A Bayesian methodology for hybrid degradation prognostics

E. Jaber[1,2,3],
E. Remy[1], V. Chabridon[1], M. Mougeot[2], D. Lucor[3],

1. EDF R&D / PRISME Department
2. Université Paris-Saclay, ENS Paris-Saclay, CNRS, Centre Borelli
3. Laboratoire Interdisciplinaire Des Sciences Du Numérique, LISN-CNRS

INI Workshop - Calibrating prediction uncertainty: statistics and machine learning perspectives

06/04/2025

Table of contents

Clogging of steam generators (SGs)

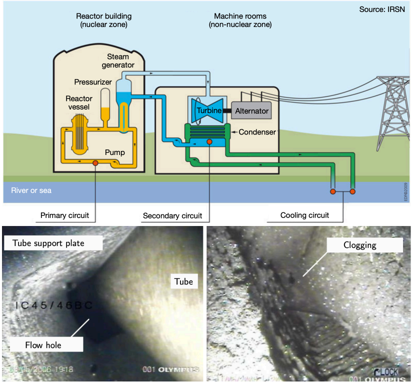
- Clogging of SGs is a complex multiphysics phenomenon that occurs following long operational periods in pressurized-water reactors (PWR) of the French nuclear fleet $\rightarrow$ undermines performance $\&$ weakens the structures $\rightarrow$ *may require chemical cleanings*
- 

Figure: PWR scheme, and example of video examination during a PWR outage (© IRSN, EDF)

Clogging of SGs

- No state-of-the-art model allowing for ground insights on diagnosis and prognosis of clogging rate τ_c $\rightarrow$ very hard to model $\&$ challenging to create reproducible lab experiment for model validation $+$ not a lot of literature [Srikantiah and Chappidi, 2000; Prusek et al., 2013; Girard, 2014; Yang et al., 2017]
- Available scarce video field data as well as indirect measurements $\rightarrow$ allow to construct data-driven regression algorithms [Pinciroli et al., 2021] $\approx$ not enough data to have robust predictive models
- Another tool is the physical clogging model developed by [Prusek et al., 2013] $\rightarrow$ subsequent numerical model THYC-Puffer-DEPO [Feng et al., 2023] $\approx$ lack of enough trustworthy field data for precise validation
- Necessary decision-making on chemical cleaning planning under uncertainty $\rightarrow$ ***how to make use of the available knowledge and models for achieving reliable predictions?***

Introduction

- Industrial engineering systems such as airplane blades, concrete structures in bridges, components in nuclear reactors $\rightarrow$ subject to complex physics and regular loads $\rightarrow$ degrade over time, need maintenance or replacement especially in critical applications
- Degradation level $t \mapsto \delta(t)$ for an industrial system $\rightarrow$ objective is to predict remaining useful life (RUL) [Biggio and Kastanis, 2020] for a fixed threshold $D \in \mathbb{R}_+$:

$$\mathrm{RUL}(D) = \underset{t_1 < t \leq t_N}{\mathrm{argmin}} \{\delta(t) \geq D\} \tag{1}$$

- Usually relies on physics-based simulation codes, and/or data driven methods
- RUL prediction with each individual approach is not robust $\rightarrow$ high level of uncertainty $\&$ individual predictions not fully reliable

Introduction

Available tools:

- *Physics-based computer simulation model* $g : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}^N$ with prior uncertainty on input variables $\boldsymbol{X} = (X_1, \ldots, X_d) \sim \mu_{\boldsymbol{X}} \to$ one input value $\boldsymbol{x}_0$ gives the trajectory $g(\boldsymbol{x}_0) = (g(t_1, \boldsymbol{x}_0), \ldots, g(t_N, \boldsymbol{x}_0))$ where $\mathrm{pr}_\ell \circ g(\boldsymbol{X}) := g(t_\ell, \boldsymbol{X})$ approximates $\delta(t_\ell)$
- *Surrogate modeling strategy* $\widehat{g}$ if code is time-costly such that $\widehat{g}$ approximates g with less computation effort
- *q heterogeneous degradation data groups* $\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q$ with different sizes $\boldsymbol{y}^i \in \mathbb{R}^{m_i} \to$ corresponding to different time indices in $\mathcal{J}_i$ so that $\mathcal{J} = \cup_{i=1}^q \mathcal{J}_i$ and $|\mathcal{J}| = m_1 + \ldots + m_q$, we suppose that:
$$y^i(t_\ell) = g(t_\ell, \boldsymbol{X}) + \eta_\ell^i, \tag{2}$$
with $\eta_\ell^i \sim \mathcal{N}(0, \sigma_i^2) \to$ homoskedastic noise for each data group
- *How to fuse these tools for hybrid RUL estimation of the system?*

Offline data assimilation

- A single input parameter $\boldsymbol{X} = \boldsymbol{x}_0$ produces an entire degradation trajectory $g(\boldsymbol{x}_0) = (g(t_1, \boldsymbol{x}_0), \ldots, g(t_N, \boldsymbol{x}_0))$, which is generally not a Markov chain $\rightarrow$ cannot use data assimilation (considered state of the art hybrid method [Jouin et al., 2016])
- Scarcity of data, packed in groups $\rightarrow$ no arrival of new data points on the fly $\rightarrow$ *offline* data assimilation is suitable for this context, similar to Bayesian calibration of computer models
- The objective is to estimate the posterior distribution $\widehat{p}(\theta|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q)$ of influential parameters $\theta \in \boldsymbol{X}$
- This enables obtaining an updated distribution for the state variable via the pushforward $g\#\widehat{p}(\theta|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q)$
- The probabilistic RUL is determined by its conditioned cumulative distribution function:

$$\mathbb{P}(\mathrm{RUL}(D) \leq t_\ell|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q) = \int_{\mathbb{R}} \mathbf{1}\{z \geq D\}(\mathrm{pr}_{\ell+1} \circ g)\#\widehat{p}(\theta|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q)(z)dz$$

Table of contents

Methodology

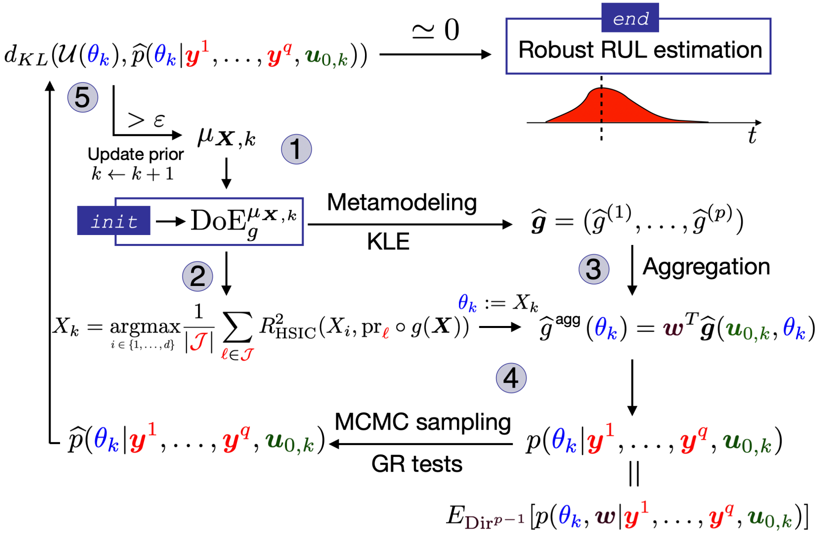
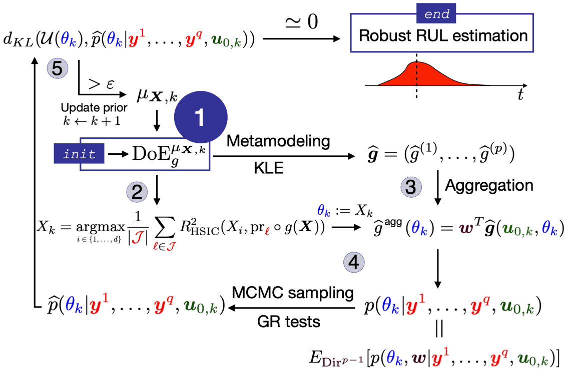


Figure: Proposed 5-steps algorithm

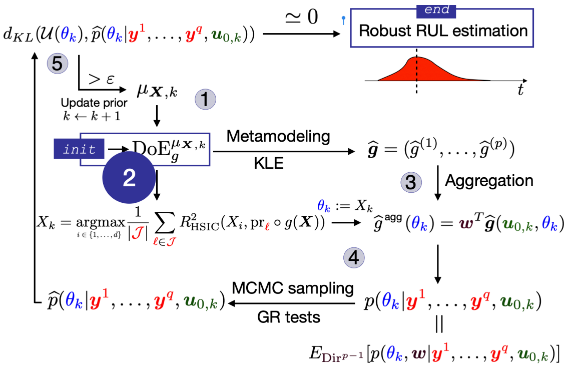
Step 1



Perform k iterations where $1 \leq k \leq d$:

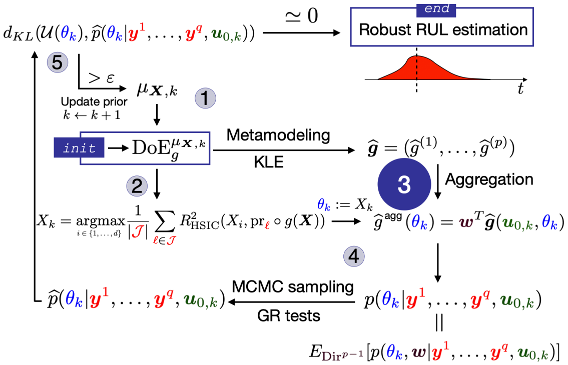
1. If $k = 0$, assume uniform independent priors $\mu_{\boldsymbol{X},k} \simeq \mathcal{U}[-1, 1]^{\otimes d} \rightarrow$ generate a design of experiments $\mathrm{DoE}_g^{\mu_{\boldsymbol{X},k}} = \{(\boldsymbol{X}^{(j)}, g(\boldsymbol{X}^{(j)}))\}_{1 \leq j \leq n}$

Step 2



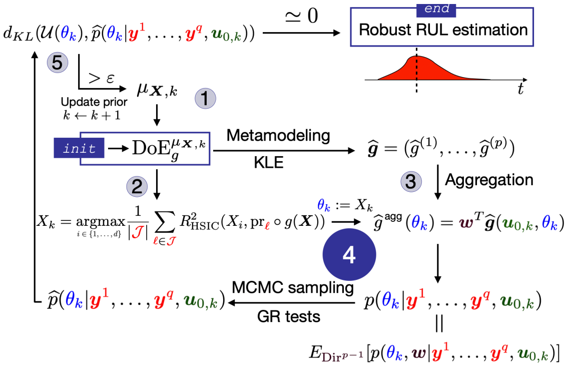
2. Compute **HSIC indices** [Gretton et al., 2005] between input variables and outputs at data time instances $\rightarrow$ **given data** sensitivity analysis method to assess *individual* input variable influence on the output

Step 3



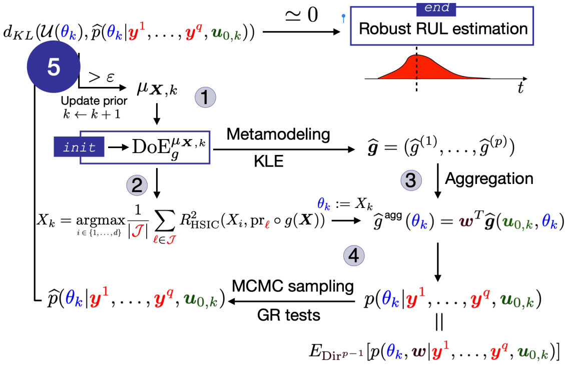
3. If g is time-costly, build and validate p metamodels $\widehat{\boldsymbol{g}} = (\widehat{g}^{(1)}, \ldots, \widehat{g}^{(p)})$ with chosen strategy $\rightarrow$ avoid metamodeling bias with *convex aggregation* on the unit-simplex chosing $\boldsymbol{w} \in \Delta^{p-1} := \{\boldsymbol{w} \in [0,1]^p, \ \|\boldsymbol{w}\|_1 = 1\}$, fix nominal value of $\boldsymbol{U}_{0,k} = \boldsymbol{u}_{0,k}$ by taking the mean

Step 4



4. Estimate the posterior distribution $\widehat{p}(\theta_k|\boldsymbol{y}^1, \dots, \boldsymbol{y}^q, \boldsymbol{u}_{0,k})$ with an MCMC sampling procedure

Step 5



5. Compute the Kullback-Leibler divergence d_{KL} between prior distribution $\mathcal{U}(\theta_k)$ and the estimated density:
   - If $d_{KL} > \varepsilon$, update the prior $\mu_{\boldsymbol{X},k}$ by replacing marginal $\mathcal{U}(\theta_k)$ with $\widehat{p}(\theta_k|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q, \boldsymbol{u}_{0,k})$ and continue $k \leftarrow k+1$
   - Otherwise, stop and obtain an *updated* RUL prediction by computing $g\#\mu_{\boldsymbol{X},k}$

Bayesian updating step ④

Proposition

Assume $\lambda := 1/\sigma_{\boldsymbol{\eta}}^2 \sim \mathcal{G}(\frac{m}{2}, \frac{1}{2}\|\mathbf{y} - f(\theta)\|^2)$ *(Gamma distribution), where* m *is the number of data points in* $\mathbf{y}$; $\theta \sim \mathcal{U}(\theta)$, *and* $p(\theta, \lambda) \propto \lambda^{-1}$. *Then:*

$$p(\theta|\mathbf{y}) \propto \|\mathbf{y} - f(\theta)\|^{-m} \tag{3}$$

Moreover, if multiple groups of data at different time-instances are considered, $\mathbf{y}^1, \ldots, \mathbf{y}^q$, *with respective priors on the inverse of their standard deviations* $\lambda_i \sim \mathcal{G}(\frac{m_i}{2}, \frac{1}{2}\|\mathbf{y}^i - f(\theta)\|^2)$, *then the generalization is:*

$$p(\theta|\mathbf{y}^1, \ldots, \mathbf{y}^q) \propto \prod_{i=1}^{q} \|\mathbf{y}^i - f(\theta)\|^{-m_i} \tag{4}$$

Proof. Bayes' theorem and simplifications.

Bayesian updating step (4)

$$p(\theta_k|\boldsymbol{y}^1,\ldots,\boldsymbol{y}^q,\boldsymbol{u}_{0,k}) \propto \frac{1}{M}\sum_{r=1}^{M}\prod_{i=1}^{q}\|\boldsymbol{y}^i - \langle \boldsymbol{w}^{(r)}, \widehat{\boldsymbol{g}}(\boldsymbol{u}_{0,k},\theta_k)\rangle\|^{-m_i} \tag{5}$$

- Use Random Walk Metropolis-Hastings (RWMH) MCMC algorithm [Sullivan, 2015] to sample from (5)
- Monte-Carlo integration using sample $\{\boldsymbol{w}^{(r)}\}_{r=1}^{M}$ from the Dirichlet-$\mathbf{1}_p$ distribution on the simplex $\rightarrow$ integrate hyperparameter
- Test convergence of RWMH chains with Gelman-Rubin test [Gelman and Rubin, 1992]
- Updated densities are conditioned on nominal values $\boldsymbol{u}_{0,k}$ of *other* $d-1$ *input variables* $\rightarrow$ future work on how to integrate uncertainty
- Use log-sum-exp trick for numerical computation

Table of contents

Results

- Computer code THYC-Puffer-DEPO, complex multiphysics [Jaber et al., 2024b] , chaining of 3 codes $\rightarrow$ allows to simulate SG clogging on entire lifespan of the asset integrating past chemical cleanings and predicting future τ_c levels
- Two data groups $q = 2$, corresponding to field data and regression data

Input variable	Distribution
α	$\mathcal{U}(100, 103)$
β	$\mathcal{U}(0.02, 0.025)$
ϵ_e	$\mathcal{U}(0.2, 0.5)$
ϵ_c	$\mathcal{U}(0.01, 0.3)$
d_p	$\mathcal{U}(0.5, 10.0) \times 10^{-6}$
$\Gamma_p(0)$	$\mathcal{U}(1.0, 8.0) \times 10^{-9}$
a_v	$\mathcal{U}(0, 15) \times 10^{-4}$

Table: Probabilistic modeling of uncertain input variables

Results: posterior distributions

- 3 independent calibrations for scenarios after maintenances, $p = 12$ metamodels, 5 MCMC chains are launched for GR convergence test, use uniform proposal distributions
- Computing time around 40 min $\rightarrow 5/7$ distributions are informed by the data, distinct modes for a_v

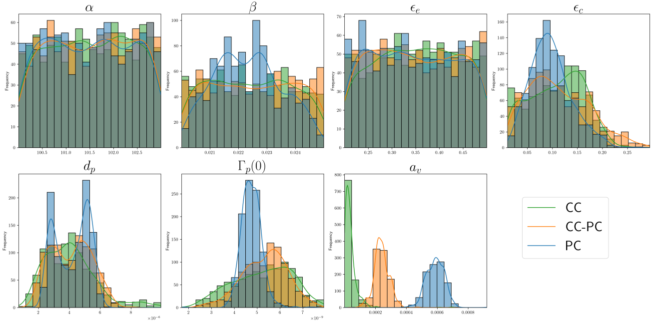


Figure: Posterior distributions of TPD clogging simulation code

Results: posterior trajectories

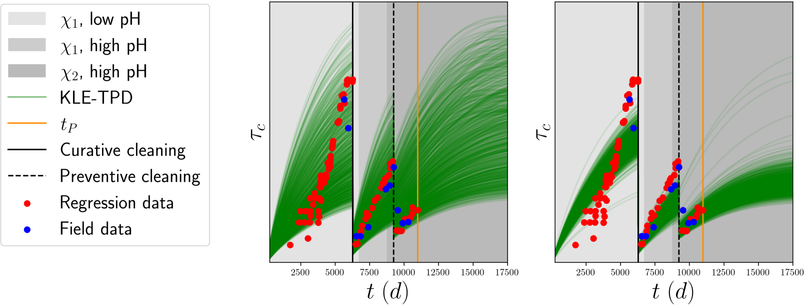
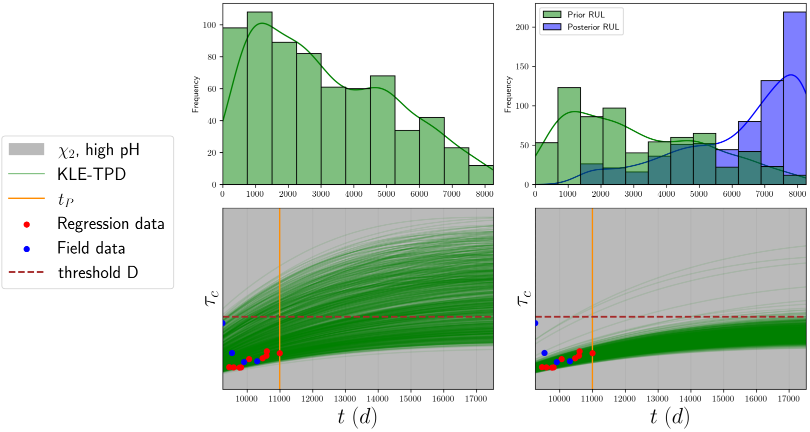


Figure: Prior/posterior TPD emulations with Karhunen-Loève expansion metamodel

Results: posterior RUL



- RUL prediction uncertainty substantially reduced and mean of the distribution is shifted compared to the prior $\rightarrow$ positive impact for maintenance planning

Table of contents

Summary

- Presented an iterative algorithm leveraging kernel sensitivity analysis (HSIC) to identify individual influential variables and update priors $\rightarrow$ acting sequentially on each marginal to keep independence assumption for all dimensions $\rightarrow$ avoids cross-correlation in MCMC and curse of dimensionality
- Methodology works with a metamodeling step, enriched at each iteration by an optimization + aggregation of the metamodels on the refined DoEs to avoid bias in the posteriors
- The method integrates the noise uncertainty and works with heteroskedastic groups of data points
- Demonstrated the approach on industrial steam generator clogging, showing improved posterior inference and reduced RUL uncertainty
- Methodology is general and can be adapted to other industrial prognostics problems with scarce and heterogeneous data $\rightarrow$ GitHub repository

Some extensions and future work

- How to integrate uncertainty in nominal parameters $\boldsymbol{u}_k$?
- Prior work on adaptive conformal prediction for GP surrogate models validation [Jaber et al., 2024a] $\rightarrow$ to appear in Journal of Machine Learning for Modeling and Computing
- We define the cross-conformal estimator at a new point $\boldsymbol{X}_{n+1}$ using the posterior mean of the GP $\widetilde{g}$ and the posterior variance $\widetilde{\gamma}$:

$$\widehat{C}^{J+GP}_{n,\alpha}(\boldsymbol{X}_{n+1}) = \left[\widehat{q}^{\,\pm}_{n,\alpha}\left\{\widetilde{g}_{-i}(\boldsymbol{X}_{n+1}) \pm R_i^{LOO\gamma} \times \widetilde{\gamma}_{-i}(\boldsymbol{X}_{n+1})\right\}\right] \quad (6)$$

  where $R_i^{LOO\gamma}$ is the Leave-One-Out error normalized by $\widetilde{\gamma}$
- Since the intervals are adaptive, one can use it as a proxy for metamodel accuracy $\rightarrow$ perform active learning during MCMC evaluations to refine surrogates
- Available GitHub repository

Thank you for your attention!
Any questions?

Figure: Bayesian fusion

Figure: GitHub repository

Figure: CP+GP

reach me out at `edgar.jaber@ens-paris-saclay.fr`

Table of contents

Sensitivity analysis: HSIC

- Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005], kernel method $\rightarrow$ evaluates sensitivity of a single-input in a given-data context, no need for surrogate models
- Theoretical result for all $i \in \{1, \ldots, d\}, k \in \{1, \ldots, N\}$:

$$\text{HSIC}(X_i, g(\boldsymbol{X}, t_k)) = 0 \Longleftrightarrow X_i \perp g(\boldsymbol{X}, t_k) \tag{7}$$

- The index disposes of U-stat and V-stat estimators $+$ hypothesis testing with corresponding p-value $\rightarrow$ implemented in the OpenTURNS
- The normalized R^2_{HSIC} index is better suited for interpretation:

$$R^2_{\text{HSIC}}(X_i, g(\boldsymbol{X}, t_k)) = \frac{\text{HSIC}(X_i, g(\boldsymbol{X}, t_k))}{\sqrt{(\text{HSIC}(X_i, X_i)\text{HSIC}(g(\boldsymbol{X}, t_k), g(\boldsymbol{X}, t_k)))}} \in [0, 1]$$

- Empirical evidence suggests that R^2_{HSIC} can be used confidently for variable ranking $\rightarrow$ HSIC-ANOVA decompositions also exist *but* only pathological cases create stark differences (see [Sarazin et al., 2022])

Metamodeling step 3

The metamodeling process involves:

- *Data generation:* Using the DoE of g at n input samples $\{\boldsymbol{X}^{(i)}\}_{i=1}^{n} \sim \mu_{\boldsymbol{X}}$, assemble the data matrix:

$$\boldsymbol{Y} = \left[g(\boldsymbol{X}^{(1)}), \ldots, g(\boldsymbol{X}^{(n)}) \right] \in \mathbb{R}^{N \times n} \tag{8}$$

- *Dimensionality reduction:* Apply a Karhunen–Loève (KL) decomposition [Sullivan, 2015] using the empirical covariance matrix $\widehat{C} = \frac{1}{n} \boldsymbol{Y}\boldsymbol{Y}^{\top}$. Perform singular value decomposition (SVD):

$$\boldsymbol{Y} = \boldsymbol{V} \Sigma \boldsymbol{W}^{\top}, \tag{9}$$

  where $\boldsymbol{V}$ contains the KL modes $\{\Phi_k\}_{k=1}^{m}$, and $\boldsymbol{\Sigma}$ holds the singular values.

- *Mode selection:* Retain m modes to capture a prescribed variance (e.g., 99%). Project trajectories onto the retained modes:

$$\xi_k(\boldsymbol{X}^{(i)}) = g(\boldsymbol{X}^{(i)})^{\top} \Phi_k, \quad k = 1, \ldots, m \tag{10}$$

Metamodeling step 3

- *Surrogate modeling:* For each mode k, construct a surrogate model $\widehat{\xi}_k(\boldsymbol{X})$ using a Gaussian process [Rasmussen and Williams, 2006] with identical prior mean and kernel for all modes
- *Reconstruction:* Reconstruct the full trajectory using the surrogate models:

$$\widehat{g}(\boldsymbol{X}) = \sum_{k=1}^{m} \widehat{\xi}_k(\boldsymbol{X}) \boldsymbol{\Phi}_k \tag{11}$$

- *Aggregation:* Combine multiple surrogate models $\{\widehat{g}^{(i)}\}_{i=1}^{p}$ using convex aggregation weights $\boldsymbol{w} \in \Delta^{p-1}$ to form the aggregated surrogate model:

$$\widehat{g}^{\text{agg}}(\boldsymbol{X}) = \sum_{i=1}^{p} w_i \widehat{g}^{(i)}(\boldsymbol{X}) \tag{12}$$

  This ensures robustness by leveraging multiple models while minimizing bias

References I

Biggio, L. and Kastanis, B. (2020). Prognostics and health management of industrial assets: Current progress and road ahead. *Frontiers in Artificial Intelligence*, 3:578613.

Fang, C., Liu, H.-J., Lam, H.-F., Adeagbo, M. O., and Peng, H.-Y. (2022). Practical model updating of the ting kau bridge through the mcmc-based bayesian algorithm utilizing measured modal parameters. *Engineering Structures*, 254:113839.

Feng, Q., Nebes, J., Bachet, M., Pujet, S., You, D., and Deri, E. (2023). Tube support plates blockage of PWR steam generators: thermalhydraulics and chemical modeling. Proceedings of the International Conference on Water Chemistry in Nuclear Reactor Systems (NPC 2023), Juan-les-Pins.

Gelman, A. and Rubin, D. B. (1992). Inference from iterative simulation using multiple sequences. *Statistical Science*, 7(4):457 – 472.

Girard, S. (2014). *Clogging of recirculating nuclear steam generators*. Springer International Publishing.

References II

Gretton, A., Bousquet, O., Smola, A., and Schölkopf, B. (2005). Measuring statistical dependence with Hilbert-Schmidt norms. In *Proceedings Algorithmic Learning Theory*, pages 63–77. Springer-Verlag.

Jaber, E., Blot, V., Brunel, N., Chabridon, V., Remy, E., Iooss, B., Lucor, D., Mougeot, M., and Leite, A. (2024a). Conformal Approach To Gaussian Process Surrogate Evaluation With Coverage Guarantees.

Jaber, E., Chabridon, V., Remy, E., Baudin, M., Lucor, D., Mougeot, M., and Iooss, B. (2024b). Sensitivity analyses of a multi-physics long-term clogging model for steam generators. *International Journal for Uncertainty Quantification*.

Jouin, M., Gouriveau, R., Hissel, D., Péra, M.-C., and Zerhouni, N. (2016). Particle filter-based prognostics: Review, discussion and perspectives. *Mechanical Systems and Signal Processing*, 72-73:2–31.

References III

Liu, J., Wang, D., Kong, J.-Z., Li, N., Peng, Z., and Tsui, K.-L. (2024). New look at bayesian prognostic methods. *IEEE Transactions on Automation Science and Engineering*, pages 1–16.

Moravej, H., Chan, T. H., Nguyen, K.-D., and Jesus, A. (2019). Vibration-based Bayesian model updating of civil engineering structures applying Gaussian process metamodel. *Advances in Structural Engineering*, 22(16):3487–3502.

Peng, T., He, J., Xiang, Y., Liu, Y., Saxena, A., Celaya, J., and Goebel, K. (2015). Probabilistic fatigue damage prognosis of lap joint using Bayesian updating. *Journal of Intelligent Material Systems and Structures*, 26(8):965–979.

Pinciroli, L., Baraldi, P., Shokry, A., Zio, E., Seraoui, R., and Mai, C. (2021). A semi-supervised method for the characterization of degradation of nuclear power plants steam generators. *Progress in Nuclear Energy*, 131:103580.

References IV

Prusek, T., Moleiro, E., Oukacine, F., Adobes, A., Jaeger, M., and Grandotto, M. (2013). Deposit models for tube support plate flow blockage in steam generators. *Nuclear Engineering and Design*, 262:418–428.

Rasmussen, C. E. and Williams, C. K. I. (2006). *Gaussian Processes for Machine Learning*. The MIT Press, Massachusetts.

Rocchetta, R., Broggi, M., Huchet, Q., and Patelli, E. (2018). On-line Bayesian model updating for structural health monitoring. *Mechanical Systems and Signal Processing*, 103:174–195.

Sarazin, G., Marrel, A., Da Veiga, S., and Chabridon, V. (2022). Test d'indépendance basé sur les indices HSIC-ANOVA d'ordre total. Proceedings des 53èmes Journées de Statistique de la SFdS.

Srikantiah, G. and Chappidi, P. (2000). Particle deposition and fouling in PWR steam generators. *Nuclear Engineering and Design*, 200(1-2):285–294.

Sullivan, T. J. (2015). *Introduction to uncertainty quantification*. Texts in Applied Mathematics, 63. Springer-Verlag.

References V

Yang, G., Pointeau, V., Tevissen, E., and Chagnes, A. (2017). A review on clogging of recirculating steam generators in pressurized-water reactors. *Progress in Nuclear Energy*, 97:182–196.

Zárate, B. A., Caicedo, J. M., Yu, J., and Ziehl, P. (2012). Bayesian model updating and prognosis of fatigue crack growth. *Engineering Structures*, 45:53–61.