A Bayesian neural network approach to multi-fidelity surrogate modeling

UQSay # 70

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A BAYESIAN NEURAL NETWORK APPROACH TO MULTI-FIDELITY SURROGATE MODELING

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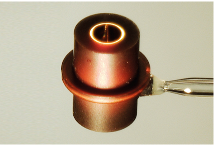
Motivation of surrogate modeling

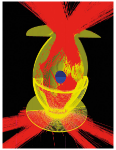
Megajoule laser experiment [CEA DAM, 2021]

- **Physical system** (Inertial confinement fusion)
  - Manufacture of targets $\sim$ 1 year
  - Set up of the installation $\sim$ 2 months
  - Performing an experiment $\sim$ 1 day



- **Computer code**
  - Computation of a numerical experiment $\sim$ 1 week

  $\rightarrow$ Uncertainty quantification requires "many" simulations, intractable with this computer code.

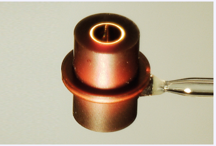


- **Surrogate model**
  - Computing a surrogate experiment $\sim$ 1 second

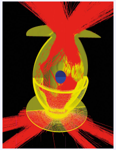
Motivation of surrogate modeling

Input parameters x

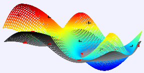
Physical system



Computer code



Surrogate model



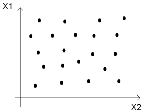
$z_{\mathrm{exp}}(x)$ $\approx$ $z(x)$ $\approx$ $\tilde{z}(x)$

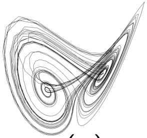
Experimental | Simulate | Predict

Multi-fidelity surrogate model

- **Two versions** of the code are available:

Low Fidelity Code (Cheap)



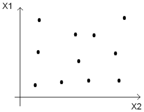


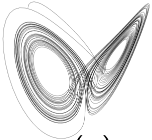
$\longrightarrow$ Low Fidelity

x $\qquad$ $z_L(x)$

High Fidelity Code (Expensive)

Enriched





$\longrightarrow$ Surrogate Model

x $\qquad$ $z_H(x)$

Goal: Construct a surrogate from $\left(z_L(x^{(i)})\right)_{i=1}^{N_L}$ and $\left(z_H(x^{(i)})\right)_{i=1}^{N_H}$ $N_H < N_L$

Hierarchical 2 levels multi-fidelity

2 versions of the same code

- **Low-fidelity** : cheap and approximation
- **High-fidelity** : expensive and very accurate

$$Z_H(x) \quad = \quad \rho\left(x,\ Z_L(x) \quad\right) + \quad \delta(x)$$

- The interaction between code depends on the model.
- Low-fidelity is learn with an independant surrogate model.

Hierarchical 2 levels multi-fidelity

2 versions of the same code

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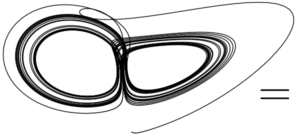
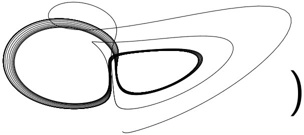
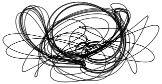


$= \rho(x,$



$) +$



- The interaction between code depends on the model.
- Low-fidelity is learn with an independant surrogate model.

Goal

Method for surrogate modeling in a multi-fidelity framework

Stat-of-the-art methods:

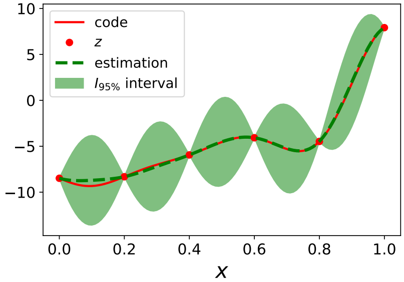
- Multi-fidelity surrogate modeling with simple interactions and uncertainties quantification,
- Multi-fidelity surrogate modeling with complexe interactions and without uncertainties quantification.

Challenges:

- Take into-account non-linear interactions and non-given interactions between fidelities.
- Quantify the prediction uncertainties associated with the surrogate model.

Simple fidelity Gaussian process regression

- Hypothesis: $z(x)$ is a realization of a Gaussian process (GP) $Z(x)$
- We have N observations $z(x^{(i)}) = y^{(i)}$, $i = 1, \cdots, N$.
- The conditional GP gives a prediction of $z(x)$, with analytical expressions for mean and variance.



This framework is presented in [Williams and Rasmussen, 2006].

Multi-fidelity with scalar outputs

Problem: We want to predict a costly code outputs $a_H(x) \in \mathbb{R}$, with $x \in \mathbb{R}^d$. We also have access to a cheaper code $a_L(x)$ with more observations available.

Multi-fidelity with scalar outputs

Problem: We want to predict a costly code outputs $a_H(x) \in \mathbb{R}$, with $x \in \mathbb{R}^d$. We also have access to a cheaper code $a_L(x)$ with more observations available.

State-of-the-art GP-based methods:

- Multi-fidelity AR(1) Gaussian process regression [Kennedy and O'Hagan, 2000].
- Multi-fidelity with Deep Gaussian processes [Perdikaris et al., 2017].
- Neural network for multi-fidelity [Meng et al., 2020].

Multi-fidelity AR(1) Gaussian process regression

- Hypothesis: The emulator is a Gaussian process $(A_H(x), A_L(x))$.

- Autoregressive CoKriging model from [Kennedy and O'Hagan, 2000] :

$$A_H(x) = \rho(x)A_L(x) + \delta(x),$$

where $\delta(x)$ GP independent of $A_L(x)$ and $\rho(x)$ adjustment linear form.

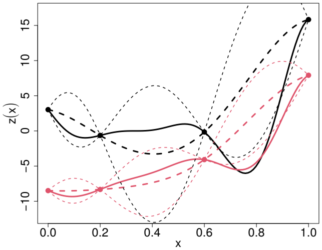
- Estimation of hyperparameters: Maximum likelihood [Le Gratiet and Garnier, 2014], [Ma, 2020].

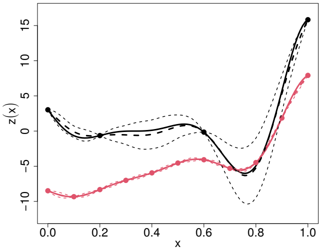
- Prediction: We have

$$[A_H(x)|\text{data}, \text{hyperparameters}] \sim \mathcal{GP}(m_{A_H}(x), \sigma^2_{A_H}(x)),$$

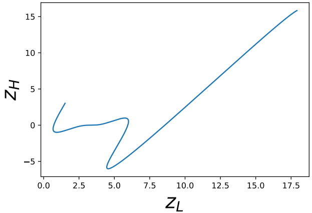
the quantities $m_{A_H}(x)$ and $\sigma^2_{A_H}(x)$ have analytical expressions.

Illustration AR(1) surrogate model





Linear interactions between low- and high-fidelity:



AR(1) multi-fidelity $\longrightarrow$ for linear interactions

If the interaction between fidelities is non-linear ?

Deep Gaussian process for multi-fidelity [Perdikaris et al., 2017]

- Hypotheses :
  - There is a known relation between fidelity
  - The output of the code is a realization of a Gaussian process

$$f_L(\mathbf{x}) = h_L(\mathbf{x}),$$

$$f_L(\mathbf{x}) = h_H(\mathbf{x}, f_L(\mathbf{x})) + \delta(\mathbf{x}),$$

with $h_{L,H}$ two GPs and δ a GP.
The GP prior f_L with the GP posterior from the previous inference level $f_L^\star(\mathbf{x})$. Then, using the additive structure , along with the independence assumption between the GPs f_L and δ, we can summarize the autoregressive scheme as

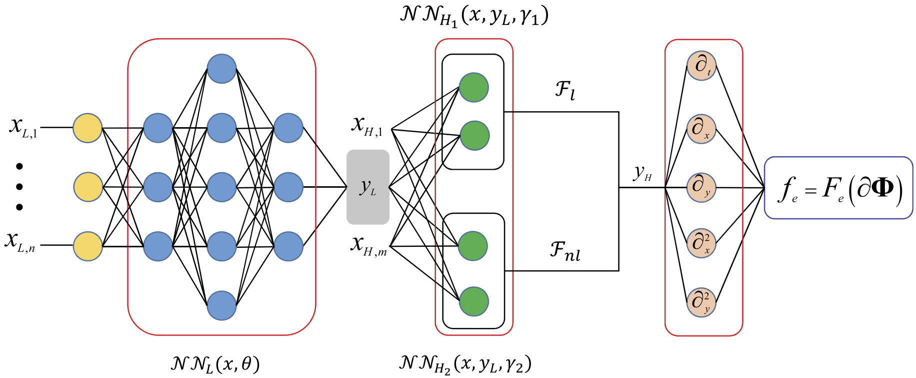
$$f_L(\mathbf{x}) = g_L(\mathbf{x}, f_L^\star(\mathbf{x})),$$

where $g_L \sim \mathcal{GP}\left(f_L|\mathbf{0}, k_2((\mathbf{x}, f_1^\star(\mathbf{x})), (\mathbf{x}, f_1^\star(\mathbf{x})), \theta)\right)$. θ is the hyperparameters of the model.

The machine learning option

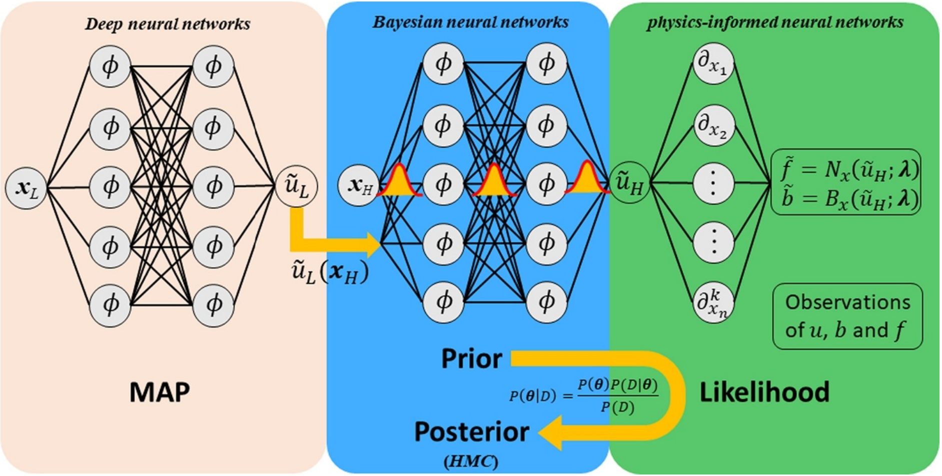
Multi-fidelity neural networks [Meng et al., 2020]

X. Meng, G.E. Karniadakis / Journal of Computational Physics 401 (2020) 109020



The machine learning option

Multi-fidelity Bayesian neural networks [Meng et al., 2020]



Multi-fidelity with scalar outputs

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- Neural network for multi-fidelity [Meng et al., 2020].

Proposed approach:

- Gaussian process and Bayesian Neural network combined (GP-BNN) [Kerleguer, et al., 2024].

Bayesian Neural Network (BNN)

- Bayesian neural network (BNN) for regression.
- We start from the same formalism as a neural network:

$$y = g(w_1 x + \beta_1)$$

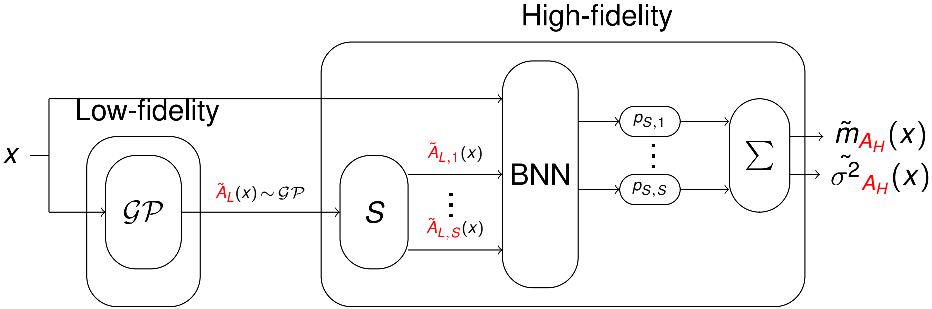
$$BNN(x) = w_2 y + \beta_2$$

$w_1 \in \mathbb{R}^{q\times d}$, $\beta_1 \in \mathbb{R}^q$, $w_2 \in \mathbb{R}^q$, $\beta_2 \in \mathbb{R}$ and g activation function.

- The parameters w_i and β_i follow the Bayesian formalism.
- To predict we use Markov-Chain Monte-Carlo methods like Hamiltonian Monte Carlo.

GP-BNN [Kerleguer, et al., 2024]

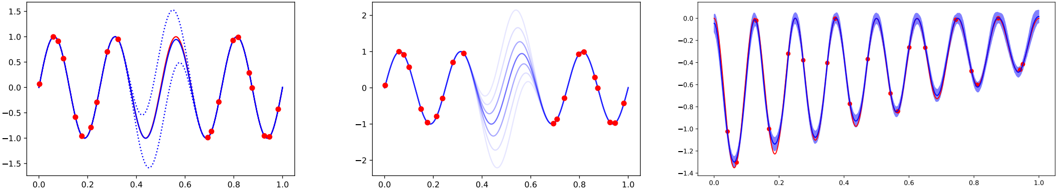
- The low-fidelity code is modeled by a Gaussian process.
- The High-fidelity and high-low interaction is modeled by a Bayesian Neural Network.
- The predictive distribution of the low-fidelity is transfered to the BNN using Gauss-Hermite quadrature.



GP-BNN estimators

The Gauss-Hermite sampling in the GP-BNN method.

Low-fidelity Sampling High-fidelity



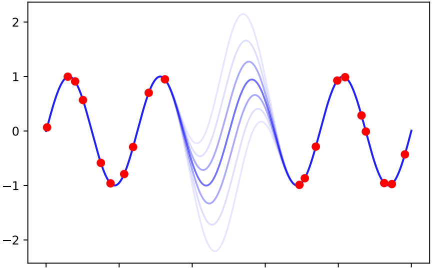
- GP-BNN $\longrightarrow$ for non-linear interactions

Sampling of $\tilde{A}_L(\mathbf{x})$

- Let $z_{S,i}$ be the roots of the Hermite polynomials $H_S(x) = (-1)^S e^{x^2} \partial_x^S e^{-x^2}$, $S \in \mathbb{N}$.
- For each input $\mathbf{x}$ the GP posterior law has mean $\mu_L(\mathbf{x})$ and covariance $C_L(\mathbf{x}, \mathbf{x})$.
- Therefore, the ith realization in the Gauss-Hermite quadrature formula is:

$$\tilde{f}_{L,i}(\mathbf{x}) = \mu_L(\mathbf{x}) + z_{S,i}\sqrt{C_L(\mathbf{x}, \mathbf{x})},$$

- the associated weight is $p_{S,i} = \frac{2^{S-1} S! \sqrt{\pi}}{S^2 H_{S-1}^2(z_{S,i})}$, for $i = 1, \ldots, S$.



The High-fidelity BNN

- The inputs: $\mathbf{x}$ and $\tilde{f}_{L,i}(\mathbf{x})$
- Output: $BNN_{\theta}(\mathbf{x}, \tilde{f}_{L,i}(\mathbf{x}))$
- The estimator of the predictive mean of the output of the high-fidelity model is:

$$\tilde{f}_H(\mathbf{x}) = \frac{1}{N_v} \sum_{j=1}^{N_v} \sum_{i=1}^{S} p_{S,i} BNN_{\theta_j}(\mathbf{x}, \tilde{f}_{L,i}(\mathbf{x})),$$

and the estimator of the predictive variance is:

$$\tilde{C}_H(\mathbf{x}) = \frac{1}{N_v} \sum_{j=1}^{N_v} \left(\sum_{i=1}^{S} p_{S,i} BNN_{\theta_j}(\mathbf{x}, \tilde{f}_{L,i}(\mathbf{x})) \right)^2 - \tilde{f}_H^2(\mathbf{x}) + \frac{1}{N_v} \sum_{j=1}^{N_v} \left(\sum_{i=1}^{S} p_{S,i}^2 \right) \sigma_j^2 .$$

$\rightarrow$ Also available for Mean-Standard Deviation Method, Quantiles Method

Hyperparameters of the model

Low fidelity model

- Prior mean and parameters (null mean and classical DICEkriging priors)
- Kernel function (Matèrn $\frac{5}{2}$)
- (Low fidelity Sampler)

High fidelity

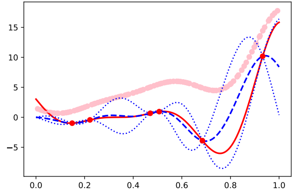
- Dimension of the neural network (Set at 100)
- Number of samples in the MCMC estimator ($N_v = 500$ explaine in [Kerleguer, et al., 2024])
- Number of samples of the low-fidelity Gaussian process S (Explain in the following)

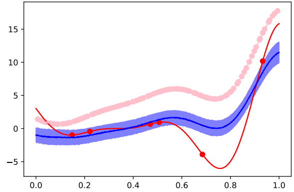
Multi-Fidelity scalar illustration

Interaction	AR(1)	GP-BNN

Linear

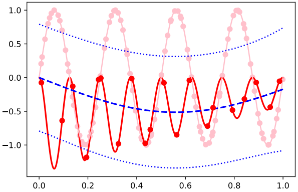
[Forrester et al., 2007]

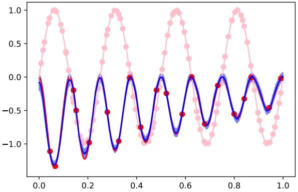




Non-linear

sin-sin^2





Evaluation of surrogate models

Q^2

$$Q^2_{\mathrm{T}} = 1 - \frac{\sum_{i=1}^{N_{\mathrm{T}}} \left[\tilde{\mu}_H(\mathbf{x}_{\mathrm{T}}^{(i)}) - f_H(\mathbf{x}_{\mathrm{T}}^{(i)})\right]^2}{N_{\mathrm{T}} \mathbb{V}_{\mathrm{T}}\left(f_H\right)},$$

with $\mathbb{V}_{\mathrm{T}}(f_H) = \frac{1}{N_{\mathrm{T}}} \sum_{i=1}^{N_{\mathrm{T}}} \left[f_H(\mathbf{x}_{\mathrm{T}}^{(i)}) - \frac{1}{N_{\mathrm{T}}} \sum_{j=1}^{N_{\mathrm{T}}} f_H(\mathbf{x}_{\mathrm{T}}^{(j)})\right]^2$.

- A highly predictive model gives a Q^2_{T} close to 1 while a less predictive model has a smaller Q^2_{T}.

Evaluation of the uncertainty interval

- The uncertainty prediction interval is not taken into account with Q^2. Two metrics are therefore introduced: the coverage probability and the mean predictive interval width. Both were studied in [Acharki et al., 2023] and [Kerleguer, et al., 2024].

Evaluation of surrogate models

Coverage probability (CP)

- CP_α: probability for $f_H(\mathbf{x}_\mathrm{T})$ to be within the prediction interval with confidence level α :

$$\mathrm{CP}_\alpha = \frac{1}{N_\mathrm{T}} \sum_{i=1}^{N_\mathrm{T}} \mathbf{1}_{f_H(\mathbf{x}_\mathrm{T}^{(i)}) \in \mathcal{I}_\alpha(\mathbf{x}_\mathrm{T}^{(i)})},$$

  with $\mathbf{1}$ the indicator function and $\mathcal{I}_\alpha(\mathbf{x})$ the prediction interval at point $\mathbf{x}$ with confidence level α.

- The prediction uncertainty of the surrogate model is well characterized when CP_α is close to α.

Mean Predictive Interval Width

- The mean predictive interval width MPIW_α is the average width of the prediction intervals:

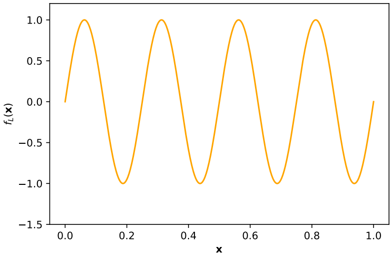
$$\mathrm{MPIW}_\alpha = \frac{1}{N_\mathrm{T}} \sum_{i=1}^{N_\mathrm{T}} \left|\mathcal{I}_\alpha(\mathbf{x}_\mathrm{T}^{(i)})\right|,$$

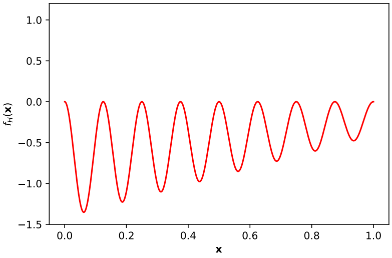
  where $|\mathcal{I}_\alpha(\mathbf{x})|$ the length of the prediction interval $\mathcal{I}_\alpha(\mathbf{x})$.

- The prediction uncertainty of the surrogate model is small when MPIW_α is small.

Parameters of the surrogate model

A test multi-fidelity function [Perdikaris et al., 2017]

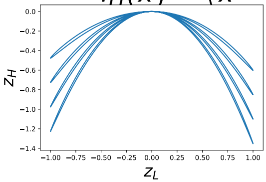




$$f_L(x) = \sin 8\pi x$$

$$f_H(x) = (x - \sqrt{2})\, f_L^2(x)$$

Interactions :



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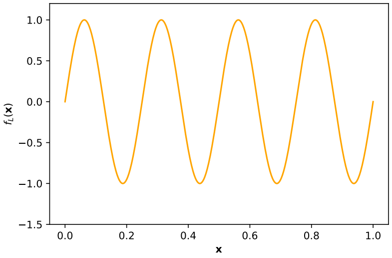
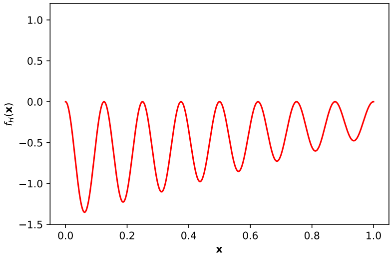




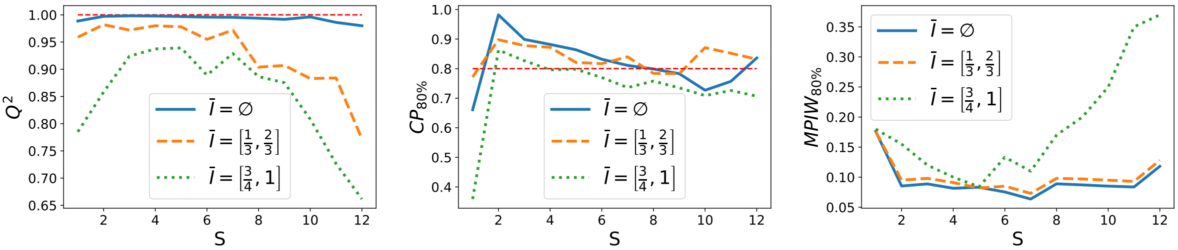
Low fidelity learning intervals

The low-fidelity learning interval is $I = [0, 1] \backslash \bar{I}$

$\bar{I}$	$\emptyset$	$[\frac{1}{3}, \frac{2}{3}]$	$[\frac{3}{4}, 1]$
Q^2_{L}	0.99	0.98	0.84

Optimal S for this example

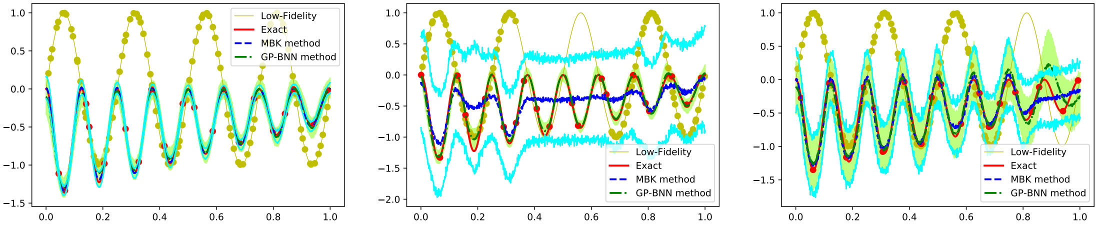
- GPBNN performance with different values of S



$\rightarrow$ $S = 5$, number of neurons $N_n = 100$ and number of samples $N_v = 500$

Performance of the surrogate model

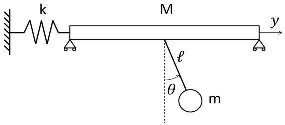
MBK method is proposed in [Meng et al., 2020]



→ Prediction performance is equivalent, but in areas where low fidelity is poorly reconstructed, GPBNN performs better.

→ The uncertainty interval is more relevant in all cases for the GPBNN method

Double pendulum



	GP 1F	AR(1)	[Perdikaris et al., 2017]	[Meng et al., 2020]	[Kerleguer, et al., 2024]
Q^2_{T}	0.93	0.94	**0.95**	0.54	**0.95**
$\mathrm{CP}_{80\%}$	**0.81**	**0.78**	0.62	0.88	**0.80**
$\mathrm{MPIW}_{80\%}$	0.154	0.146	0.069	0.859	**0.101**

Q^2_{T}: represent the quadratic error.
$\mathrm{CP}_{80\%}$: coverage probabilité of the Uncertainty Quantification.
$\mathrm{MPIW}_{80\%}$ size of the Uncertainty interval.

Perspectives

Gaussian-Process Bayesian Neural Network:

- Modele available on [Kerleguer, et al., 2024]
- **Uncertainty prediction** for both high- and low-fidelity
- Interactions between high- and low-fidelity **linear and non-linear**

Adaptations needed:

- Growing the **dimension of output**
- Image processing
- **Non-hierarchical** Multi-fidelity surrogate modeling

Hierarchical Multi-fidelity is more than

MF : Multi-Fidelity, GP : Gaussien Process, NN : Neural Network

	Scalar	Time-series
Linear	Co-Kriging MF x x autorecursive MF x x	MF time series x x
Non-linear	Deep GP x x **GPBNN** x x Deep MF Transfert learning	Deep MF (MF wavelet GP x x) Transfert learning

Today's methods
(work in progress)

x Avec quantification d'incertitudes
x Small Data

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