Approches multi-fidélité basées sur les processus gaussiens profonds

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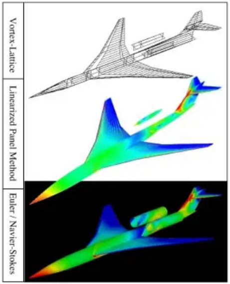
Multi-fidelity modeling

- High-fidelity (HF) models → **accurate data** but on a **limited dataset**.
- Low-fidelity (LF) models → **large amount of data** of **approximated data**.
- Use of multi-fidelity model to exhibit correlations between datasets of s increasing levels of fidelity $(X^t, \mathbf{y}^t), \forall 1 \leq t \leq s$, to improve prediction accuracy.

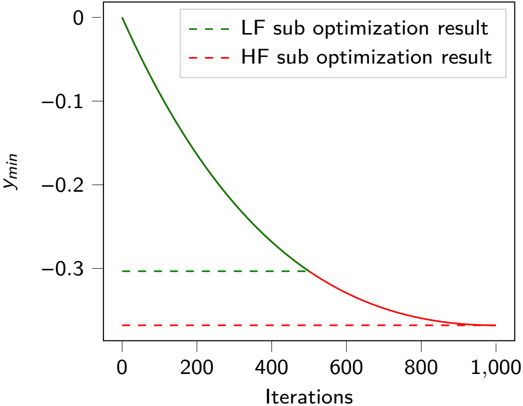


[Choi et al., 2004]

Types of fidelities

Different types of fidelity modeling approaches [Fernández-Godino et al., 2016] :

- numerical relaxation,
- different assumptions about the physical model,
- different levels of space or time discretization.



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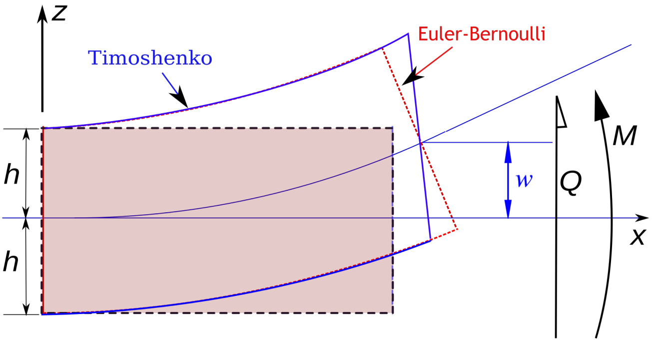

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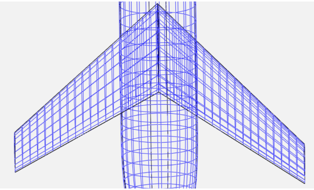

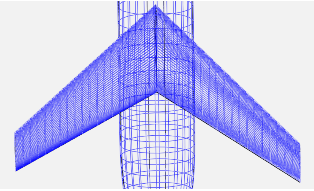

Multi-fidelity models

Multiple machine learning models have been used to exhibit correlations between HF and LF models.

Suport vector machines	Artificial Neural Networks	Gaussian Processes	...
[Shi et al., 2019]	[Kim et al., 2007] [Minisci and Vasile, 2013]	[Kennedy and O'Hagan, 2001] [Le Gratiet and Garnier, 2014] [Perdikaris et al., 2017] [Cutajar et al., 2019]	

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Gaussian Process Regression

Gaussian process [Rasmussen and Williams, 2006]

A Gaussian Process is used to describe a distribution over function. It is a collection of infinite random variables, **any finite number of which have a joint Gaussian distribution**.

It is defined by its mean function and covariance function (Kernel) :

$f(.) \sim \mathcal{GP}(\mu(.), k^{\Theta}(.))$

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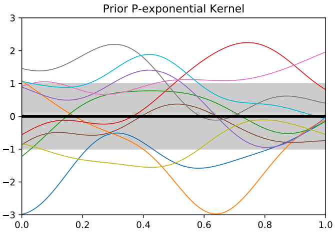
Automatic Relevance Determination p-exponential kernel :

$$K^{\Theta}(\mathbf{x}, \mathbf{x'}) = \sigma^2 \exp\left(- \sum_{i=1}^{d} \theta_i . |x_i - x_i^{'}|^{p} \right)$$

Prior Gaussian Process



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$$\hat{\Theta}, \hat{\mu} = \underset{\boldsymbol{\Theta}, \mu}{\operatorname{argmax}} \log(p(\mathbf{y}|X))$$

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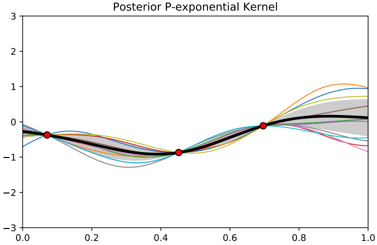
Posterior Gaussian Process



$$f(\cdot)|\mathbf{y}, X \sim \mathcal{N}\left(f^*(\cdot), s^*(\cdot)\right)$$

Linear Auto-regressive

Auto-Regressive model (AR1) [Kennedy and O'Hagan, 2001] :

$$f_t(\mathbf{x}) = \rho_{t-1} f_{t-1}(\mathbf{x}) + \gamma_t(\mathbf{x})$$

$f_t(\cdot)$	Fidelity function of level t	$(\mathcal{GP})$
$f_{t-1}(\cdot)$	Fidelity function of level $t-1$	$(\mathcal{GP})$
ρ_{t-1}	Scaling factor of the lower-fidelity	(constant)
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| Linear correction with a scaling factor ρ_{t-1} and a bias $\gamma_t(\cdot)$ $\rightarrow$ captures only linear correlations between fidelities.

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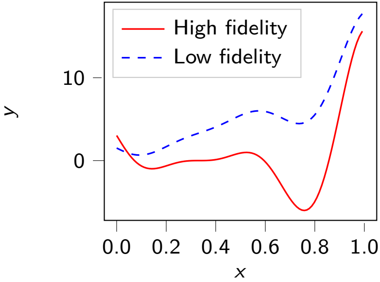

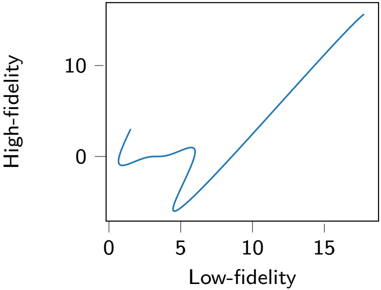

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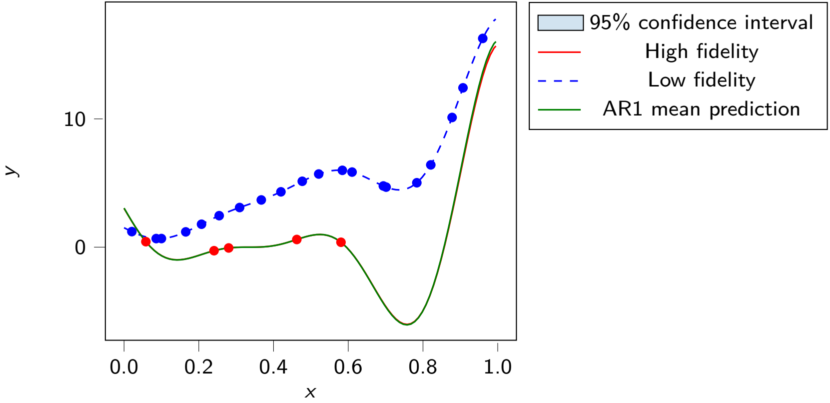

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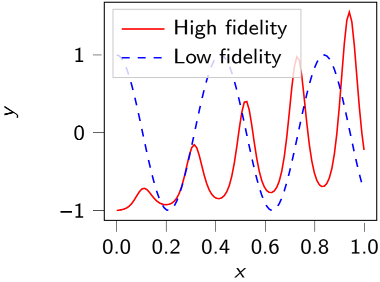
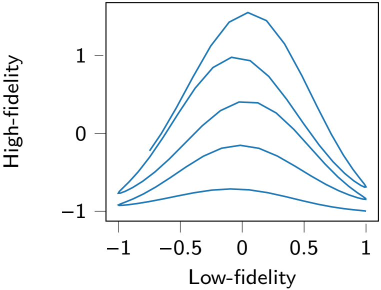
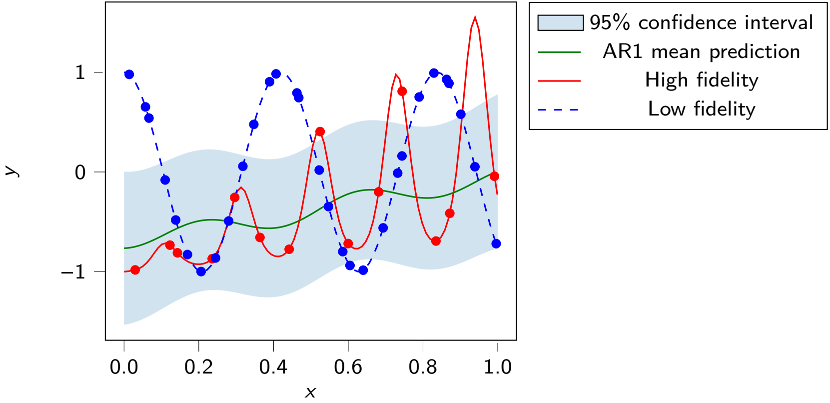




Review of GP based MF models

Auto-Regressive model (AR1) [Kennedy and O'Hagan, 2001] :



Variations of AR1

A parametric function $\rho_{t-1}(\cdot)$ as a scaling factor instead of a constant [Qian and Wu, 2008] :

$$f_t(\mathbf{x}) = \rho_{t-1}(\mathbf{x}).f_{t-1}(\mathbf{x}) + \gamma_t(\mathbf{x})$$

- Increases the expressive power of the model,
- Supposes a known parametric form of the function $\rho_{t-1}(\cdot)$.

Variations of AR1

A sequential training of the fidelities by considering the mean posterior of to lower-fidelity $f^*_{t-1}(\cdot)$ instead of the GP prior $f_{t-1}(\cdot)$ [Le Gratiet and Garnier, 2014] :

$$f_t(\mathbf{x}) = \rho_{t-1}(\mathbf{x}).f^*_{t-1}(\mathbf{x}) + \gamma_t(\mathbf{x})$$

- Reduces the computational complexity of AR1,
- Supposes a nested structure of the DoE.

Non-Linear Auto-Regressive

Non-linear relationship between fidelities

$$f_t(\mathbf{x}) = \rho_{t-1}(f_{t-1}(\mathbf{x})) + \gamma_t(\mathbf{x})$$

$\rho_{t-1}(\cdot)$ Non-linear transformation of the lower-fidelity $(\mathcal{GP})$

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$\downarrow$ independency

$$f_t(\mathbf{x}) = g_{t-1}(f_{t-1}(\mathbf{x}), \mathbf{x})$$

Input space augmented by absorbing $\gamma_t(\cdot)$ and $\rho_{t-1}(\cdot)$ into the $\mathcal{GP}$ $g_{t-1}(\cdot)$

Non-Linear Auto-Regressive

Non-Linear Auto-Regressive model (NARGP) [Perdikaris et al., 2017] :

$$f_t(\mathbf{x}) = g_{t-1}(f^*_{t-1}(\mathbf{x}), \mathbf{x})$$

$f_t(\cdot)$	Fidelity function of level t	$(\mathcal{GP})$
$f^*_{t-1}(\cdot)$	mean of the posterior of the $\mathcal{GP}$ $f_{t-1}(\cdot)$	(Real function)
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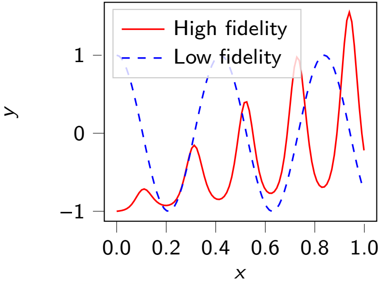

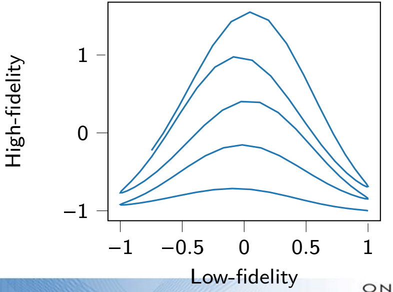

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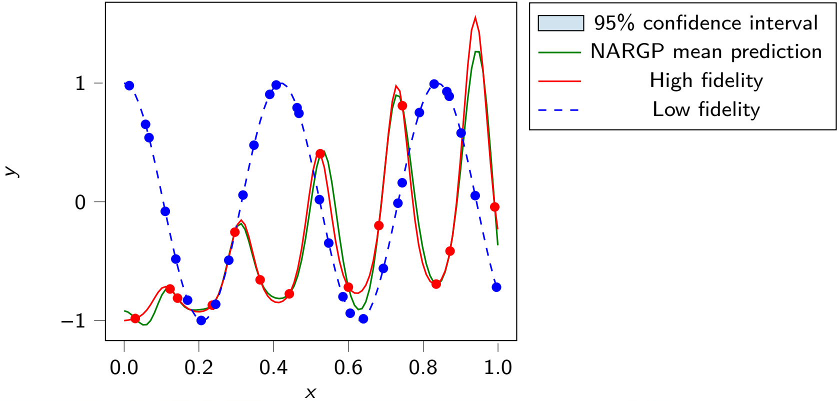

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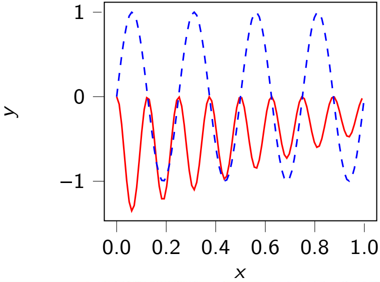

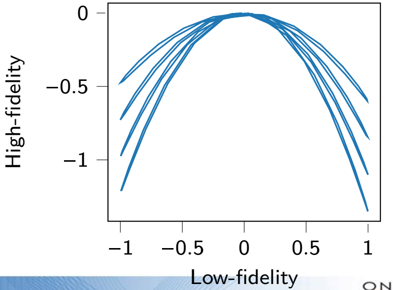

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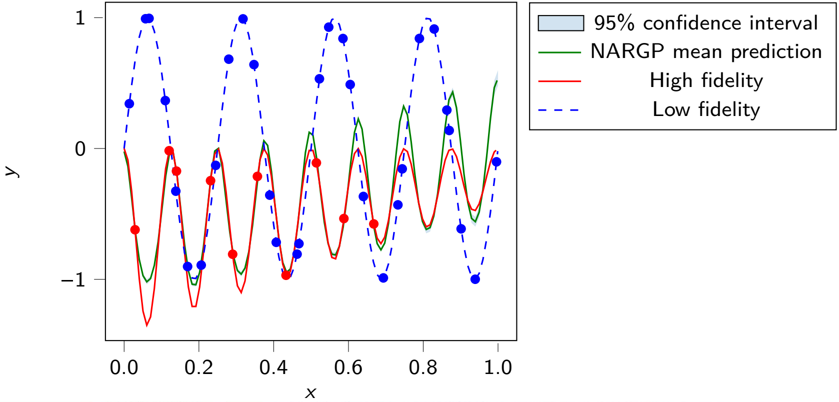

MF-DGP

Multi-fidelity Deep Gaussian Process model (MF-DGP) [Cutajar et al., 2019] :

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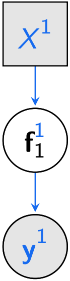

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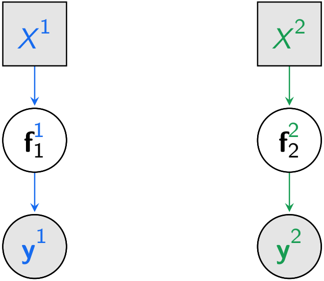

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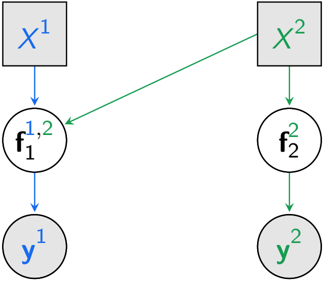

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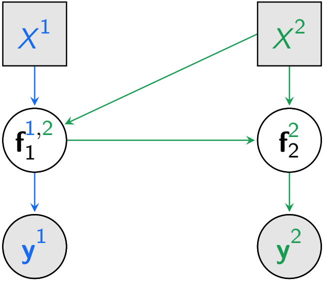

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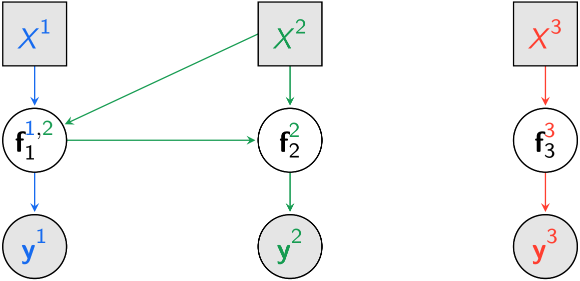

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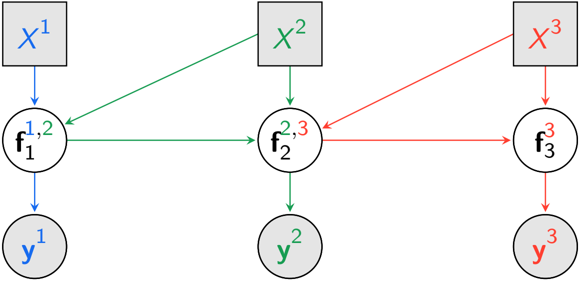

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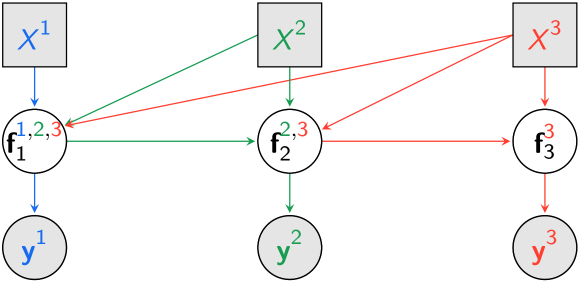
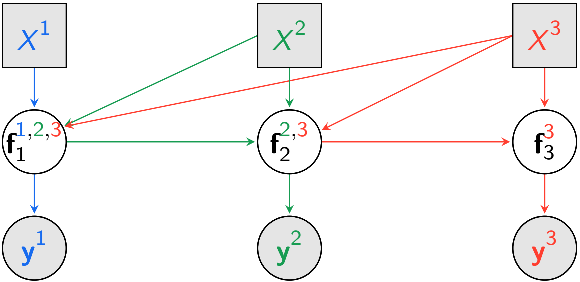


MF-DGP

- Keeping the GP prior $f_{t-1}(\cdot)$ implies a composition of GPs → Deep Gaussian Processes

✓ Joint optimization of the different fidelities. $p\left(\mathbf{y}^1, \ldots, \mathbf{y}^s | X^1, \ldots, X^s\right)$
✓ Well-calibrated uncertainty quantification.



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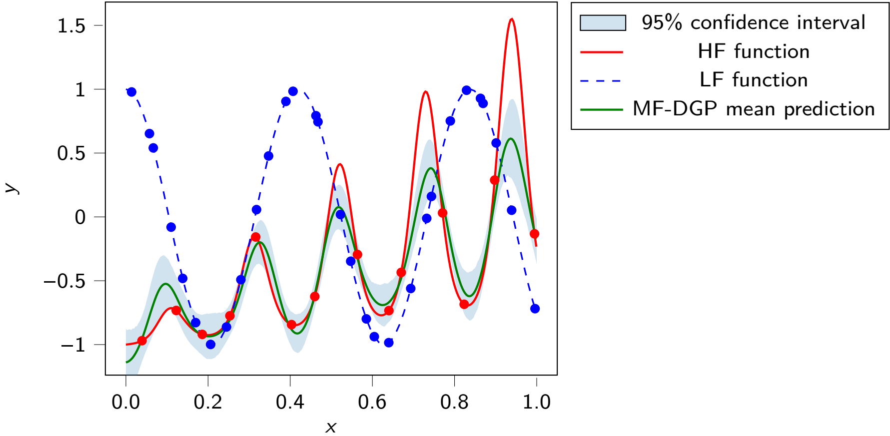
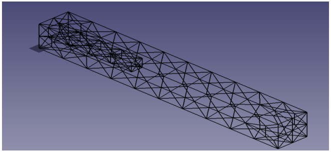


A structural problem

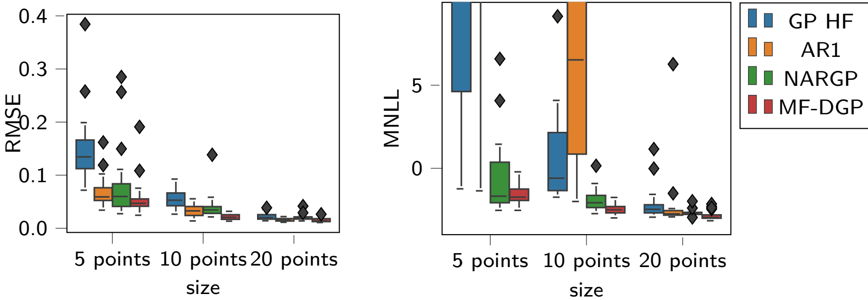
Modeling of the maximum distortion criterion of a :

- Rectangular cantilever beam with a rectangular bore along its horizontal axis.
- Characterized by its length L, its width d, the applied force at its extremity F and also the length L_b and width d_b of the rectangular bore . (5 Variables)
- The computation of the maximum distortion is computed using a finite element (FE) analysis with Calculix solver.
- The difference between the **low-fidelity** and **high-fidelity** is at the level of the density of the mesh.



A structural problem

Results on 20 repetitions with 30 LF data points.



Synthesis

Models	Handling of non-linear correlation	Quality of the uncertainty estimate	Training time	Number of parameters
AR1	−	−	−	−
NARGP	+	−	−	−
MF-DGP	+	+	+	+

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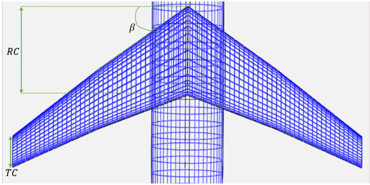
Multi-fidelity with varying input spaces

Multi-fidelity with varying input spaces

In some industrial problems each fidelity can be characterized by its own input space due to :

- Different modeling approaches in each fidelity,
- Omission of some variables in the lower fidelities.



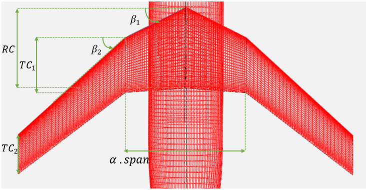


FIGURE – A one-section wing characterized by 3 design variables (left) can be used as a low-fidelity model of a two-sections wing characterized by 6 design variables (right).

Nominal mapping

A nominal mapping $g_0(\cdot)$ is an input mapping based on theoretical insight of the multi-fidelity problem at hand.
Ex1 : The LF design variables are included in the HF design variables, the nominal mapping is the identity.

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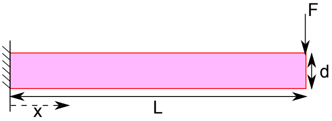
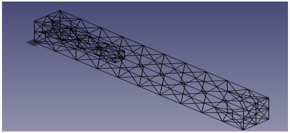


$$\mathbf{x}^{lf} = \begin{bmatrix} L \\ d \\ F \end{bmatrix} \xleftarrow{g_0(\cdot)} \mathbf{x}^{hf} = \begin{bmatrix} L \\ d \\ F \\ L_b \\ d_b \end{bmatrix}$$



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Ex2 : The mapping maps the design variables of the HF into the LF space to obtain an identical defined quantity of interest (*e.g.* the volume defined by the HF variables equals to the volume defined by the mapped HF variables)

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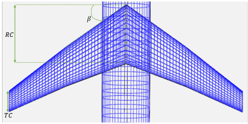
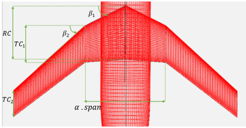


$$S\left(g_0(\mathbf{x}^{hf})\right) = \qquad S\left(\mathbf{x}^{hf}\right)$$

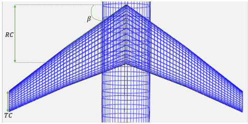


$$\mathbf{x}^{lf} = \begin{bmatrix} R_C \\ T_{C1} + (1-\alpha)TC_2 + (\alpha)RC \\ \alpha\beta_1 + (1-\alpha)\beta_2 \end{bmatrix} \xleftarrow{g_0(\cdot)} \mathbf{x}^{hf} = \begin{bmatrix} R_C \\ T_{C1} \\ T_{C2} \\ \beta_1 \\ \beta_2 \\ \alpha \end{bmatrix}$$

Nominal mapping

A nominal mapping $g_0(\cdot)$ is an input mapping based on theoretical insight of the multi-fidelity problem at hand.

Ex2 : The mapping maps the design variables of the HF into the LF space to obtain an identical defined quantity of interest (*e.g.* the volume defined by the HF variables equals to the volume defined by the mapped HF variables)



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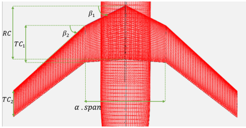


$$\mathbf{x}^{lf} = \begin{bmatrix} R_C \\ T_{C1} + (1-\alpha)TC_2 + (\alpha)RC \\ \alpha\beta_1 + (1-\alpha)\beta_2 \end{bmatrix} \quad \xleftarrow{g_0(\cdot)} \quad \mathbf{x}^{hf} = \begin{bmatrix} R_C \\ T_{C1} \\ T_{C2} \\ \beta_1 \\ \beta_2 \\ \alpha \end{bmatrix}$$

The input mapping may be computationally expensive.

Nominal mapping

A nominal mapping $g_0(\cdot)$ is an input mapping based on theoretical insight of the multi-fidelity problem at hand.
Classic approach : Bias correction with nominal mapping.

$$f_{hf}(\mathbf{x}^{hf}) = f_{lf}(g_0(\mathbf{x}^{hf})) + \gamma(\mathbf{x}^{hf})$$

Input Mapping Calibration

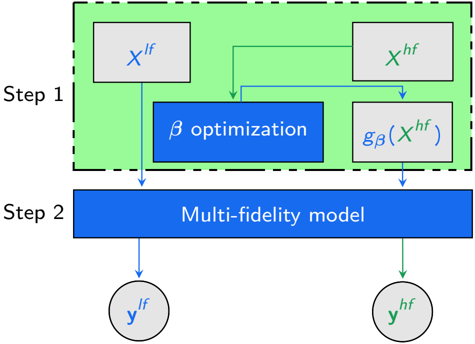
Input Mapping Calibration (IMC) [Tao et al., 2019] as a space mapping approach corrects the inputs instead of the output of a fidelity.

A parametric input mapping g_β is used to map the HF data into the LF space.

The parameters β are estimated by minimizing a distance between the HF response and the LF response of the input transformation of these HF input data points :

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \left(\sum_{i=1}^{n_{hf}} \left(|| f_{hf}(\mathbf{x}^{hf^{(i)}}) - f_{lf}^{\text{exact}} \left(g_\beta(\mathbf{x}^{hf^{(i)}}) \right) || \right) + R(\beta, \beta_\mathbf{0}) \right)$$

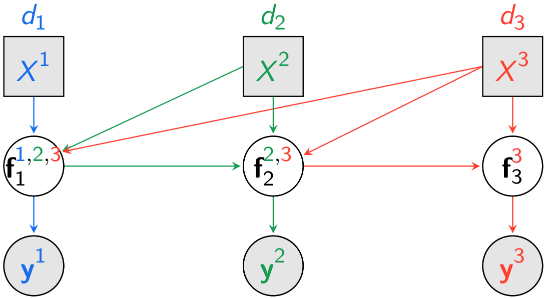
Input Mapping Calibration



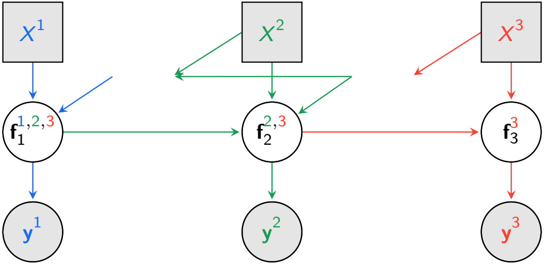
Classic approach for multi-fidelity with varying input spaces [Tao et al., 2019].

- Use of the exact low-fidelity model,
- Disjoint optimization of the mapping parameters and the multi-fidelity model,
- Training only on the lower fidelity input space.

MF-DGP for varying input space parametrizations



Proposed model : A two-level DGP



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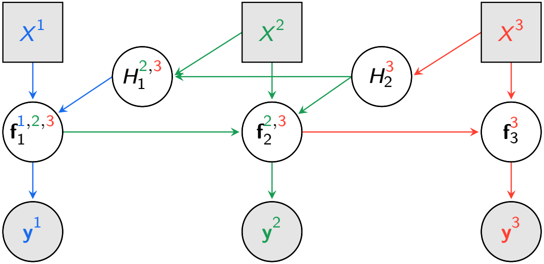
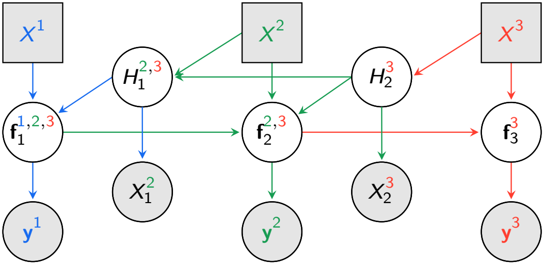


- Multi-output GPs $H_t^{t+1} : d_{t+1} \rightarrow d_t$,
- Conditioning of the GPs input mapping on the nominal mapped values of the training data X_t^{t+1}.

Proposed model : A two-level DGP



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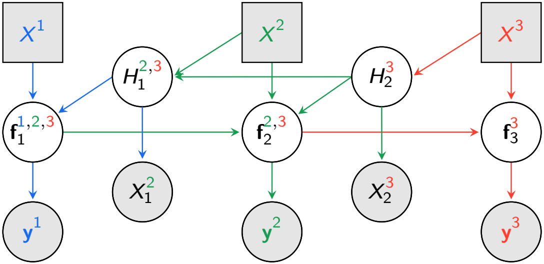
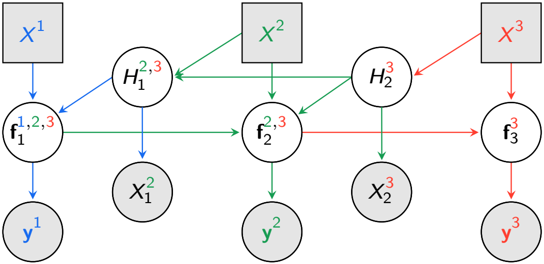


MF-DGP Embedded mapping (MF-DGP-EM) graphical representation

- ✓ Joint optimization of the mapping and the multi-fidelity model $p\left(\mathbf{y}^1, \dots, \mathbf{y}^s, X_1^2 \dots, X_{s-1}^s | X^1, \dots, X^s\right)$,
- ✓ Correlation computed in the original input space of each fidelity,
- ✓ Adapted to computationally expensive nominal input mapping,
- ✓ Uncertainty quantification on the input space mapping.

Proposed model : A two-level DGP



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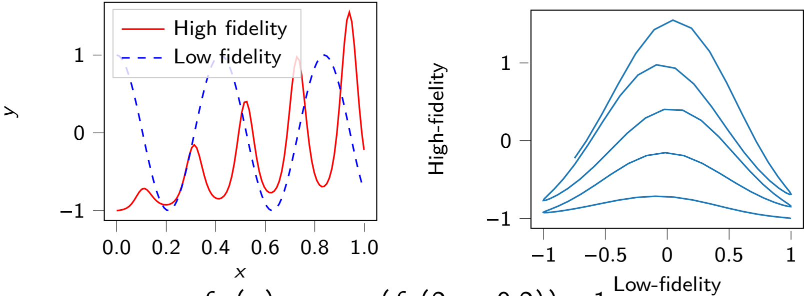
Hebbal, A., Brevault, L., Balesdent, M., Talbi, E., and Melab, N., Multi-fidelity modeling using DGPs : Improvements and a generalization to varying input space dimensions. 4th workshop on Bayesian Deep Learning (NeurIPS 2019).

Illustrative problem



$$f_{hf}(x) = x\exp\left(f_{lf}(2x-0.2)\right) - 1$$

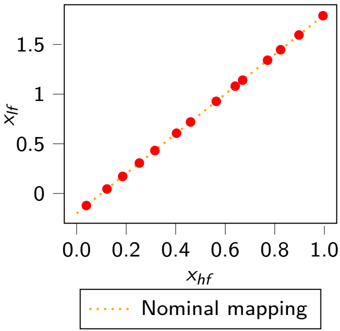
where f_{lf} is :

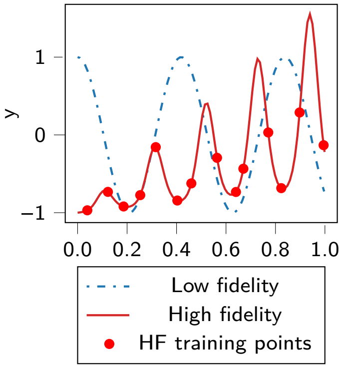
$$f_{lf}(x) = \cos(15x)$$

A possible nominal mapping can be defined as :

$$g_0(x_{hf}) = 2x_{hf} - 0.2$$

Illustrative problem





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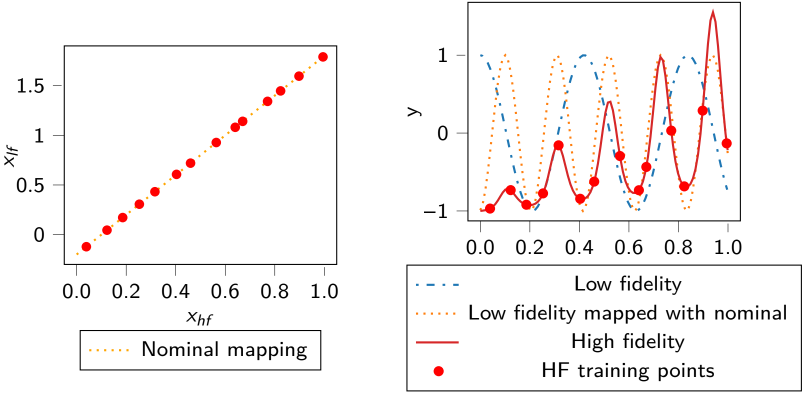

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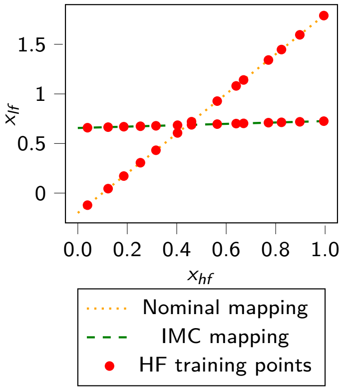

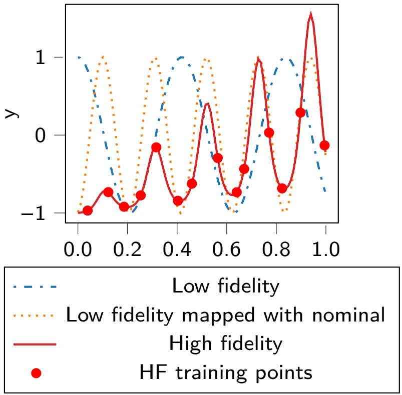

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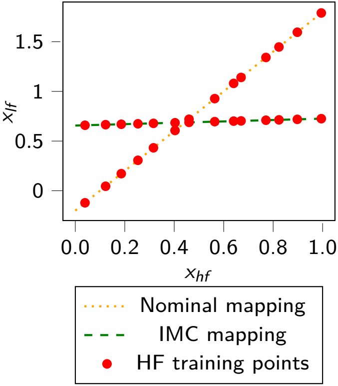

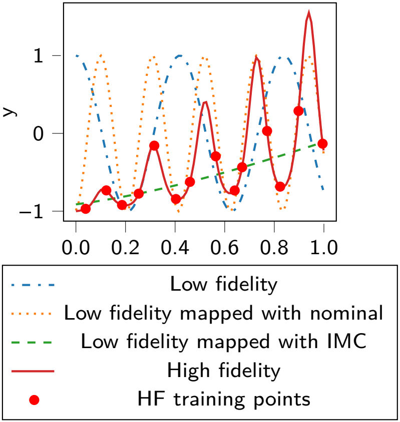

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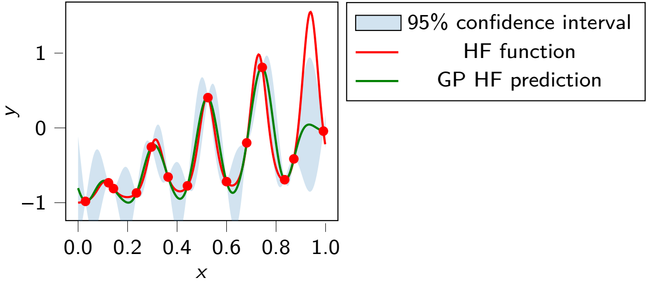
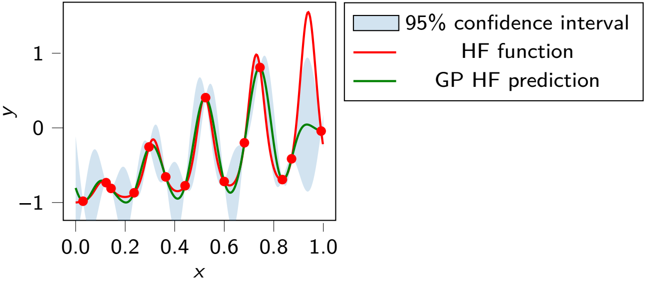
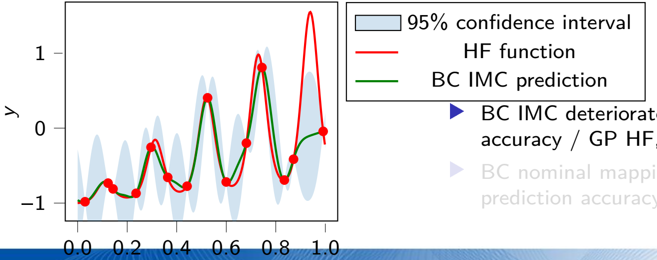


- BC IMC deteriorates the prediction accuracy / GP HF,
- BC nominal mapping improves the prediction accuracy / GP HF.

Illustrative problem





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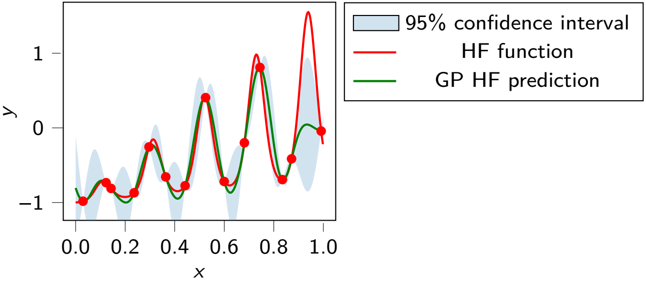

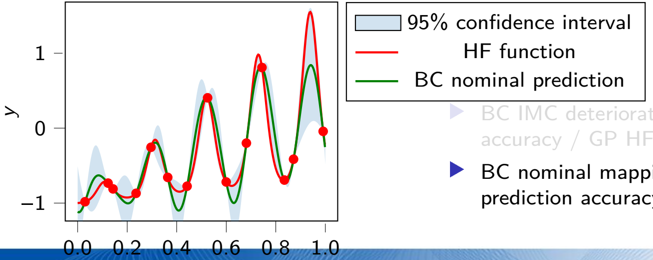

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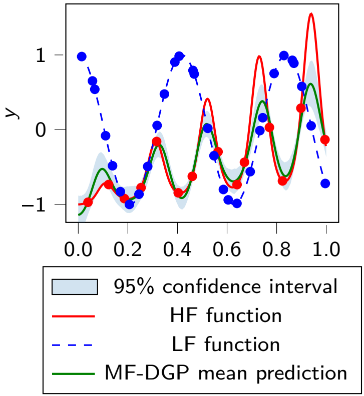
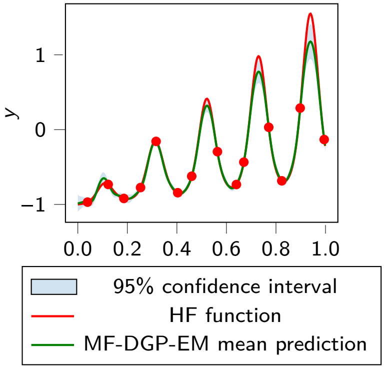


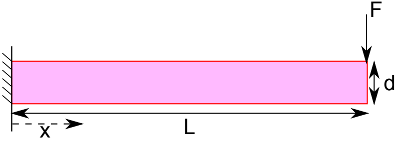


- MF-DGP-EM embeds the input mapping relationship between the HF and LF → better prediction accuracy and uncertainty quantification.

Structural problem

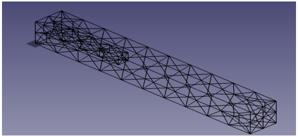
Modeling of the maximum distortion criterion of :

Low-fidelity :



- Standard solid rectangular cantilever beam.
- Characterized by its length L, its width d, and the applied force at its extremity F. (3 Variables)
- The computation of the maximum distortion is computed analytically using the von Mises equation.

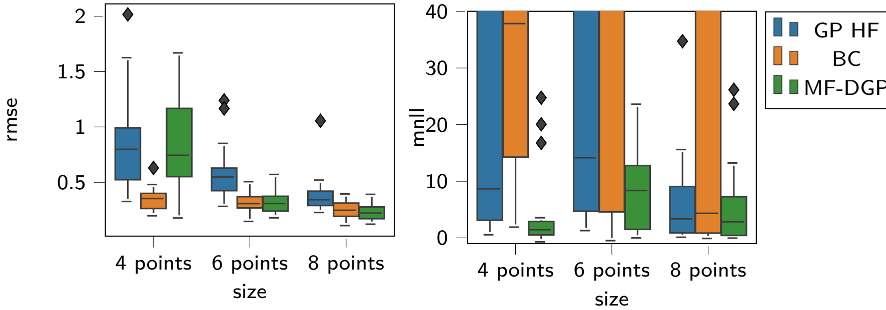
High-fidelity :



- Rectangular cantilever beam with a rectangular bore along its horizontal axis.
- Characterized by its length L, its width d, the applied force at its extremity F and also the length L_b and width d_b of the rectangular bore . (5 Variables)
- The computation of the maximum distortion is computed using a finite element (FE) analysis with Calculix solver.

Structural problem

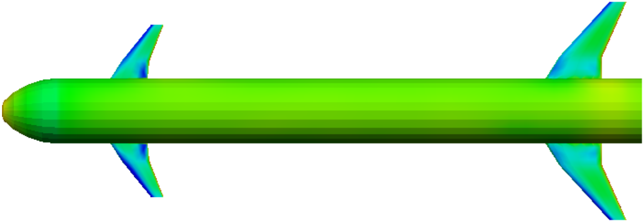
Results on 20 repetitions with 30 LF data points.



- BC has better prediction accuracy with only few information ← the relationship between the two fidelities is well approximated by a linear function
- MF-DGP-EM gives better uncertainty quantification even in the case when the mapping is not learned well enough ← uncertainty on the nominal mapping.

Aerodynamic Problem

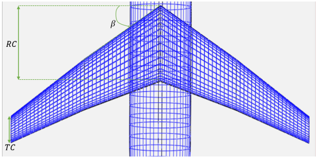
Modeling of the lift coefficient (CL) of a winged reusable launch vehicle composed of a core, two wings, and two canards.



The Vortex lattice method (VLM), is used for the computation of CL using openVSP.

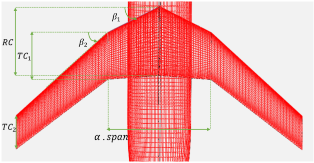
Aerodynamic Problem

Low-fidelity :



- The main wing and canards are considered as one-section wings.
- Main wings and canards characterized by 3 variables each, root chord, tip chord, and sweep angle. (**6 variables**)

High-fidelity :



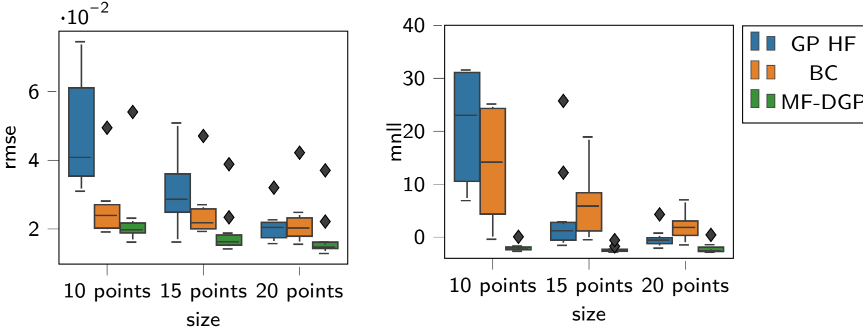
- The main wing and canards are two-section wings.
- Main wings and canards characterized by 6 variables each, root chord, tip chord 1, tip chord 2, sweep angle 1, sweep angle 2, relative span of the first section. (**12 variables**)
- **Meshes densified**

The surface of the main wings and the canards are fixed for the two fidelities.

A possible nominal mapping : for a set of HF design variables maps LF design variables with the same canard and main wings span.

Aerodynamic Problem

Results on 10 repetitions with 120 LF data points.



- With a DoE size of only 4 points for HF, the MF-DGP-EM already obtains a robust and efficient result in prediction accuracy and uncertainty quantification
- No improvement when the number of HF data points cross the threshold of 8 points for BC compared to GP HF.

Table of Contents

Conclusions

Conclusions :

- Review of the different GPs based multi-fidelity approaches,
- Proposition of MF-DGP Embedded Mapping model for varying input spaces with a nominal mapping to be learned,
- Experimentations on analytical and physical test cases confirm the efficiency of the proposed model,

Future works :

- Experimentations on more than two fidelities,
- Multi-fidelity optimization with varying input space dimensions.

Merci pour votre attention !

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