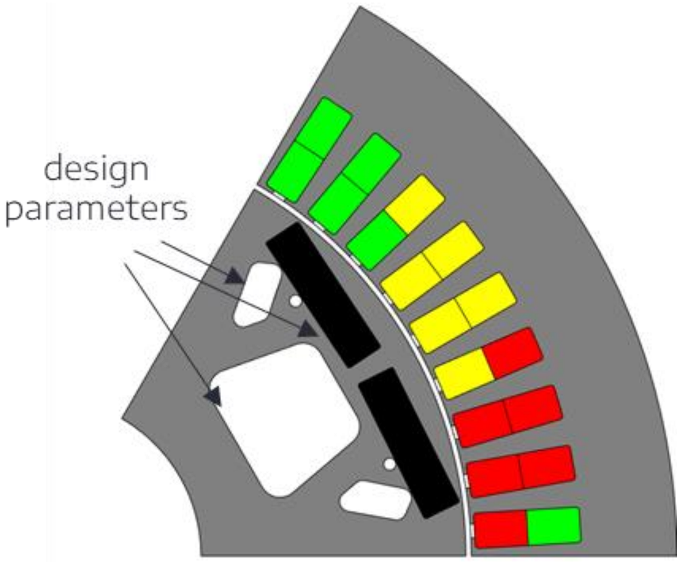


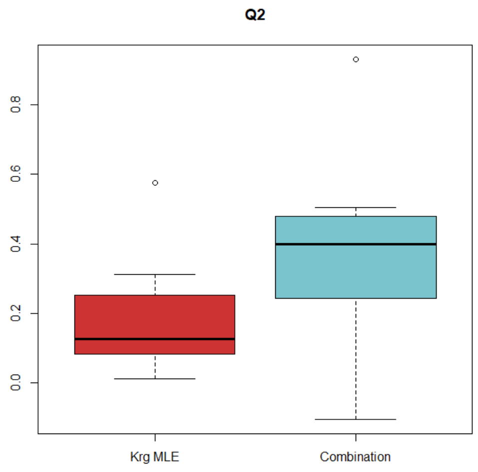
Average computational time:

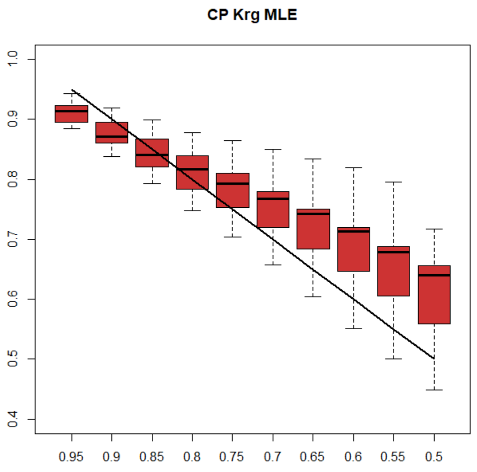
- Krg MLE: 3,4 mins
- Combination : 0,33 mins

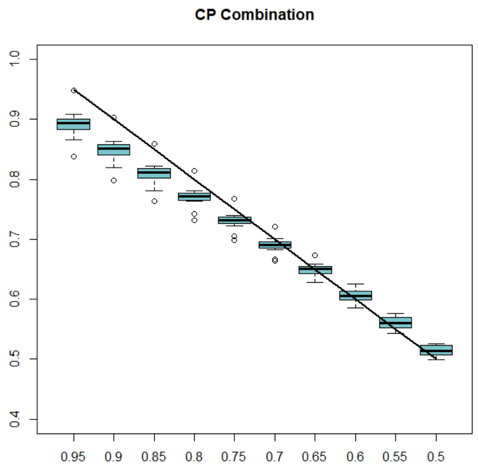
- Study of an electrical machine:

- 37 design variables,
- 500 training points,
- 4500 test points,
- 2 objectives and 10 constraints to surrogate,
- Average results over 10 runs.









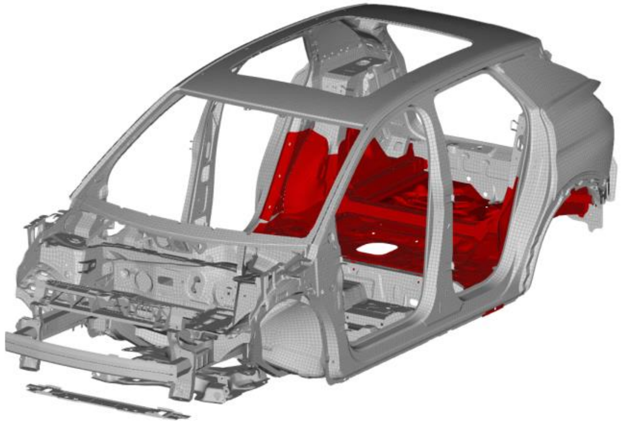
Average computational time:

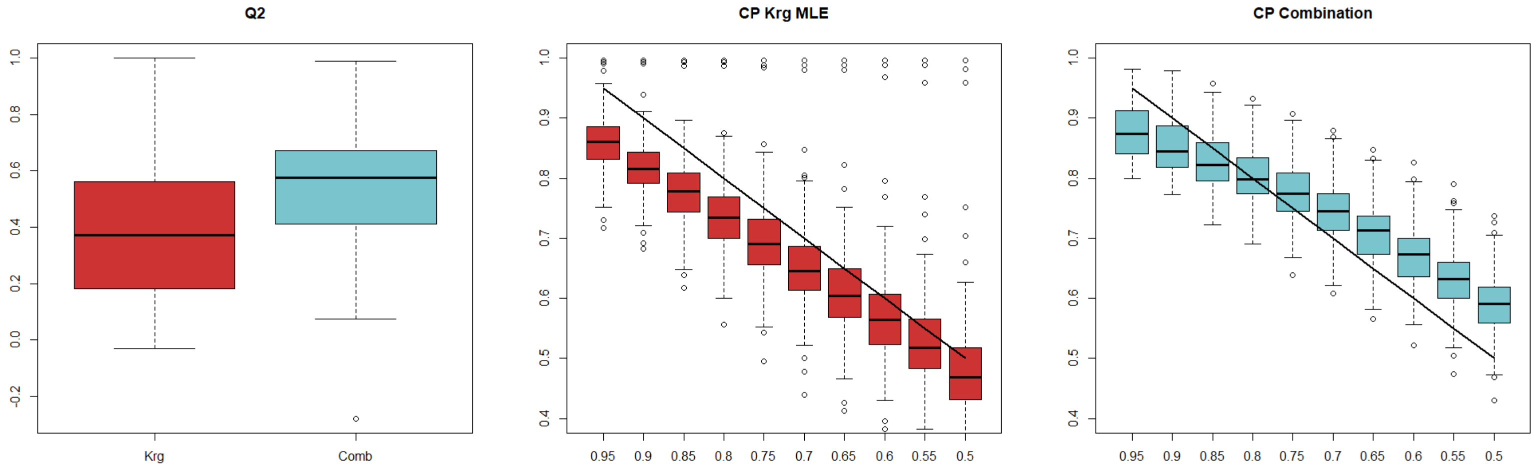
- Krg MLE: 17,1 mins
- Combination : 3,0 mins

NUMERICAL RESULTS – REAL-WORLD APPLICATIONS

- Study of the Peugeot 3008 (vibratory comfort and rear crash safety) :

  - 48 design variables,
  - 300 training points,
  - 327 test points,
  - 2 objectives and 413 constraints (a surrogate model is built only for 190 constraints).





Computational time:

- Krg MLE: 220 mins
- Combination : 15,8 mins

- We developed **a model with better accuracy than the ordinary Kriging** in high dimension, especially when the length-scales are poorly estimated using MLE, and which is both easier and faster to construct.

- We also gave a method to obtain the prediction error for the combined model which gives prediction interval that are overall well-calibrated and suitable for Bayesian optimization.

Future work :

- Apply the combined model for Bayesian optimization and see the potential gains in both construction time and number of iterations required to find the optimum.

- There are still challenges in the acquisition criterion for Bayesian optimization:
- The acquisition function is very flat with only a few peaks which can be hard to find, especially so in high dimension.
- In high dimension, the volume near the borders of the design space becomes dominant. This can result in adding most of the new points near the borders.

- We can also diversify the sub-models using subsets of points or subsets of design variables for example.

- …

Thank you for your attention !

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