UQ and ML in Industry: Current Practices and Challenges in Industrial Applications for Low-Carbon Electricity Production

AISSAI Workshop on Artificial Intelligence and the Uncertainty Challenge in Fundamental Physics, November 27th, 2023, SCAI @ Sorbonne Université, 4 Pl. Jussieu, 75005 Paris

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Foreword and acknowledgements



This talk is given in the context of the AISSAI Workshop on Artificial Intelligence and the Uncertainty Challenge in Fundamental Physics (https://indico.in2p3.fr/event/30589/)



Acknowledgements

- □ To the **organizers** of the workshop (CNRS AISSAI & CNRS IN2P3)
- To the hosts (SCAI / Sorbonne Université, Institut Pascal / Université Paris-Saclay)
- To all the colleagues, Postdoc/PhD/Master students, and academic/industrial collaborators who helped in a direct or indirect manner to create the content of these slides!

Doing Research and Development @ EDF R&D



Figure 1: Key figures 2022-2023 for EDF R&D - part 1 (Source: EDF).

Doing Research and Development @ EDF R&D



Figure 2: Key figures 2022-2023 for EDF R&D - part 2 (Source: EDF).

Doing Research and Development @ EDF R&D

Our (local) research environment

- <u>Lab</u>: EDF Lab Chatou (Western Paris, Island of Impressionists)
- Department: "Performance, Industrial Risk, Monitoring for Maintenance and Operating" (≈ 130 people)
- □ Group: "Asset Management, Uncertainty Quantification and Statistical Learning" (≈ 20 permanent researchers, ≈ 4 to 8 PhD/MSc students)





Introduction

• Beyond the electricity bill...

- □ EDF is a leading international energy supplier ⇔ the ambition to produce zero carbon electricity in complete safety
- □ EDF operates a large panel of industrial assets
 - ➡ nuclear power plants, dams and penstocks, wind turbines, etc.
- □ Electricity production facilities ⇔ highly-safe complex industrial systems
 - \Im risk-sensitive industrial applications
 - \supset performance and safety are subject to several sources of uncertainty

Industrial context and motivations

A road trip through uncertainties!



Figure 3: Dealing with uncertainties in an industrial process (©EDF).

More about UQ in industrial practice: [DRDT08, DR12]

Industrial context and motivations

• Why do we need UQ of computer models in our industry?

- Computational modeling and simulation at EDF
 - Needed to model, design & predict the behavior of complex engineering systems (e.g., using digital twins)
 - Simulators Substitute to / complementary to (costly or unfeasible) experiments (e.g., rare/extreme/undesired/risky configurations)
- Our simulators can be:
 - Static / time-dependent / spatiotemporal
 - Deterministic / stochastic
 - ► Low / high-fidelity \Rightarrow cheap / costly-to-evaluate
 - Run on HPC / cannot!
 - Scalar-valued / vector-valued / mapping between functional inputs and functional outputs
 - Involve several codes (computational chain)
- Boths inputs and models are tainted with uncertainties
- M Uncertainties play a key role at several stages (design, operation & maintenance, risk and safety assessment, production, ...)

◆ Sources of uncertainty (⚠ from Engineers' point of view)

Natural variability / randomness / stochasticity

- intrinsic heterogeneity between individuals
- w.r.t. time or/and space
 - ➡ soil mechanical properties, part manufacturing process, etc.
- Modeling errors
 - modeling errors / model form inadequacy
 - ➡ numerical approximation, simplified equations, scenarios, etc.
 - input modeling uncertainties
 - ⇒ statistical uncertainty, measurement uncertainty, etc.

Industrial context and motivations

◆ Aleatoric vs. epistemic: does it (really) matter?

Etymology

- ► Aleatory rightarrow alea (Latin) \equiv "rolling of a dice"
- **>** Epistemic $\Rightarrow \epsilon \pi \iota \sigma \tau \eta \mu \eta$ (Greek) \equiv "knowledge"
- Aleatory uncertainty
 - Can be seen as "irreducible" within a specific context
 - Seems to be rather "objective"
- □ Epistemic uncertainty
 - Can be seen as a lack-of-knowledge, thus potentially "reducible" within a specific context
 - Seems to be rather "subjective"
 - ➤ How? ▷ By adding more information (higher-order modeling, more data, more expert knowledge, etc.)
- □ Any consensus to decide whether sth is aleatoric or epistemic?
 - ➤ No scientific consensus! But... ☞ [DKD09]
 - ... a pragmatic approach is possible to it depends on the context!
 - This distinction is debated not only in UQ, but also, recently, in ML
 IHW21]

◆ The goals of this talk are ...

- ✓ To briefly introduce the UQ framework and a few links with ML
- ✔ To provide an overview of a few motivating real-world applications
- ✔ To give a highlight of related works we did in order to tackle them!
- ✓ To make some advertisement for our tools and software!

This talk will not ...

- X Present a rigorous lecture about UQ
- X Present use cases that can be easily reproduced

1. Introduction

- 2. A few reminders about UQ and ML
- 3. Two challenging industrial use cases & related works
- 4. Open source tools and software for UQ
- 5. Conclusion

2. A few reminders about UQ and ML

◆ Verification, Validation & Uncertainty Quantification (VV&UQ)

Numerous scientific societies defined common engineering practices for VV&UQ (e.g., AIAA, ASME)

** https://www.asme.org/codes-standards/publicationsinformation/verification-validation-uncertainty

- □ Verification ⇒ to determine if the computational model fits the mathematical description
- ❑ Validation ⇒ to determine if the model accurately represents the real world application
- □ Uncertainty Quantification ⇒ to determine how variations in the numerical and physical parameters affect simulation outcomes

To go further: [OR10]

◆ Verification, Validation & Uncertainty Quantification



Figure 4: VV&UQ framework (©EDF).

🖙 [Smi13, Sul15]

Step A – Problem specification

- Dependence of interest: physical, chemical phenomenon, etc.
- $\begin{tabular}{ll} \Box & Computational modeling: $\mathcal{M}:\mathcal{X}\longrightarrow\mathcal{Y}$ \\ \end{tabular}$
- \Box Input (physical) variables: $\mathbf{x} = (x_1, \dots, x_d)$

 \Box Output variable of interest (VoI): $y = \mathcal{M}(\mathbf{x})$

(+ a first hint in order to drive the next UQ steps)

□ Quantity of Interest (QoI): QoI(Y) ► Central tendency analysis: ► QoI(Y) := $\mathbb{E}[Y]$ or QoI(Y) := Var(Y) ► Tail (risk/reliability) analysis: ► QoI(Y) := $q_{\alpha}(Y)$ (e.g., $\alpha = 0.90/0.95/0.99$) or QoI(Y) := $\mathbb{P}(Y > y_{th})$

◆ Step B – Quantification of uncertainty sources

Assume you have:

- > Data (measurements, experiments, monitoring data, etc.)
- Expertise (prior knowledge, bounds/constraints, distributions, feasible/unfeasible values, etc.)
- Standards (recommendations, common engineering practice, etc.)
- \Box Uncertain input (physical) variables: $\mathbf{X} = (X_1, \dots, X_d) \sim P_{\mathbf{X}}$
 - ► If the variables are independent $rightarrow P_{\mathbf{X}} := \prod_{j=1}^{d} P_{X_j}$
 - ➤ If they are dependent ⇔ to learn d marginal probability distributions and the copula r [Nel06, Leb13]
- □ How to construct this joint probability distribution?
 - Using parametric statistics (inference and tests)
 - Using nonparametric statistics (kernel smoothing, n.p. copula fitting)
 - Using Bayesian statistics
 - Using expert elicitation in order to derive bounds and supports



◆ Step C – Propagation of uncertainties

□ Black-box model (with scalar output):

$$\mathcal{M}: \begin{vmatrix} \mathcal{X} \subseteq \mathbb{R}^d & \longrightarrow & \mathcal{Y} \subseteq \mathbb{R} \\ \mathbf{X} & \longmapsto & Y = \mathcal{M}(\mathbf{X}) \end{vmatrix}$$
(1)

 \triangle "Black-box" here \equiv nonintrusive w.r.t. the code $\mathcal M$

 \Box Depending on the nature of the Qol(*Y*):

Central tendency estimation

⇒ analytical formulas, Monte Carlo simulations, ... 🖙 [RK08]

Rare event estimation

 \blacktriangleright approximation-based methods, variance reduction techniques

(e.g., Quasi-Monte Carlo, Importance sampling), splitting techniques, etc. 🖙 [MB15, DK22]

 \Box \bigtriangleup If \mathcal{M} is costly-to-evaluate \diamondsuit surrogate models $\widetilde{\mathcal{M}}$

Gaussian processes, polynomial chaos expansions, support vector machines, ...

🖙 [LGMS17, Bou18]

◆ Step C' – (Global) Sensitivity Analysis

- □ SA settings "revisited" = Goal of the study 🖾 [DGIP21]
 - 1. Model exploration
 - 2. Factor fixing (\equiv Qualitative screening)
 - 3. Factor priotization (\equiv Quantitative ranking)
 - 4. Robustness analysis (w.r.t. input distributions)
- \Box A zoology of methods rightarrow How to choose?
 - Dependence structure in P_X
 - \blacktriangleright Linearity / nonlinearity of \mathcal{M}
 - ► Input dimension and output dimension
 - ► The nature of the Qol(*Y*) (target and conditional analyses)
 - Computational constraints (limited simulation budget)
 - ► (If you already have a surrogate model $\widetilde{\mathcal{M}}$ or not)
 - ➤ ...

🖙 [SRA+08, IL15, RJS+21, DGIP21]

◆ Step C' – (Global) Sensitivity Analysis



Figure 5: SA methods (Source: adapted from [IL15] by [Mar21]).

Supervised Machine Learning vs. UQ?

• Supervised Machine Learning ... (not that much different from UQ)



Figure 6: Supervised ML framework (©EDF).

♦ A few recent links between supervised ML and UQ

□ Several analogies between VV&UQ and (supervised) ML:

- Validation techniques of statistical learning (surrogate / ML) models
 \$\vee\$ using kernel-based methods such as Kernel Herding \$\vee\$ [FIM⁺22a]
- UQ for for robust prediction in ML
 Conformal Prediction framework [JBB⁺23]
- Global SA (given-data) as a tool for ML Interpretability /

Explainability

⇔ Regression-based importance measures 🖙 [ICT22, CIC⁺nt]

⇔ Kernel-based indices (HSIC) 🖙 [GBSS05, DV15]

▷ Importance measures derived from Random Forests I [B21]



3. Two challenging industrial use cases & related works

Overview of the overview

- □ Two **use cases** (**UC**) are presented for the main electricity production assets
- □ They arise from real-world engineering-related questions and challenges, focusing on **various goals**:
 - > Safety analysis, risk and reliability assessment
 - Operating (statistical lifetime analysis, prognostics & health monitoring, maintenance optimization)
 - Robust design (under uncertainty) of new components and assets
 - Predictive analysis and new electricity usage
 - ➤ ...



Figure 7: A typical French pressurized water reactor (source: IRSN).

☆ The 3 safety barriers.

▷ (#1) cladding, (#2) primary circuit, (#3) reactor building

Context of UC#1

- □ Scenario: Intermediate-Break Loss-Of-Coolant Accident (IBLOCA)
- \Box Computer model: the CATHARE2 code (1 call \approx 1 hour)



Figure 8: IBLOCA in a PWR (©CEA) / PCT trajectories from CATHARE2 (©EDF).

Context of UC#1

- □ Scenario: Intermediate-Break Loss-Of-Coolant Accident (IBLOCA)
- **\Box** Computer model: the CATHARE2 code (1 call \approx 1 hour)
- Inputs:
 - ► Type #1: Initial/boundary conditions \square probabilistic (U, trunc. N)
 - ► Type #2: Physical parameters $\stackrel{\circ}{\rightarrow}$ probabilistic ($\mathcal{U}, \mathcal{LU}, \text{trunc. } \mathcal{N}, \mathcal{LN}$)
 - ➤ Type #3: Scenario parameters ▷ not probabilistic (lower/upper bounds)
- □ Output QoI: Second peak of cladding temperature (PCT) ⇔ scalar QoI

☆ Main scientific/technical objectives.

- **(O1)** How to find the most penalizing values of Type #3 parameters?
- (O2) How to derive robustness indicators of risk-estimates w.r.t. input probabilistic modeling?
- **(O3)** How to detect functional outliers in transient simulations?

Context of UC#1



Figure 9: Nuclear fuel schematic (Source: US DoE and this website).

\hookrightarrow (O1) How to find the most penalizing values of Type #3 parameters?

\Lambda Main challenges:

- ▶ $d \approx$ 100 input variables, computational cost & nonlinearity
- Single input-output MC sample available ("given-data" framework)
- Proposed approach: ICSCREAM methodology [MIC22]

Main ingredients

- $\Box \quad \text{Qol} \, \mathfrak{i} \, \widehat{q}_{0.90}(Y)$
- Use of global and target SA using the Hilbert-Schmidt Independence Criterion (HSIC) [DV15, MC21]
- □ Gaussian process (GP) regression
- Optimization under uncertainty
- Tracking nonmonotonic relationships



Figure 10: HSIC and GP regression.

\hookrightarrow (O1) How to find the most penalizing values of Type #3 parameters?



Figure 11: Illustration on 1D and 2D cases (Source: [MIC22]).

\hookrightarrow (O2) How to derive robustness indicators of risk-estimates w.r.t. input probabilistic modeling?

- ▲ Main challenges: (same as before, plus...)
 - Qol \varphi a risk measure (e.g., failure probability / high-order quantile / a super-quantile)
 - Several sources of epistemic uncertainties (e.g., input distributions, model uncertainties)
- Proposed approaches:
 - (A.) Using **perturbation-based robustness measures** [Lem14, LSA⁺15, SID17, IVL22, GSSI22]
 - (B.) Using the **Optimal Uncertainty Quantification** (OUQ) framework [Ste20, SGKI20, SGK21]
 - (C.) Using the Info-Gap (IG) framework and extra-probabilistic modeling [Aje22, AAC⁺22, AAC⁺23]

 \hookrightarrow (O2) How to derive robustness indicators of risk-estimates w.r.t. input probabilistic modeling?

(A.) Using perturbation-based robustness measures [Lem14, LSA⁺15, SID17, IVL22, GSSI22]

Main ingredients

- □ Perturbed-law based (PLI) indices: $S_{j,\delta} = \frac{\operatorname{Qol}(f_j^{\delta}) - \operatorname{Qol}(f_j)}{\operatorname{Qol}(f_j)}$
- MC and IS-based estimators for several Qols with asymptotic guarantees
- Extensions to several Qols and multivariate perturbations
- Generalization through Information
 Geometry and the Fisher-Rao
 distance (Optimal Fisher-based PLI)



Figure 12: PLI and OF-PLI ([IVL22, GSSI22]).

\hookrightarrow (O2) How to derive robustness indicators of risk-estimates w.r.t. input probabilistic modeling?

(B.) Using the Optimal Uncertainty Quantification (OUQ) framework [Ste20, SGK120, SGK21]

Main ingredients

□ OUQ principles [OSS⁺13] Evaluation of a maximum risk measure over a class of admissible measures

 $\inf_{\mu \in \mathcal{A}_{\Delta}} \mathbb{P}(G(\mathbf{X}) \leq h)$

- □ Relies on the **Reduction Theorem** optimal solution of Qol optimization is a product of discrete measures
- ❑ Set of input measures reparameterized using Canonical Moments ♀ facilitates the optimization problem



Figure 13: OUQ and canonical moments ([Ste20, SGKI20]).

\hookrightarrow (O2) How to derive robustness indicators of risk-estimates w.r.t. input probabilistic modeling?

(C.) Using the Info-Gap (IG) framework and extra-probabilistic modeling [Aje22, AAC⁺22, AAC⁺23]

Main ingredients

- □ IG [BH06]
 decision-theoretic
 framework under severe uncertainty
- Relies on the concepts of horizon of uncertainty and robustness curve
- □ Coupled with **random sets** [Mol17] ⇒ generic framework for hybrid reliability assessment
- Proposition of efficient strategies based on advanced sampling and surrogate modeling





\hookrightarrow (O3) How to detect functional outliers in transient simulations?

- ⚠ Main challenges: (same as before, plus...)
 - ► No off-the-shelf method for expensive-to-evaluate computer simulations
- Proposed approach: Functional Outlier Detection (FOD) methodology adapted to strongly nonlinear nuclear transients [RDP21, RDPCI⁺21]

Main ingredients

- To measure the outlyingness both in the magnitude and shape senses
 [RDP21, RDPCI⁺21]
- Various features used (h-mode depth or DTW)
- Using HSIC indices in order to better interpret outliers



Figure 15: FOD on transients ([RDP21]).

Context of UC#2

- <u>Scenario</u>: reliability analysis of an offshore wind turbine (OWT)
- Computer model: complex computational chain



Figure 16: Monopile OWT diagram [FCMI23].



Figure 17: Computational chain [FCMI23].

Context of UC#2

- □ <u>Scenario</u>: reliability analysis of an offshore wind turbine (OWT)
- Computer model: complex computational chain (TurbSim - DIEGO - Damage)
- Inputs:
 - Environmental variables X
- Output Qol: mean fatigue damage in the structure w.r.t. the environmental conditions

☆ Main scientific/technical objectives.

- (O1) How to build an input probabilistic model when inputs have a complex dependence structure?
- □ (O2) How to efficiently propagate uncertainties in a costly-to-evaluate computational chain?

\hookrightarrow (O1) & (O2) Learning complex dependence structure + Efficient uncertainty propagation?

\Lambda Main challenges:

- Large dataset of environmental conditions (given-data)
- Complex dependence structures among inputs
- Proposed approach: Using the empirical Bernstein copula and Kernel Herding [FCMI23]

Main ingredients

- ❑ Nonparametric copula fitting ⇒ empirical Bernstein copula [Las22, FCMI23]
- □ Use of Kernel Herding [CWS10] ⇒ subsampling and efficient propagation of uncertainties [FIM⁺22b, FCMI23]



 \hookrightarrow (O1) & (O2) Learning complex dependence structure + Efficient uncertainty propagation?



Figure 19: Kernel Herding applied to a 2D and OWT cases (Source: [FCMI23]).

4. Open source tools and software for UQ

OpenTURNS: an open-source library for UQ

OpenTURNS in a few words:

- An Open source initiative for the Treatment of Uncertainties, Risks'N Statistics
 [BDIP17]
- ► Started in 2004...
- ► Last version: 1.21 (summer 2023, 2 releases / year)
- Developed (LGPL License) by
 Airbus EDF IMACS ONERA Phimeca
- ≻ 🮯 core & 🟓 API

conda/pip install openturns

□ More information?

- ► <u>Website</u>: https://openturns.github.io/www/
- <u>Github</u>: https://github.com/openturns/openturns
- ▶ <u>Discourse</u>: https://openturns.discourse.group/
- <u>Gitter</u>: chatting for short questions and problems
- ► <u>Stack Overflow</u>: tag 'openturns'
- ▶ <u>OT modules</u>: several specific 🥏 modules (packages) on this page



OpenTURNS: an open-source library for UQ



Data analysis

Probabilistic modeling

Meta modeling



Sample analysis Distribution fitting Statistical hypothesis testing Estimate dependency and copulas



Copulas Stochastic processes



Figure 20: OpenTURNS' webpage.

OpenTURNS: an open-source library for UQ

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all categories All tags Categories Latest	New (1) Ur	nread (1)	Тор	+ New Topic
Category	Topics	Latest		
Methodology Discussion on the uncertainty quantification methodology in studies	2 / month	6	Metamodel to substitute a Code_Aster study Methodology polynomial-chaos	5 1d
Development Everything about hacking the library.	2 / month 1 new	6	Comparaison Point/Sample vs numpy array • Development	0 1d
Python usage Get help using openturns from its Python module	1 / month 1 unread		Why does the LHS class exist? Python usage reliability	8 2d
Announcements Infos on new releases, events, etc	1 / month	0	Version 1.22 RC1 available	0 7d
Installation Installation troubleshooting	9	0	Computing Conditional Quantiles Python usage	3 19d
Site Feedback Discussion about this site, its organization, how it works, and how we can improve it.	2	0	SubsetSampling intermediary quantiles estimation ()	4 23d

Figure 21: OpenTURNS' Discourse forum.

Persalys: an open-source GUI for UQ and data analysis

D Persalys in a few words:

- GUI based on OpenTURNS
- ► Interface available in French or in English
- Open source software, developed by a partnership between Phimeca & EDF (and a collaboration with the OpenTURNS consortium)



□ More information?

- Website: https://persalys.fr/index.php
 Iust fill in the form (Level 1) and download it for free!
- <u>Github</u>: https://github.com/persalys/persalys
- Discourse: https://persalys.discourse.group/

'sensitivity': global sensitivity analysis and ML interpretability

□ 'sensitivity' in a few words:

- R package for the sensitivity analysis of model outputs
- Now contains a few methods for ML interpretability I [ICT22]
- Last version: 1.29.0 (Published: 2023-08-31)
- Many contributors (academic / industrial / students)
- Maintainer: Bertrand looss (EDF R&D)
- ► Companion book 🖙 [DGIP21]

More information?

- CRAN webpage: https://persalys.fr/index.php
- Reference manual:

https://cran.r-project.org/web/packages/sensitivity/sensitivity.pdf



Conclusion

Conclusion

- ◆ A few (positive) take-home messages...
 - ✓ UQ is now a mature field in several industrial fields (energy, aerospace, automotive, etc.)
 - ✓ UQ benefits from a (very) high-level of academic research (in probability, statistics, optimization, machine learning, signal processing, geometry, topology, ...)
 - ✓ Many open source tools and software are available!
 ▲ Be careful about "blind/naive use" of these methods and tools!
 - Safety authorities and regulators recognize this field as being of major interest
- ◆ ... and a few (personal) disappointments
 - X UQ is still underrepresented in some fields
 - ✗ UQ suffers (sometimes) from a lack of attractiveness compared to ML

Conclusion

◆ A few open questions and/or perspectives

□ Going deeper into the links between UQ and ML:

- > Several connections about the way uncertainties are taken into account
- On-going works about kernel methods
- > The use of conformal prediction for doing UQ in ML models
- Strong links between eXplainable AI and global sensitivity analysis
- Anomaly detection vs. rare event estimation, any links?
- Hybridation between UQ and ML
 - Robustess of "Physics-informed" strategies (complex simulation models)
 - Hybridation using other methods than neural networks
- □ Challenges for industrial UQ:
 - UQ for input/output fields
 - ▶ UQ and the "transposition" problem (\approx transfer learning)
 - UQ based on images/videos
 - ► UQ for complex models (environmental, biological, etc.)

Scientific dissemination & the French UQ community?

Main organizations and networks

- □ GdR MASCOT-NUM ⇔ a French Research Group dealing with stochastic methods for the analysis of numerical codes
- □ GIS LARTISSTE ⇒ a French Scientific Consortium about UQ @ Paris-Saclay
- □ SINCLAIR AI Lab. ⇒ the Saclay INdustrial Collaborative Laboratory for Artificial Intelligence Research (SINCLAIR), gathering researchers from EDF, Thales and TotalEnergies
- □ **frENBIS** ⇒ the French local network of the European Network for Business and Industrial Statistics (ENBIS)

Main seminars and scientific events

- □ UQSay seminars ⇔ series of online seminars on the broad area of UQ, ML and related topics
- □ ETICS Annual Research Schools

 Thematic Research School on Uncertainty in Scientific Computing

Thank your for your attention! Any question?

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