A Bayesian methodology for hybrid degradation prognostics

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UNCECOMP 2025 - MS7 - Surrogate models for UQ: new trends

06/16/2025

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Clogging of steam generators (SGs)

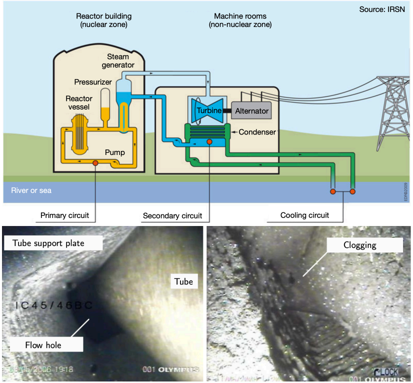
- Clogging of SGs is a complex multiphysics phenomenon that occurs following long operational periods in pressurized-water reactors (PWR) of the French nuclear fleet $\rightarrow$ undermines performance $\&$ weakens the structures $\rightarrow$ *may require chemical cleanings*
- 

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:

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

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Methodology

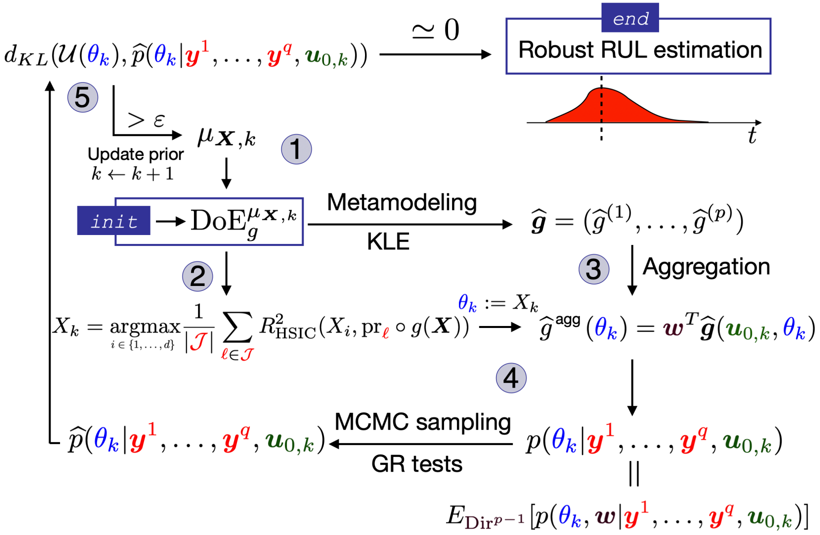
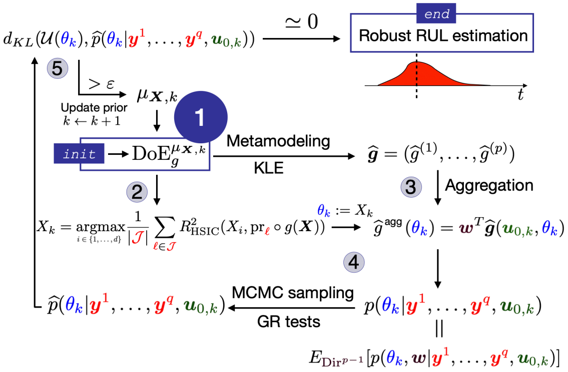


Figure: Proposed 5-steps algorithm

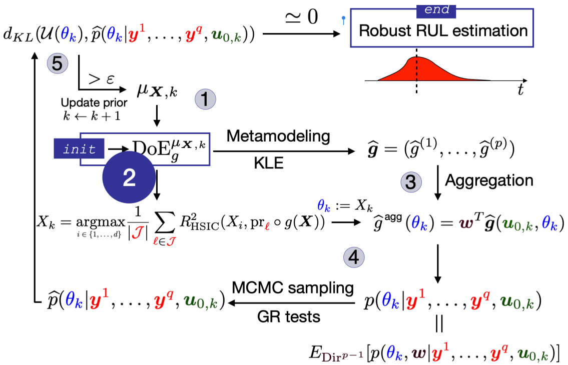
Step 1



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

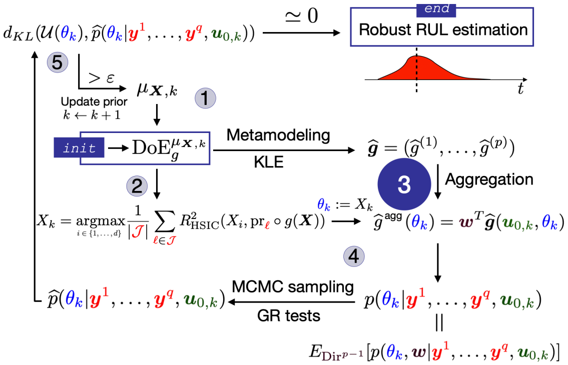
1. If $k = 0$, assume uniform independent priors $\mu_{\boldsymbol{X},k} \simeq \mathcal{U}[-1,1]^{\otimes d} \rightarrow$ generate a design of experiments $\mathrm{DoE}_g^{\mu_{\boldsymbol{X},k}} = \{(\boldsymbol{X}^{(j)}, g(\boldsymbol{X}^{(j)}))\}_{1 \leq j \leq n}$

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 $\widehat{\boldsymbol{g}} = (\widehat{g}^{(1)}, \dots, \widehat{g}^{(p)})$ 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

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:

$$\boldsymbol{Y} = \left[g(\boldsymbol{X}^{(1)}), \ldots, g(\boldsymbol{X}^{(n)}) \right] \in \mathbb{R}^{N \times n} \tag{3}$$

- *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):

$$\boldsymbol{Y} = \boldsymbol{V}\Sigma\boldsymbol{W}^{\top}, \tag{4}$$

  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:

$$\xi_k(\boldsymbol{X}^{(i)}) = g(\boldsymbol{X}^{(i)})^{\top}\Phi_k, \quad k = 1, \ldots, m \tag{5}$$

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:

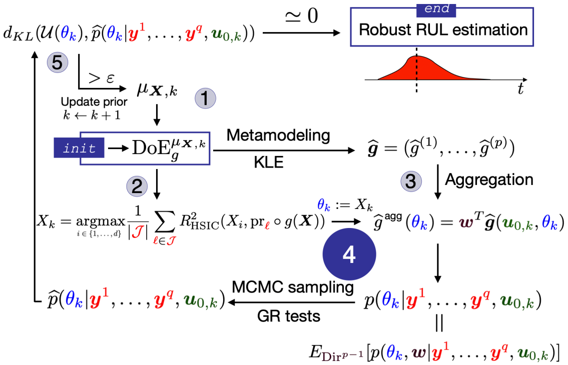
$$\widehat{g}(\boldsymbol{X}) = \sum_{k=1}^{m} \widehat{\xi}_k(\boldsymbol{X}) \boldsymbol{\Phi}_k \tag{6}$$

- *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:

$$\widehat{g}^{\text{agg}}(\boldsymbol{X}) = \sum_{i=1}^{p} w_i \widehat{g}^{(i)}(\boldsymbol{X}) \tag{7}$$

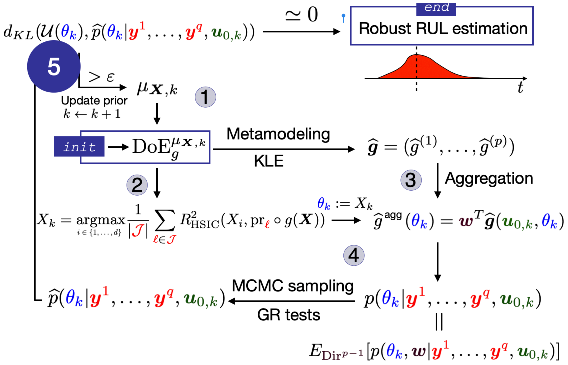
This ensures robustness by leveraging multiple models while minimizing bias

Step 4



4. Estimate the posterior distribution $\widehat{p}(\theta_k|\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q, \boldsymbol{u}_{0,k})$ 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:*

$$p(\theta|\mathbf{y}) \propto \|\mathbf{y} - f(\theta)\|^{-m} \tag{8}$$

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:*

$$p(\theta|\mathbf{y}^1, \ldots, \mathbf{y}^q) \propto \prod_{i=1}^{q} \|\mathbf{y}^i - f(\theta)\|^{-m_i} \tag{9}$$

Proof. Bayes' theorem and simplifications.

Bayesian updating step 4

$$p(\theta_k | \mathbf{y}^1, \dots, \mathbf{y}^q, \mathbf{u}_{0,k}) \propto \frac{1}{M} \sum_{r=1}^{M} \prod_{i=1}^{q} \| \mathbf{y}^i - \langle \mathbf{w}^{(r)}, \widehat{\mathbf{g}}(\mathbf{u}_{0,k}, \theta_k) \rangle \|^{-m_i} \qquad (10)$$

- Use Random Walk Metropolis-Hastings (RWMH) MCMC algorithm [Sullivan, 2015] to sample from (10)
- Monte-Carlo integration using sample $\{\mathbf{w}^{(r)}\}_{r=1}^{M}$ from the Dirichlet-$\mathbb{1}_p$ 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 $\mathbf{u}_{0,k}$ of *other $d-1$ input variables* $\rightarrow$ future work on how to integrate uncertainty
- Use log-sum-exp trick for numerical computation

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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

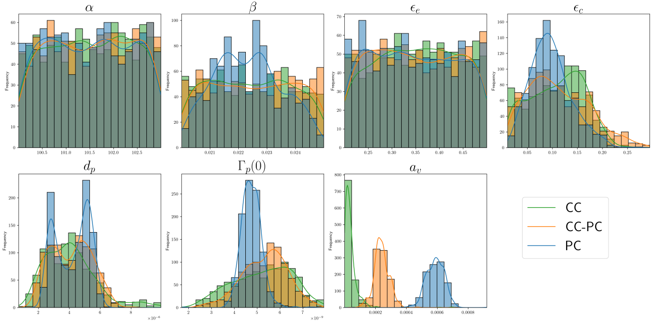


Figure: Posterior distributions of TPD clogging simulation code

Results: posterior trajectories

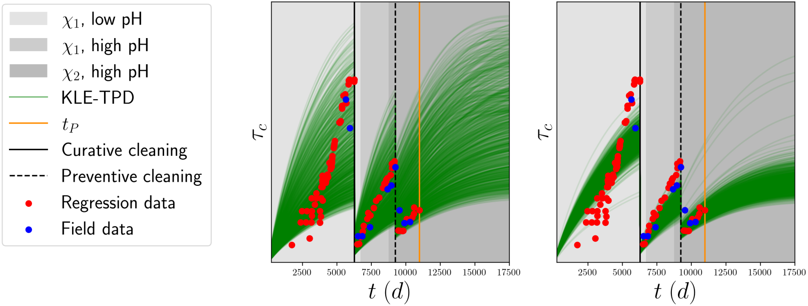
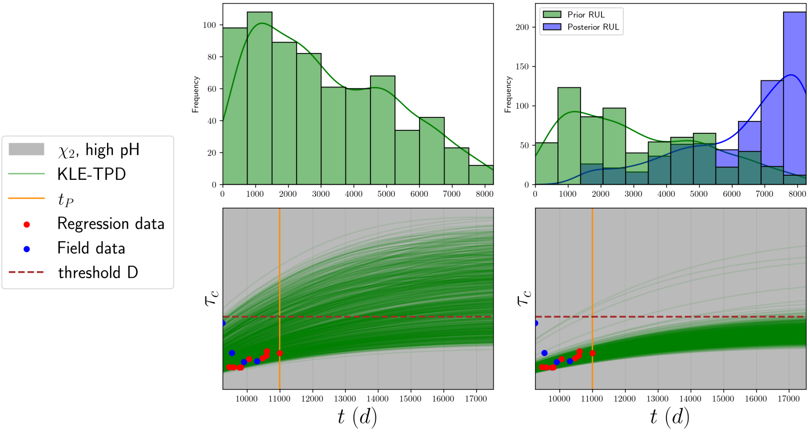


Figure: Prior/posterior TPD emulations with Karhunen-Loève expansion metamodel

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

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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 $\widetilde{\gamma}$:

$$\widehat{C}_{n,\alpha}^{J+GP}(\boldsymbol{X}_{n+1}) = \left[\widehat{q}_{n,\alpha}^{\,\pm} \left\{\widetilde{g}_{-i}(\boldsymbol{X}_{n+1}) \pm R_i^{LOO\gamma} \times \widetilde{\gamma}_{-i}(\boldsymbol{X}_{n+1})\right\}\right] \quad (11)$$

  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

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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 $i \in \{1, \ldots, d\}, k \in \{1, \ldots, N\}$:

$$\text{HSIC}(X_i, g(\boldsymbol{X}, t_k)) = 0 \iff X_i \perp g(\boldsymbol{X}, t_k) \tag{12}$$

- 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])

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