Kernel methods for uncertainty propagation and sensitivity analysis

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Foreword and acknowledgements

◆ Foreword

❑ This course is given in the context of the HIPERWIND Summer School

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About 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 seminars on the broad area of UQ, ML and related topics
- ❑ **ETICS Annual Research Schools** ➪ Thematic Research School on Uncertainty in Scientific Computing

Doing Research and Development @ EDF R&D

- **Our research group**
  - 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 students and Master students)

- **The main tools we develop for UQ/ML**
  - OpenTURNS ➪ an open source library for UQ (Python / C++)
  - Persalys ➪ a friendly GUI (open source) for performing UQ, data visualization, ...
  - `sensitivity` ➪ R package for sensitivity analysis of model outputs
  - `mistral` ➪ R package for structural reliability methods

Introduction

Industrial context and motivations

◆ **A road trip through uncertainties!**

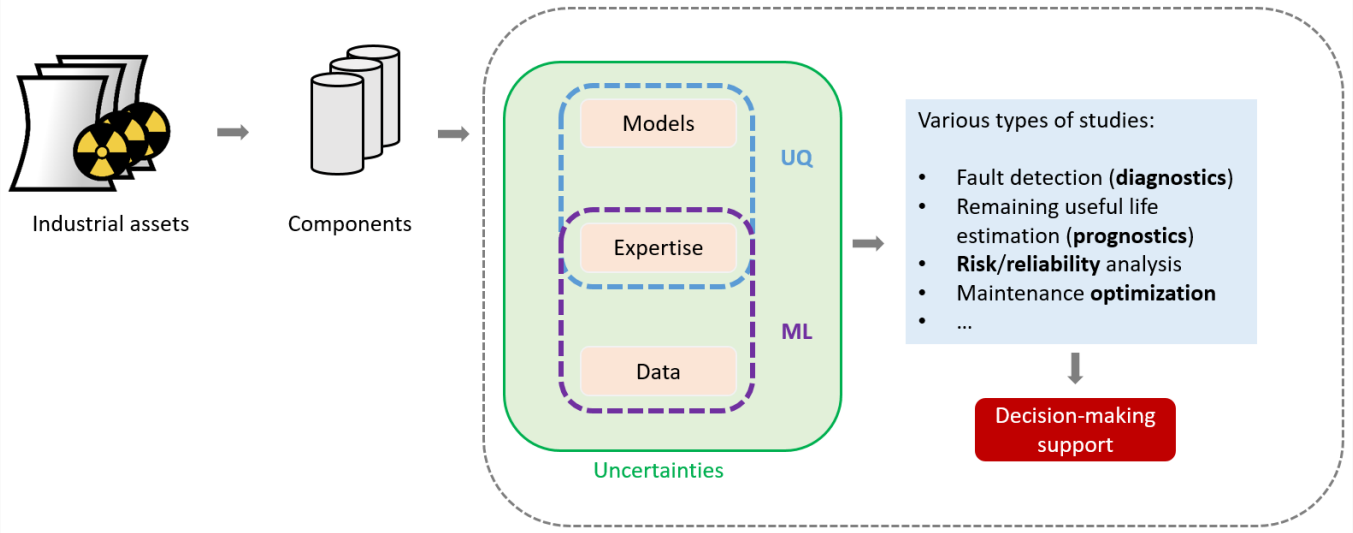

Figure 1: Dealing with uncertainties in an industrial process (©EDF).

☞ About UQ in industrial practice: [DRDT08, DR12]

Uncertainty Quantification in a nutshell!

◆ Verification, Validation & Uncertainty Quantification

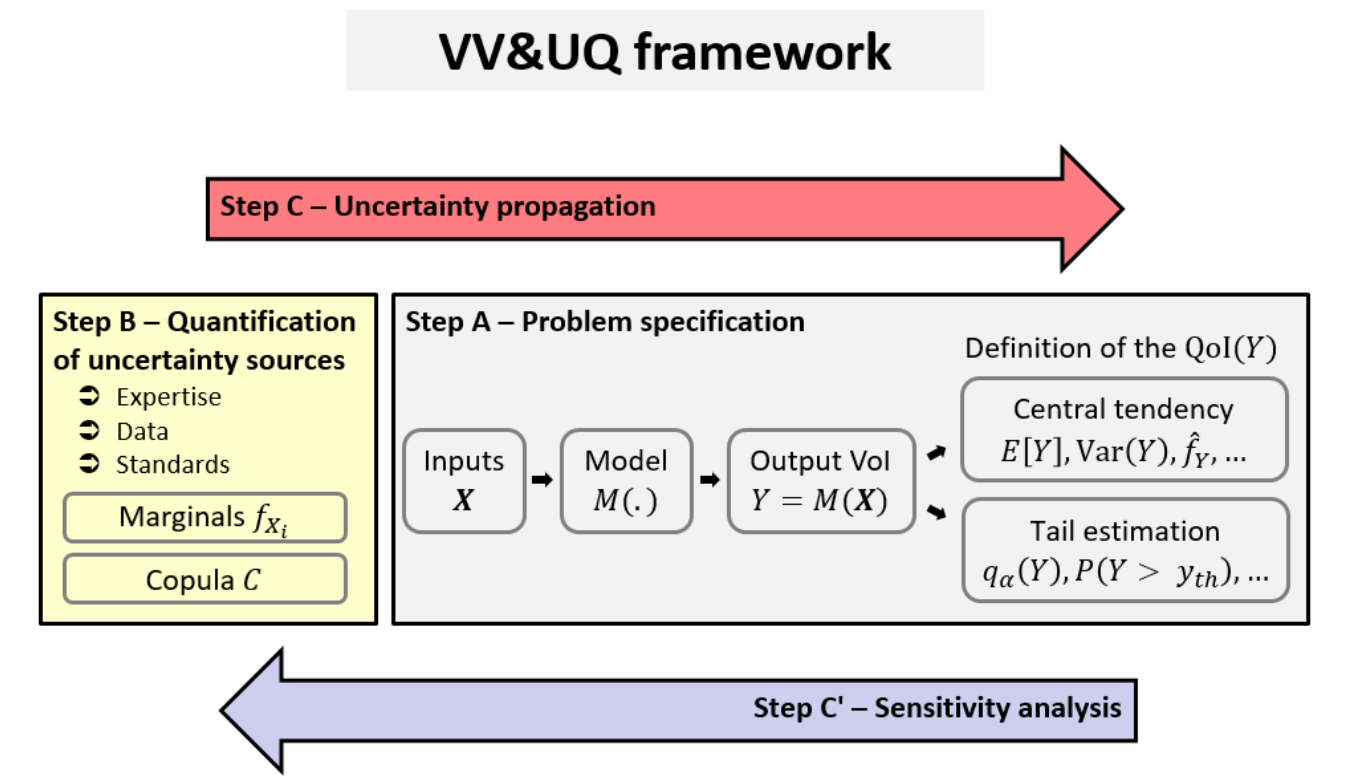

Figure 2: VV&UQ framework (©EDF).

☞ To go further into UQ in general: [Smi13, Sul15]
☞ To go further into Uncertainty Propagation: [MB15, DK22]
☞ To go further into Surrogate Modeling: [Bou18]
☞ To go further into SA: [SRA+08, DGIP21]

Supervised Machine Learning in a nutshell!

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

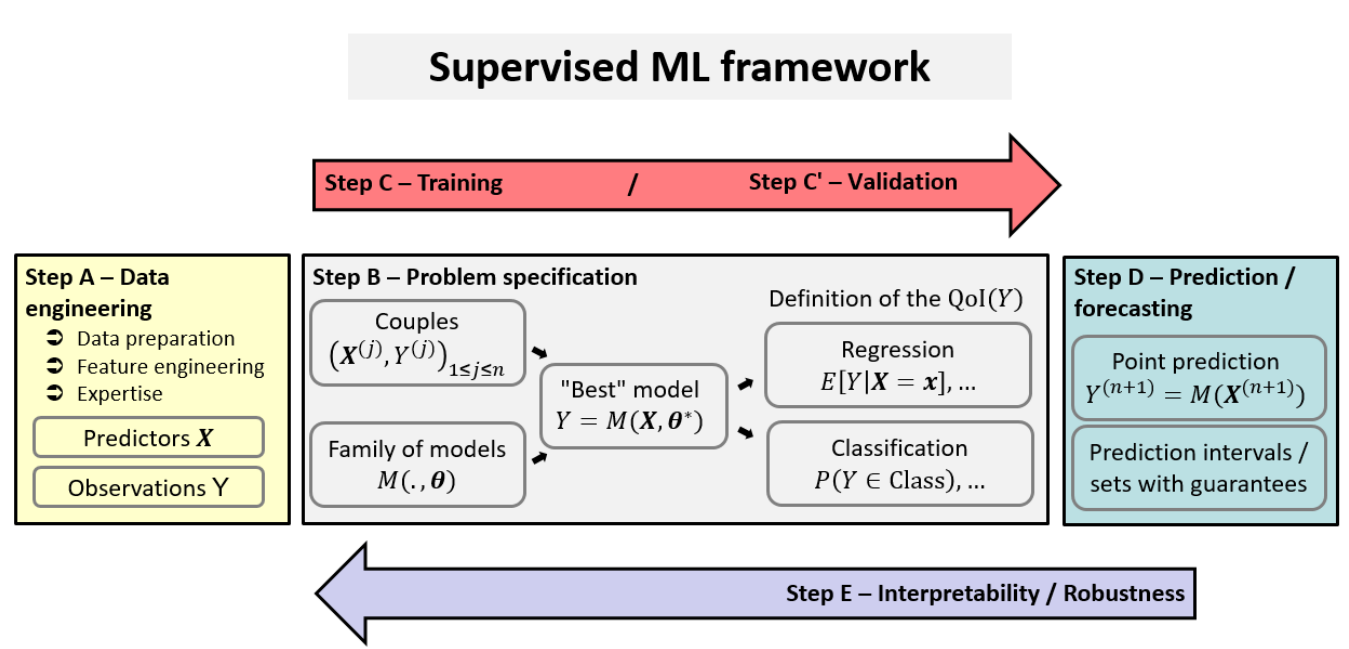

Figure 3: Supervised ML (©EDF).

☞ To further into ML in general: [Bis06, HTF09]
☞ To go further into the links between SQ (UQ) and Interpretability/Explainability (ML): [Mol22, ICT22]

Main objectives of this course

◆ **What about the possible links between UQ and ML?**

❑ Historically, people thought UQ and ML were two distinct disciplines:

- ➤ UQ ➪ dedicated to computer experiments, based on physical / numerical models
- ➤ ML ➪ dedicated to real data, no model available

❑ Recently (> 2008-2009), people tend to see more and more similarities between UQ and ML, e.g., in the fields of:

- ➤ surrogate modeling ≡ supervised statistical learning
- ➤ global sensitivity analysis ≡ explainability/interpretability
- ➤ ...

❑ Even more recently (> 2015), people try more to adopt "hybrid approaches" by combining them!

Kernel methods

Kernel methods are one of the cornerstones between these two disciplines.

Main objectives of this course

- **With this course, you probably will ...**
  - ✔ Have an overview about "why kernels are so popular?"
  - ✔ Have a first glimpse about the mathematical foundations of these methods
  - ✔ Have access to a panel of references to go further into some topics
  - ✔ A good opportunity for discovering (only a few) kernel methods and to **use them for real!**
  - ✔ Discover the (great) **OpenTURNS software**!
- **With this course, you probably won't ...**
  - ✘ Be an expert in kernel methods
  - ✘ Be able to solve all your complicated problems with kernel methods

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2. Mathematical background about kernels for UQ and ML

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4. Kernel-based sensitivity analysis

2. Mathematical background

Why should we play with “kernels”?

◆ A few motivations

❑ Imagine you have this 1D dataset with two different labels • and •

Figure 4: A 1D dataset (source: [Sut22]).

❑ You want to do some “ML stuff” in order to have a **good classification model**!

❑ Assume a linear model: $f(x) = \beta_0 + \beta_1 x$ such that $\widehat{y}(x) = \text{sign}\left(f(x)\right)$

❑ What do you typically obtain?

Why should we play with “kernels”?

◆ **A few motivations (cont’d)**

Figure 5: 1D dataset : a first classification model (source: [Sut22]).

❑ OK! That’s clearly not a good model!

❑ Let’s extend x such that:

$$f(x) = \boldsymbol{\beta}^\top (1, x, x^2) = \boldsymbol{\beta}^\top \psi(\mathbf{x})$$

❑ What do we obtain?

Why should we play with “kernels”?

◆ **A few motivations (cont’d)**

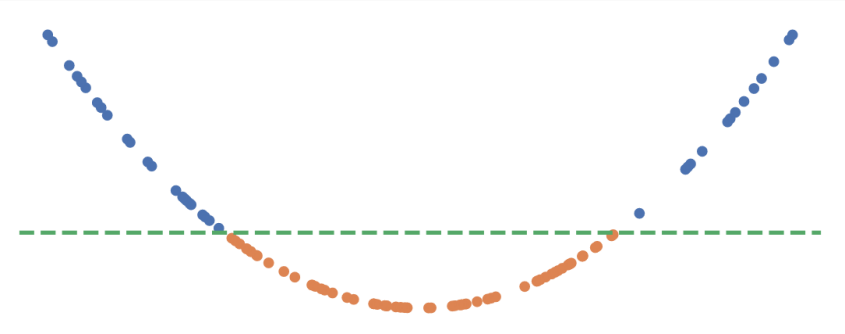


Figure 6: 1D dataset : a second classification model (source: [Sut22]).

- ❏ OK! The model does the job!
- ❏ **Kernels** are tools that enable to do this job with any (potentially) very complicated $\psi(\cdot)$ functions
- ❏ Kernels are used in modern (supervised and unsupervised) ML in order to treat very complicated data with, e.g., time series, images, graphs, text, videos, ...
- ❏ $\psi(\cdot)$ will leave in a specific mathematical space called a **reproducing kernel Hilbert space**

Which “kernels” are we talking about?

- **The word “kernel” is widely used and can be misunderstood** ⚠
  - The concept treated in this course: “positive definite kernel”, “RKHS kernel”, (“Mercer kernel”)
  - A semi-related concept: “kernel density estimation” or “kernel smoothing” (nonparametric statistics)
  - Unrelated notions[1]:
    - The kernel (null space) of a linear map (linear algebra)
    - The kernel of a convolution (image processing)
    - CUDA and Linux kernels
    - Popcorn kernels

[1] This brilliant list is directly borrowed from the wonderful course given by Danica J. Sutherland, available here: https://github.com/djsutherland/etics-kernels-22.

Kernels: definition, properties and links to RKHSs

◆ What is a kernel? A first definition!

- ❑ Let $\mathcal{Z}$ be a space of interest, e.g., such that $\mathcal{Z} \subseteq \mathbb{R}^d$
- ❑ A function $K : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ is said to be a **kernel** if it is symmetric and positive definite (pd):
  - ➤ **Symmetry**: $\forall\, z, z' \in \mathcal{Z}, K(z, z') = K(z', z)$
  - ➤ **Positive definiteness**[2]:

$$\forall\, n \geq 1, \forall\, z_1, \ldots, z_n \in \mathcal{Z}, \forall\, c_1, \ldots, c_n \in \mathbb{R}, \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(z_i, z_j) \geq 0$$

- ❑ Equivalently, the kernel function can be written following a "matrix viewpoint":

$$\mathbf{c}^\top \mathbf{K}_n \mathbf{c} \geq 0 \quad \text{with} \quad \mathbf{K}_n := [K(z_i, z_j)]_{1 \leq i,j \leq n} \quad \text{and} \quad \mathbf{c} := [c_i]_{1 \leq i \leq n}$$

- ❑ The matrix $\mathbf{K}_n$ is usually called the **Gram matrix** (or **kernel matrix**)

[2] ⚠ K is pd $\Leftrightarrow$ all Gram matrices from K are positive semi-definite (psd).

A detour through Hilbert spaces

◆ **What is an Hilbert space $\mathcal{H}$?**

- ❑ A complete (real or ~~complex~~) inner product space
- ❑ Inner product space ➪ a vector space with an **inner product**:
  - ➤ **Linearity**: $\forall\, h_1, h_2, h_3 \in \mathcal{H}, \forall\, a, b \in \mathbb{R}, \langle ah_1 + bh_2, h_3\rangle_{\mathcal{H}}$
  - ➤ **Symmetry**: $\forall\, h_1, h_2 \in \mathcal{H}, \langle h_1, h_2\rangle_{\mathcal{H}} = \langle h_2, h_1\rangle_{\mathcal{H}}$
  - ➤ **Positive definiteness**:
    $\forall\, h \in \mathcal{H}, \langle h, h\rangle_{\mathcal{H}} \geq 0$ and $\langle h, h\rangle_{\mathcal{H}} = 0 \quad \Rightarrow \quad h = 0$
- ❑ This inner product induces a **norm** on $\mathcal{H}$: $||h||_{\mathcal{H}} := \sqrt{\langle h, h\rangle_{\mathcal{H}}}$
- ❑ Completeness ➪ "well-behaved" (i.e., any Cauchy sequence in $\mathcal{H}$ converges and has a limit in $\mathcal{H}$)

◆ **Examples of well-known (and applications of) Hilbert spaces:**

➥ Lebesgue spaces, Sobolev spaces, ...

➥ Applications in Quantum Physics, Signal Processing, Probability & Statistics, ML, Computational Engineering, ...

A detour through Hilbert spaces

◆ **Do you have a map? Because I'm lost ...**

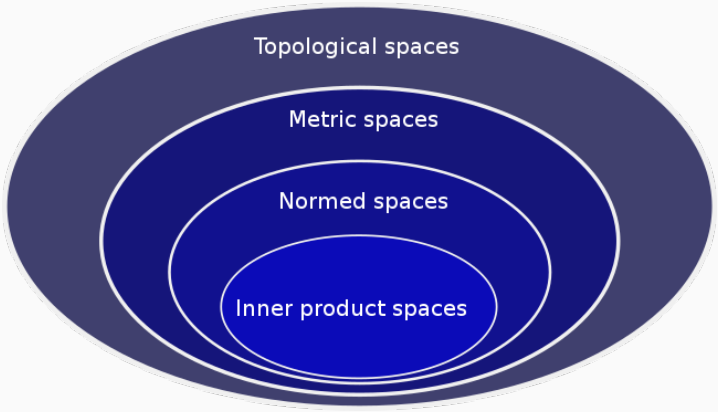


Figure 7: Hierarchy of mathematical spaces (source: Wikipedia).

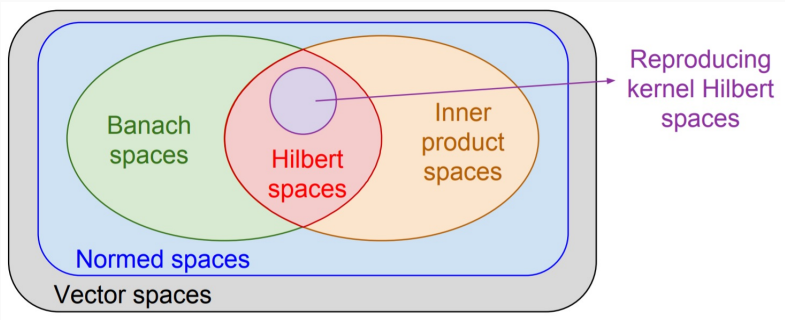


Figure 8: A more refined Venn diagram of mathematical spaces (source: https://ngilshie.github.io).

Focus in this talk

A special class of spaces will be of interest in this course:
the so-called "**reproducing kernel Hilbert spaces**" (**RKHSs**)

Kernels: definition and first properties

◆ Kernel: an inner product between feature maps

- ❑ One considers a set of interest $\mathcal{Z}$ (e.g., $\mathbb{R}^d$, functions, distributions of graphs / images, ...)
- ❑ $K : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ is a **kernel** on $\mathcal{Z}$ if there exists a Hilbert space $\mathcal{G}$ and a **feature map** $\psi : \mathcal{Z} \to \mathcal{G}$ so that:

$$\forall\, z, z' \in \mathcal{Z}, K(z, z') = \langle \psi(z), \psi(z') \rangle_{\mathcal{G}} \tag{1}$$

- ❑ Vocabulary:
  - ➤ ψ is called a **feature map**
  - ➤ $\mathcal{G}$ is called a **feature space**
  - ➤ $\psi(z)$ with $z \in \mathcal{Z}$ are the **feature functions** (or **features**)

◆ A few first properties

- ❑ $\forall\, K, \exists\, \psi$ **such that Eq.** (1) **holds, but** ψ **can be implicit**
- ❑ $\forall\, \psi : \mathcal{Z} \to \mathcal{G}$ **(with** $\mathcal{G}$ **an HS), the function** K **given by Eq.** (1) **is always a kernel**

Kernels: definition and first properties

◆ Kernel and feature map: the "hidden mechanism"

- ❑ Kernel K and feature map ψ are intimately related to each other
- ❑ The feature map ψ offers an alternative viewpoint on the kernel K
- ❑ Given two points z and z' living in an Euclidean space $\mathcal{Z}$, evaluating K leads to:
  - ➤ creating two feature functions $\psi(z), \psi(z')$ in a (possibly very sophisticated) feature space $\mathcal{G}$
  - ➤ comparing them using the existing metric in $\mathcal{G}$
- ❑ When $\mathcal{G}$ is infinite-dimensional ⇨ a much richer and subtle information is captured in $\mathcal{G}$ than in $\mathcal{Z}$
- ❑ The "kernel trick":
  - ➤ mathematically speaking ⇨ comparing $\psi(z)$ and $\psi(z')$ captures a rich information
  - ➤ numerically speaking ⇨ comparing $\psi(z)$ and $\psi(z')$ **only requires to compute** $K(z, z')$

Back to spaces: the "reproducing kernel Hilbert spaces"

◆ What is a "reproducing kernel Hilbert space" (RKHS)?

- ❑ Some basic ingredients first: let $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}}, ||\cdot||_{\mathcal{H}})$ be a Hilbert space (with inner product and associated norm) of functions mapping from some nonempty set $\mathcal{Z}$ to $\mathbb{R}$ ➪ denoted by $\mathcal{H} \subset \mathbb{R}^{\mathcal{Z}}$
- ❑ A first (desirable) property: if two functions $f \in \mathcal{H}$ and $g \in \mathcal{H}$ are close in the norm of $\mathcal{H}$, then, $f(z)$ and $g(z)$ are close for all $z \in \mathcal{Z}$
- ❑ Evaluation functional:

$$L_z : \left| \begin{array}{ccc} \mathcal{H} & \longrightarrow & \mathbb{R} \\ h & \longmapsto & L_z[h] = h(z) \end{array} \right.$$

- ❑ All those functionals are actually **linear forms**

☆ Definition (RKHS)

$\mathcal{H}$ RKHS if all the evaluation functionals (i.e., $\forall\, z \in \mathcal{Z}$) are bounded, i.e.,
$\forall\, z \in \mathcal{Z}, \exists C_z > 0 \quad$ such that $\quad |h(z)| \leq C_z ||h||_{\mathcal{H}}$.

☞ To go further: [SG15] and [PR16, Ch. 1, p. 4]

Back to spaces: the "reproducing kernel Hilbert spaces"

◆ **What is a "reproducing kernel Hilbert space" (RKHS)?**

❑ Consequences:

- ➪ functions in the RKHS are "smooth" in the sense of the previous definition
- ➪ RKHSs are particularly "well-behaved" spaces (relative to other Hilbert spaces)

☆ Corollary (norm convergence in $\mathcal{H} \Rightarrow$ pointwise convergence)

If two functions converge in RKHS norm, then they converge pointwise, i.e., if $\lim_{n\to\infty} ||h_n - h||_{\mathcal{H}} = 0$, then $\lim_{n\to\infty} h_n(z) = h(z), \forall\ z \in \mathcal{Z}$.

☞ To go further: [BTA04, Ch. 1, p. 10]

Reproducing kernel and feature maps

◆ **What about the "reproducing property"?**

❑ Riesz representation theorem: one applies it to all evaluation functionals (bounded linear operators)

$$\forall\, z \in \mathcal{Z}, \exists!\, \kappa_z \in \mathcal{H}, \quad \text{such that} \quad \forall\, h \in \mathcal{H}, L_z[h] = \langle h, \kappa_z \rangle_{\mathcal{H}}$$

➪ ⚠ this theorem ensures that, $\forall\, z \in \mathcal{Z}$, we can find a **unique** element in $\mathcal{H}$ that is a **representer** of the evaluation $h(z)$

❑ Point evaluation property: equipped with this representer, one has:

$$\forall\, z, z' \in \mathcal{Z}, K(z, z') := \langle \kappa_{z'}, \kappa_z \rangle_{\mathcal{H}} = \kappa_z(z') = \kappa_{z'}(z)$$

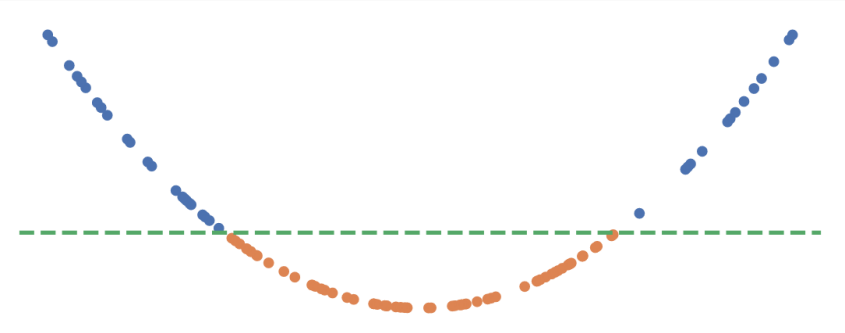
❑ Reproducing property: bringing what precedes together leads to:

$$\forall\, h \in \mathcal{H}, \forall\, z \in \mathcal{Z}, h(z) = \langle h, K(\cdot, z) \rangle_{\mathcal{H}}$$

➪ ⚠ K is the only kernel (**reproducing kernel**) that verifies this property!

Reproducing kernel and feature maps

◆ **Illustration of the reproducing property: back to the initial motivating example**



- Recall that: $\mathcal{Z} = \mathcal{X} = \mathbb{R}$ and $\psi(x) = (1, x, x^2) \in \mathbb{R}^3$
- Kernel is given by: $K(x, y) = \langle \psi(x), \psi(y) \rangle_{\mathcal{H}} = 1 + xy + x^2 y^2$
- Classifier based on a linear function f such that: $f(x) = \langle \boldsymbol{\beta}, \psi(x) \rangle_{\mathcal{H}}$
  - with $f(\cdot)$ the function itself (which corresponds to the vector $\boldsymbol{\beta} \in \mathbb{R}^3$
  - $f(x) \in \mathbb{R}$ which is the function evaluated at a point x
- Reproducing property: $f(x) = \langle f(\cdot), \psi(x) \rangle_{\mathcal{H}}$ for $f \in \mathcal{H}$

Reproducing kernel and feature maps

◆ The canonical feature map

❑ We just saw (reproducing property):

$$\forall\, h \in \mathcal{H}, \forall\, z \in \mathcal{Z}, h(z) = \langle h, K(\cdot, z)\rangle_{\mathcal{H}}$$

❑ Canonical feature map:

$$\forall\, z, z' \in \mathcal{Z}, K(z, z') = \langle \theta(z'), \theta(z)\rangle_{\mathcal{H}}$$

➪ $\theta(z) := \kappa_z$ is called the **canonical feature map**

➪ the associated RKHS is precisely the feature space $\mathcal{H}$

❑ ⚠ **This canonical feature map may be (often) not very instructive for several reasons** (not discussed here, unless questions ...)

➪ OK! Never mind! Luckily, $\exists$ many other feature maps and associated feature spaces (with very $\neq$ mathematical natures)

➪ ⚠ **There's no common rationale to establish / extract feature maps that are easy to understand!**

Reproducing kernel and feature maps

◆ **Kernel and feature maps: what do they look like?**

The dot-product (a.k.a. linear) kernel ☞ [SMDVC23]

❑ Kernel:

$$K_{\text{lin}} : \left| \begin{array}{ccc} \mathbb{R}^2 & \longrightarrow & \mathbb{R} \\ (z, z') & \longmapsto & K_{\text{lin}}(z, z') = zz' \end{array} \right.$$

❑ Feature map: ⚠ It is nonunique!

$$\begin{aligned} \forall\, z, z' \in \mathbb{R},\, K_{\text{lin}}(z, z') &= \langle \psi_1(z'), \psi_1(z) \rangle_{\mathbb{R}} \text{ with } \psi_1(z) := z \\ &= \langle \psi_2(z'), \psi_2(z) \rangle_{\mathbb{R}^2} \text{ with } \psi_2(z) := \frac{1}{\sqrt{2}}[z, z]^\top \\ &= \langle \psi_d(z'), \psi_d(z) \rangle_{\mathbb{R}^d} \text{ with } \psi_d(z) := \frac{1}{\sqrt{d}}[z, \ldots, z]^\top \end{aligned}$$

❑ Interpretation: $3 \neq$ feature spaces $(\mathbb{R}, \mathbb{R}^2, \mathbb{R}^d)$ but 3 feature maps that convey similar information ➪ here, meaningless!

Reproducing kernel and feature maps

The polynomial kernel ☞ [SMDVC23]

- Kernel:

$$K_{\text{poly}} : \left| \begin{array}{ccc} \mathbb{R}^2 & \longrightarrow & \mathbb{R} \\ (z, z') & \longmapsto & K_{\text{poly}}(z, z') = (zz' + c)^m \end{array} \right. \quad \text{with } c \in \mathbb{R}_+ \text{ and } m \in \mathbb{N}^*$$

Using binomial theorem, one has:

$$\begin{aligned} K_{\text{poly}}(z, z') &= \sum_{k=0}^{m} \binom{m}{k} (xx')^k c^{m-k} \\ &= \sum_{k=0}^{m} \left(\sqrt{\binom{m}{k}} (\sqrt{c})^{m-k} x^k \right) \left(\sqrt{\binom{m}{k}} (\sqrt{c})^{m-k} (x')^k \right) \end{aligned}$$

- Feature map: $K_{\text{poly}}(z, z') = \langle \psi_{\text{poly}}(z'), \psi_{\text{poly}}(z) \rangle_{\mathbb{R}^{m+1}}$

$$\text{with } \psi_{\text{poly}} : \left| \begin{array}{ccc} \mathbb{R} & \longrightarrow & \mathbb{R}^{m+1} \\ z & \longmapsto & \left[\sqrt{\binom{m}{k}} (\sqrt{c})^{m-k} x^k \right]_{0 \leq k \leq m} \end{array} \right.$$

- Interpretation: ψ_{poly} ➪ $m + 1$ polynomial features with increasing degrees

Reproducing kernel and feature maps

◆ Techniques for constructing new kernels

- ❑ Kernels are like "building blocks" ➪ they can be combined in order to make new kernels!
- ❑ Building valid kernels:
  - ➤ Scaling: if $\alpha \geq 0$, $K_\alpha(z, z') := \alpha K(z, z')$ is a kernel
  - ➤ Sum: $K_+(z, z') = K_1(z, z') + K_2(z, z')$ is a kernel
  - ➤ Limit: if $K_\infty(z, z') = \lim_{m \to \infty} K_m(z, z')$ exists, then K_∞ is a kernel
  - ➤ Product: $K_\times(z, z') = K_1(z, z')K_2(z, z')$ is a kernel
  - ➤ Power: $K_p(z, z') = K(z, z')^p$ is a kernel for any $p \geq 0$
  - ➤ Exponential: $K_{\exp}(z, z') = \exp[K(z, z')]$ is a kernel
  - ➤ "Sandwhich": if $f : \mathcal{Z} \to \mathbb{R}$, $K_f(z, z') = f(z)K(z, z')f(z')$ is a kernel
  - ➤ ...
- ❑ But ⚠ expliciting the feature map can be very difficult!

✎ Exercise

Starting from a very simple kernel, try to rebuild the Gaussian one!

☞ To go further: [Sut22] and [Bis06, Ch. 6, p. 296]

Links between kernels and RKHSs

◆ One-to-one mapping between kernels and RKHS

❑ Let's quickly recap:

- ➤ a **unique** reproducing kernel can be extracted from any given RKHS
- ➤ any given kernel K verifies the reproducing property for **one and only one** RKHS

☆☆ Theorem (shortened version of "Moore-Aronszajn")

For every pd function $K(\cdot, \cdot)$ on $\mathcal{Z} \times \mathcal{Z}$, there exists a unique RKHS with K as its reproducing kernel. Conversely, the reproducing kernel of an RKHS is unique and pd.

☞ To go further: [Aro50], [MFSS17, Ch. 2, Th. 2.5, p. 24] and [BTA04, Ch. 1, Th. 3, p. 19]

★★ Take-home message #1 ★★

✌ To keep in mind ✌

- We saw 4 main mathematical objects: a kernel K, a feature space $\mathcal{H}$ (RKHS), feature maps ($\psi(\cdot)$) and features ($\psi(z)$)
- If K is a (reproducing) kernel, there **always** exists a RKHS $\mathcal{G}$ and a function $\psi : \mathcal{Z} \to \mathcal{G}$ such that:

$$\forall\, z, z' \in \mathcal{Z}, K(z, z') = \langle \psi(z), \psi(z') \rangle_{\mathcal{G}}$$

- Kernel $\equiv$ inner product between feature maps in a RKHS
- The feature map is not unique! The canonical one is, often, not really informative!
- Expliciting the feature map (when possible) enables to clearly understand what is "captured" by the feature functions!

Kernel mean embedding of distributions

◆ Kernel mean embedding: a first intuition

- ❑ Roughly speaking, kernels can be used to define a sort of "(dis)similarity" between two objects (points, distributions, ...)
  - ➪ Kernels are used to **compare** two elements!
  - ➪ Usually, in UQ, we do not deal with two points, but with **probability distributions**
- ❑ Represent a point $z \in \mathcal{Z}$ as $K(\cdot, z)$: $h(z) = \langle h, K(\cdot, z) \rangle_{\mathcal{H}}$
- ❑ How to represent a distribution ν in this framework?
  - ➪ **Core idea**: to map distributions into a RKHS using a reproducing kernel!

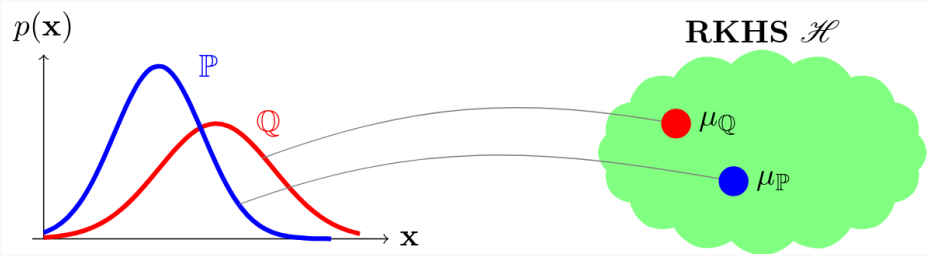


Figure 9: Embedding of two marginal distributions (source: [MFSS17]).

Kernel mean embedding of distributions

◆ Kernel mean embedding (cont'd)

❑ ⚠ I skip deliberately many details, but, only assume that:

- ➤ $\mathcal{Z}$ is always the space of our objects of interest (our **data**)
- ➤ ν is a probability measure with support in $\mathcal{Z}$ ($Z \sim \nu$)
- ➤ $\mathcal{M}_1^+(\mathcal{Z})$ is the space of all Radon probability measures ($\nu \in \mathcal{M}_1^+(\mathcal{Z})$)

❑ Represent a distribution ν:

- ➤ Consider the linear form $L_\nu : h \in \mathcal{H} \mapsto \mathbb{E}_\nu\left[h(Z)\right]$
  ➪ for any $h \in \mathcal{H}$, L_ν computes the mean value wrt. ν
- ➤ ... boundedness of the evaluation functional + Riesz representation theorem:

$$\exists!\ \mu_\nu \in \mathcal{H}, \quad \text{such that} \quad \forall\ h \in \mathcal{H}, L_\nu[h] = \langle h, \mu_\nu \rangle_{\mathcal{H}}$$

- ➤ All this process ensures that: **the initial probability measure ν admits a unique image μ_ν in the RKHS**

❑ Kernel mean embedding of ν:
➪ defined as the Riesz representation of L_ν

Kernel mean embedding of distributions

◆ **An illustration: kernel mean embedding of two probability distributions**

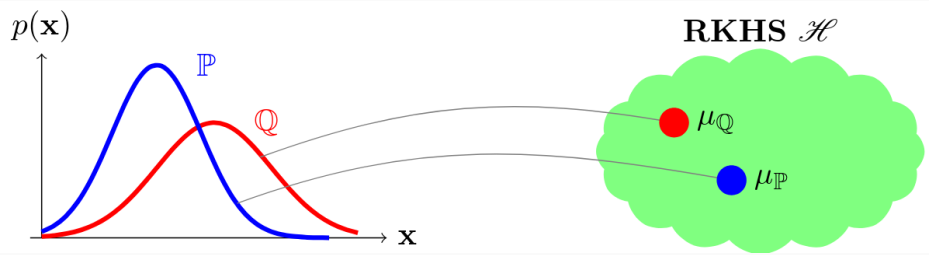


Figure 10: Embedding of two marginal distributions (source: [MFSS17]).

- (Recall) Represent a point $z \in \mathcal{Z}$ as $K(\cdot, z)$: $h(z) = \langle h, K(\cdot, z) \rangle_{\mathcal{H}}$
- Now, suppose one has $X \sim \mathbb{P}$ and $Y \sim \mathbb{Q}$
- Represent a distribution $\mathbb{P}$ as $\mu_{\mathbb{P}}$: $\mathbb{E}_{X \sim \mathbb{P}}[h(X)] = \langle h, \mu_{\mathbb{P}} \rangle_{\mathcal{H}}$
  ➪ $\mathbb{E}_{X \sim \mathbb{P}}[h(X)] = \mathbb{E}_{X \sim \mathbb{P}}[\langle h, K(\cdot, X) \rangle_{\mathcal{H}}] = \langle h, \mathbb{E}_{X \sim \mathbb{P}}[K(\cdot, X)] \rangle_{\mathcal{H}}$
  (+ assumption that $\mathbb{E}_{\mathbb{P}}\left[\sqrt{K(X, X)}\right] < \infty$)
- Thus, one has:

$$\langle \mu_{\mathbb{P}}, \mu_{\mathbb{Q}} \rangle_{\mathcal{H}} = \mathbb{E}_{X \sim \mathbb{P}, Y \sim \mathbb{Q}}[K(X, Y)]$$

- Okay! Why do we do that? ➪ **Comparing distributions!**

Maximum Mean Discrepancy

◆ Comparing two probability distributions

- ❏ Several metrics exist two compare two (or more) probability distributions (metrics, divergences, ...)
- ❏ Among this large panel of distances / divergences / metrics, one is of particular interest:
  ➪ the **Maximum Mean Discrepancy (MMD)**
- ❏ A first expression:

$$\text{MMD} : \left| \begin{array}{rcl} \mathcal{M}_1^+(\mathcal{Z}) \times \mathcal{M}_1^+(\mathcal{Z}) & \longrightarrow & \mathbb{R}_+ \\ (\nu_1, \nu_2) & \longmapsto & ||\mu_{\nu_1} - \mu_{\nu_2}||_{\mathcal{H}} \end{array} \right. \tag{2}$$

- ❏ A second (more useful) expression:

$$\begin{aligned} \text{MMD}^2(\nu_1, \nu_2) = \mathbb{E}_{\nu_1 \otimes \nu_1}\left[K(Z, Z')\right] + \mathbb{E}_{\nu_2 \otimes \nu_2}\left[K(Z, Z')\right] \\ - 2\mathbb{E}_{\nu_1 \otimes \nu_2}\left[K(Z, Z')\right] \end{aligned} \tag{3}$$

Maximum Mean Discrepancy

◆ Properties of the MMD

- ❑ MMD is a very useful tool in UQ and ML due to its interesting properties
- ❑ In short:
  - ➤ If K is a **characteristic**[3] kernel, then the mapping $\nu \mapsto \mu_\nu$ is **injective**, and thus the MMD is a **distance** on $\mathcal{M}_1^+(\mathcal{Z})$
    ➪ It gives us:

$$\mathrm{MMD}(\nu_1, \nu_2) = 0 \quad \Longrightarrow \quad \nu_1 = \nu_2 \tag{4}$$

  - ➤ Can be estimated using only samples and evaluating kernels (i.e., through Gram matrices)

[3] Not discussed in this course.

★★ Take-home message #2 ★★

✌ To keep in mind ✌

- ❏ We saw the mechanism of "kernel mean embedding"
- ❏ We can apply it to many types of data (points, distributions, ...)
- ❏ Such a tool is useful to compare, e.g., two probability distributions!
- ❏ To do so, a relevant metric exists: the **MMD**
- ❏ It has nice properties, among others:
  - ➤ being easy to estimate (because of the "kernel trick")
    - ➪ only expectations of kernels!
  - ➤ if K is **characteristic**, one has the nice property:

$$\mathrm{MMD}(\nu_1, \nu_2) = 0 \quad \Longrightarrow \quad \nu_1 = \nu_2$$

3. Kernel-based uncertainty propagation

Uncertainty propagation: a generic problem

◆ **Goal:** propagate the random vector $\mathbf{X}$ through the function g

$$\mathbb{E}[\,Y\,] = \mathbb{E}[g(\mathbf{X})] = \int_{\mathcal{D}_\mathbf{X}} g(\mathbf{x})\, f_\mathbf{X}(\mathbf{x})\, \mathrm{d}\mathbf{x} = \int_{\mathcal{D}_\mathbf{X}} g(\mathbf{x})\, \mathrm{d}\mu(\mathbf{x}) \tag{5}$$

❑ This equation can be written in terms of probability density function $f_\mathbf{X}$ or probability measure μ

❑ The integrand $g : \mathcal{D}_\mathbf{X} \to \mathbb{R}$ can be:

➤ computationally costly, nonlinear, stochastic

❑ The random input vector $\mathbf{X} \in \mathcal{D}_\mathbf{X}$ can:

➤ present a dependence structure

➤ be defined explicitly or only empirically (i.e., through a dataset)

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  - ➤ present a dependence structure
  - ➤ be defined explicitly or only empirically (i.e., through a dataset)

◆ **Remarks:**

- ❑ We can encounter this problem in various steps of the UQ framework
- ❑ It is a numerical integration problem against a density (sometimes called probabilistic integration) [BOG+19]

Approximation by a quadrature rule

A quadrature rule approximates a multivariate integral:

$$\mathbb{E}[g(\mathbf{X})] = \int_{\mathcal{D}_\mathbf{X}} g(\mathbf{x})\, f_\mathbf{X}(\mathbf{x})\, \mathrm{d}\mathbf{x} \approx \sum_{i=1}^{n} w_i\, g(\mathbf{x}^{(i)}), \quad n \in \mathbb{N} \tag{6}$$

- A quadrature rule is a weighted mean of:
  - the function g evaluated at the set of nodes $\mathbf{X}_n = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\}$
  - weighted by a set of weights $\mathbf{w}_n = \{w_1, \ldots, w_n\} \in \mathbb{R}^n$
- A "good" quadrature offers an accurate approximation for a restricted number of nodes.
- Beyond performance, convergence guarantees are essential

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- A "good" quadrature offers an accurate approximation for a restricted number of nodes.
- Beyond performance, convergence guarantees are essential

◆ **Remarks:**

- Most of the quadrature rules are built without any knowledge on the integrand g
- A strong link exists between numerical integration and space-filling design of experiments [FLQZ18]

Quadrature methods and designs of experiments

A large panel of method (see [Sul15]), among which:

- Univariate deterministic quadratures:
  - Gaussian quadrature
  - Féjer quadrature (i.e., Clenshaw-Curtis)
- Multivariate deterministic quadratures:
  - Tensor product (i.e., regular grids)
  - Smolyak grid (i.e., sparse grids)
- Latin Hypercube Sampling (LHS)
- Monte Carlo sampling
- Quasi-Monte Carlo sampling
- Kernel herding: a kernel-based sampling

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Monte Carlo

1. Generate n i.i.d samples $\mathbf{X}_n \sim f_{\mathbf{X}}$ using a pseudo-random generator (e.g., Mersenne-Twister algorithm)

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◆ **Properties:**

- ❑ The weights are all uniform
- ❑ The central limit theorem provides:
  - ➤ the variance of this estimator
  - ➤ confidence intervals of this estimator
- ❑ The convergence rate is in $o(1/\sqrt{n})$ (slow rate)
- ❑ This convergence rate does not depend on the dimension

Monte Carlo: illustration vs. regular grid

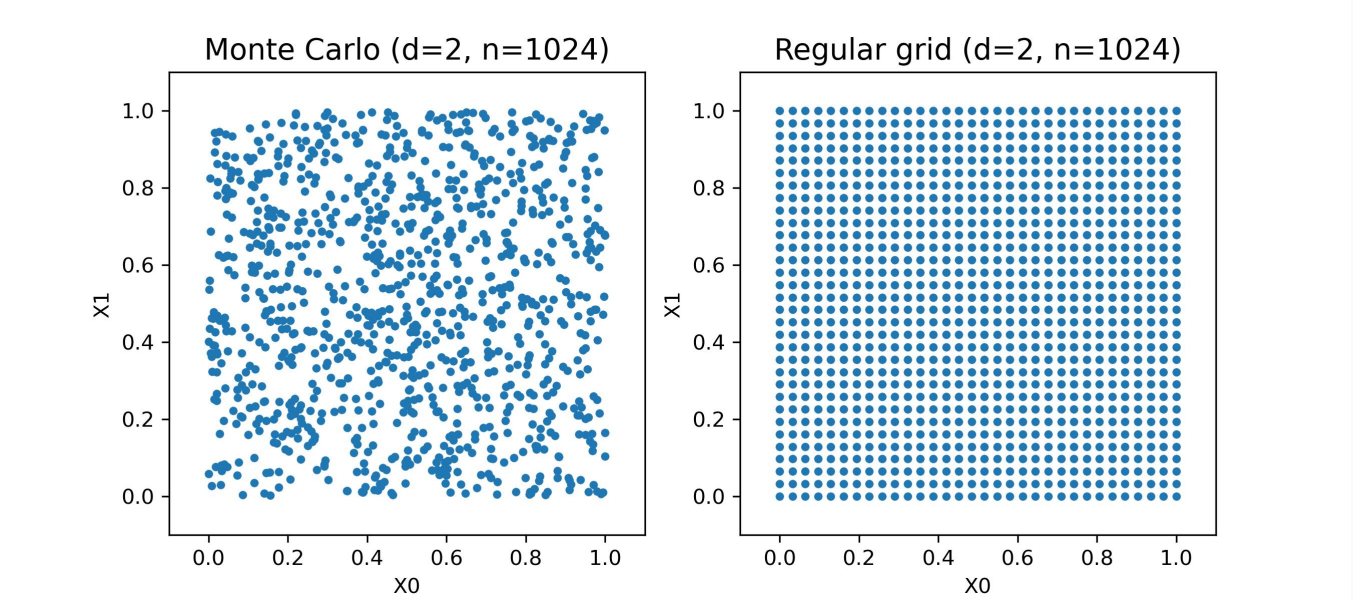

Figure 11: Sub-projection of Monte Carlo sample vs. regular grid in dim. 2 and 5.

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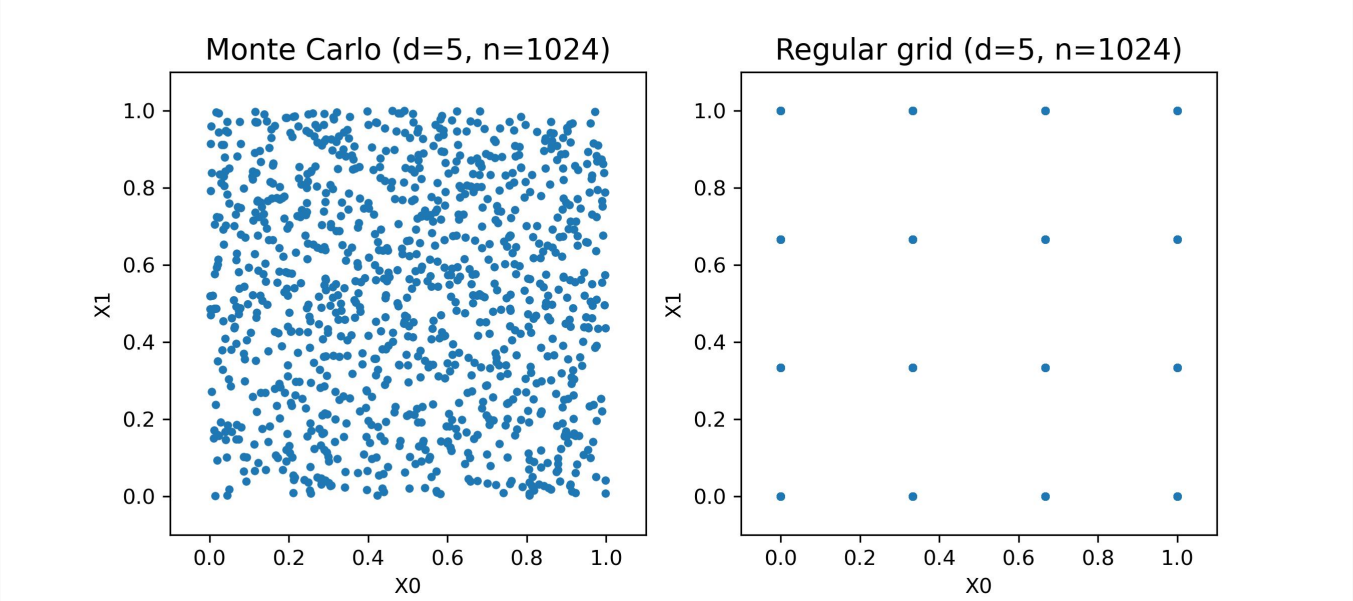

Figure 11: Sub-projection of Monte Carlo sample vs. regular grid in dim. 2 and 5.

Monte Carlo is not subject to the "curse of dimensionality"

Quasi-Monte Carlo: discrepancy and convergence guarantee

◆ Discrepancy

The discrepancy of a set of nodes $\mathbf{X}_n$ is a metric of its uniformity, e.g.:

$$D_p^*(\mathbf{X}_n) = \|\widehat{F}_{\mathbf{X}_n} - F_{\mathbf{U}}\|_p = \left(\int_{[0,1]^d} |\widehat{F}_{\mathbf{X}_n}(\mathbf{x}) - F_{\mathbf{U}}(\mathbf{x})|^p \, \mathrm{d}\mathbf{x} \right)^{1/p} \tag{8}$$

- ❑ The lowest the discrepancy, the "closest" to uniformity
- ❑ Equivalent to Kolmogorov-Smirnov statistic for $p = \infty$
- ❑ Equivalent to Cramér-Von Mises statistic for $p = 2$ (explicit formula)

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◆ Koksma-Hlawka inequality

If $g : [0,1]^d \to \mathbb{R}$ has a bounded variation, then for any $\mathbf{X}_n \in [0,1]^d$:

$$\left| \int_{[0,1]^d} g(\mathbf{x}) \mathrm{d}\mathbf{x} - \frac{1}{n} \sum_{i=1}^{n} g\left(\mathbf{x}^{(i)}\right) \right| \leq V(g) D_\infty^*(\mathbf{X}_n), \tag{9}$$

- ❑ This bound on the quadrature performance is a composed of:
  - ➤ $V(g)$, quantifying the integrand's complexity
  - ➤ $D_\infty^*(\mathbf{X}_n)$, a uniformity metric of the nodes $\mathbf{X}_n$

Quasi-Monte Carlo: low-discrepancy sequences

For numerous low-discrepancy sequences (Sobol', Halton, Faure, etc.), considering a constant $0 < C < \infty$ and specific sizes $n \in \mathbb{N}$:

$$D_{\infty}^{*}(\mathbf{X}_n) \leq C \frac{\log(n)^d}{n} \tag{10}$$

☞ To go further into quasi-Monte Carlo methods: [LP14]

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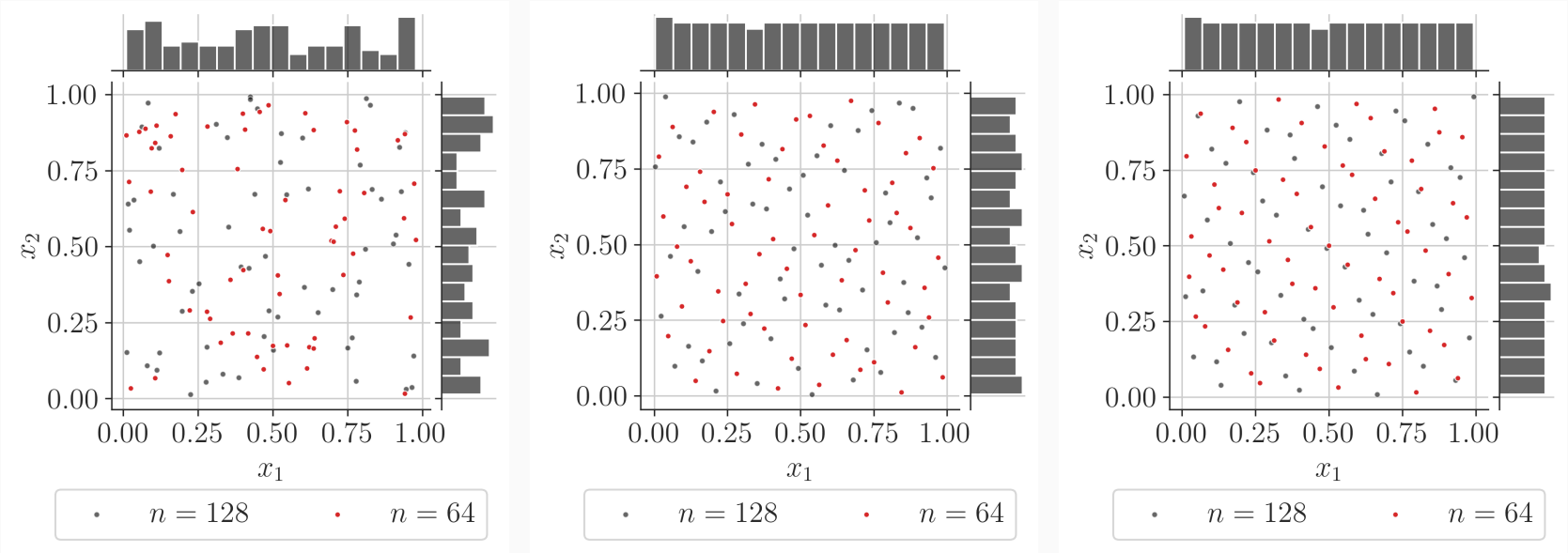
☞ To go further into quasi-Monte Carlo methods: [LP14]

◆ Properties and remarks

- ❏ Theses sequences are fully nested and deterministic
- ❏ The samples generated are not independent
- ❏ For non-uniform distribution: use inverse CDF transform
- ❏ Randomized quasi-Monte Carlo introduces a trade-off between exploration and repetitions (allowing to estimate variances [L'E18])

Quasi-Monte Carlo: low-discrepancy sequences

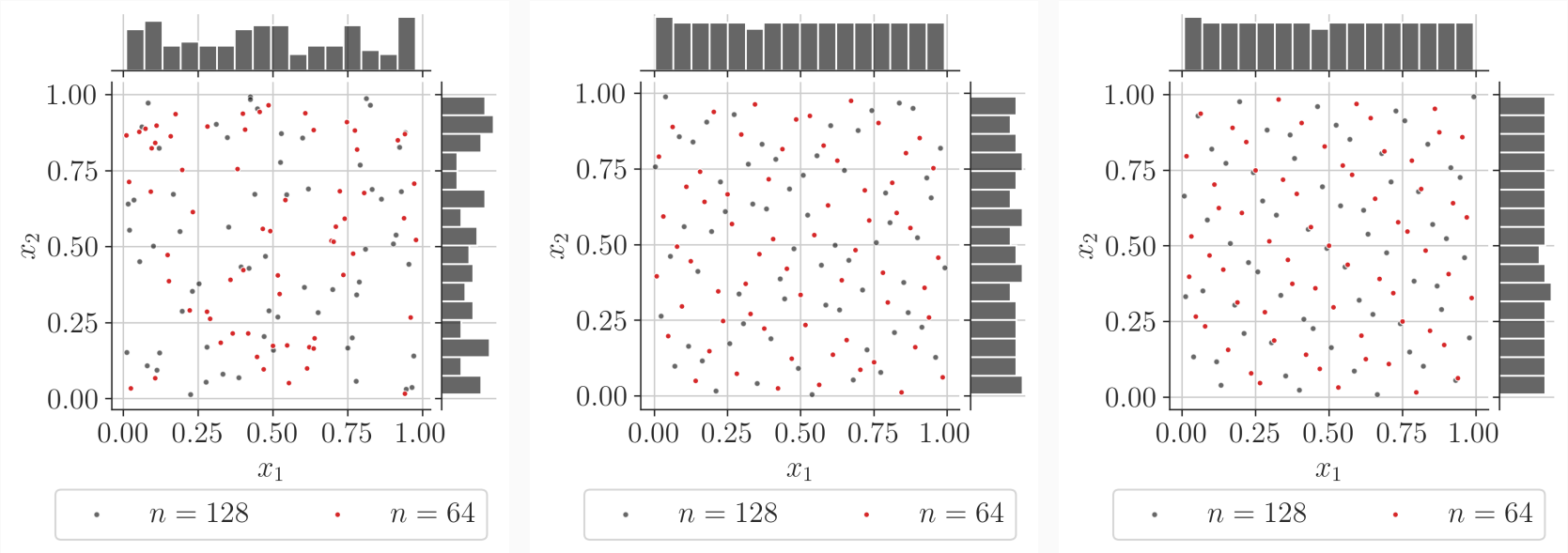


(a) Monte Carlo **(b)** Halton sequence **(c)** Sobol' sequence

Figure 12: Nested Monte Carlo and quasi-Monte Carlo designs ($n = 128$)

[4] *https://openturns.github.io/www/*

Quasi-Monte Carlo: low-discrepancy sequences



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✳ In OpenTURNS[4]:

- ❏ Sobol', Faure, Halton and Haselgrove low-discrepancy sequences
- ❏ Explicit L2-centered discrepancy

[4] *https://openturns.github.io/www/*

MMD: a generalized discrepancy [SGF+10]

- **Definition:** a discrepancy metric between any distributions μ and ζ

$$\mathrm{MMD}_K(\mu, \zeta) := \sup_{\|g\|_{\mathcal{H}(K)} \leq 1} \left| \int_{\mathcal{D}_{\mathbf{X}}} g(\mathbf{x}) \mathrm{d}\mu(\mathbf{x}) - \int_{\mathcal{D}_{\mathbf{X}}} g(\mathbf{x}) \mathrm{d}\zeta(\mathbf{x}) \right| \tag{11}$$

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1. Define a Hilbert space $\mathcal{H}(K)$ (RKHS induced by a kernel $K : \mathcal{D}_\mathbf{X}^2 \mapsto \mathbb{R}_+$)
2. The *maximum mean discrepancy* (MMD) between two probability distributions μ and ζ is given by the worst-case error for any function within $\mathcal{H}(K)$
3. For characteristic kernels, $\mathrm{MMD}_K(\mu, \zeta) = 0 \Leftrightarrow \mu = \zeta$
4. The MMD can be written as a simple difference of potentials $P_\mu(\mathbf{x}) := \int_{\mathcal{D}_\mathbf{X}} K(\mathbf{x}, \mathbf{x}') \mathrm{d}\mu(\mathbf{x}')$ of the distributions $\mathrm{MMD}_K(\mu, \zeta) = \left\| P_\mu - P_\zeta \right\|_{\mathcal{H}(K)}$

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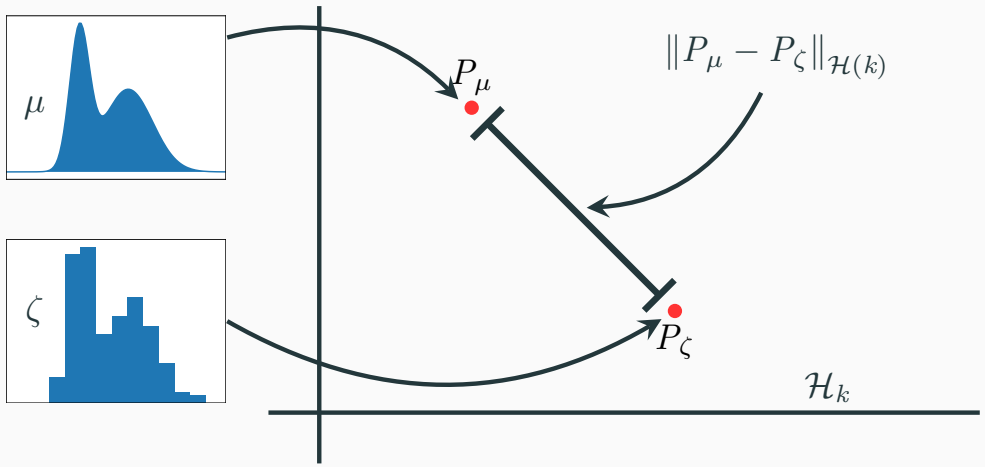

Figure 13: Kernel mean embedding of continuous and discrete distributions

Kernel herding sampling[CWS10]

- **Main idea:** iteratively pick points minimizing a MMD between the:
  - target density μ,
  - current design $\mathbf{X}_n$, represented by the density $\zeta_n = \frac{1}{n}\sum_{i=1}^{n} \delta(\mathbf{x}^{(i)})$
- **Kernel herding criterion:**

$$\mathbf{x}^{(n+1)} \in \underset{\mathbf{x}\in\mathcal{D}_\mathbf{X}}{\arg\min} \left\{ \mathrm{MMD}_K \left(\mu, \frac{1}{n+1}\left(n\zeta_n + \delta(\mathbf{x})\right)\right)^2 \right\} \Rightarrow \underset{\mathbf{x}\in\mathcal{D}_\mathbf{X}}{\arg\min} \left\{ \frac{n}{n+1} P_{\zeta_n}(\mathbf{x}) - P_\mu(\mathbf{x}) \right\} \tag{12}$$

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◆ **Candidate set $\mathcal{S}$:** is a N-sized sample ($N \gg n$) representative of μ

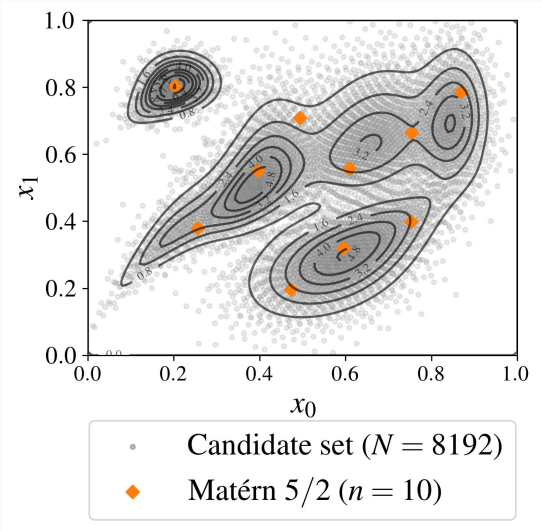
- ❑ use as a discrete domain for a greedy optimization
- ❑ used to estimate the potential $P_\mu(\mathbf{x}), \forall \in \mathcal{S}$

$$\mathbf{x}^{(n+1)} \in \arg\min_{\mathbf{x}\in\mathcal{S}} \left\{ \frac{1}{n+1}\sum_{i=1}^{n} K((\mathbf{x}, \mathbf{x}^{(i)}) - \frac{1}{N}\sum_{j=1}^{N} K(\mathbf{x}, \mathbf{x}^{(j)}) \right\} \tag{13}$$

☞ Theoretical convergence studied in [LJLB15]

Kernel herding: 2D example

- Gaussian mixture with a dependence structure



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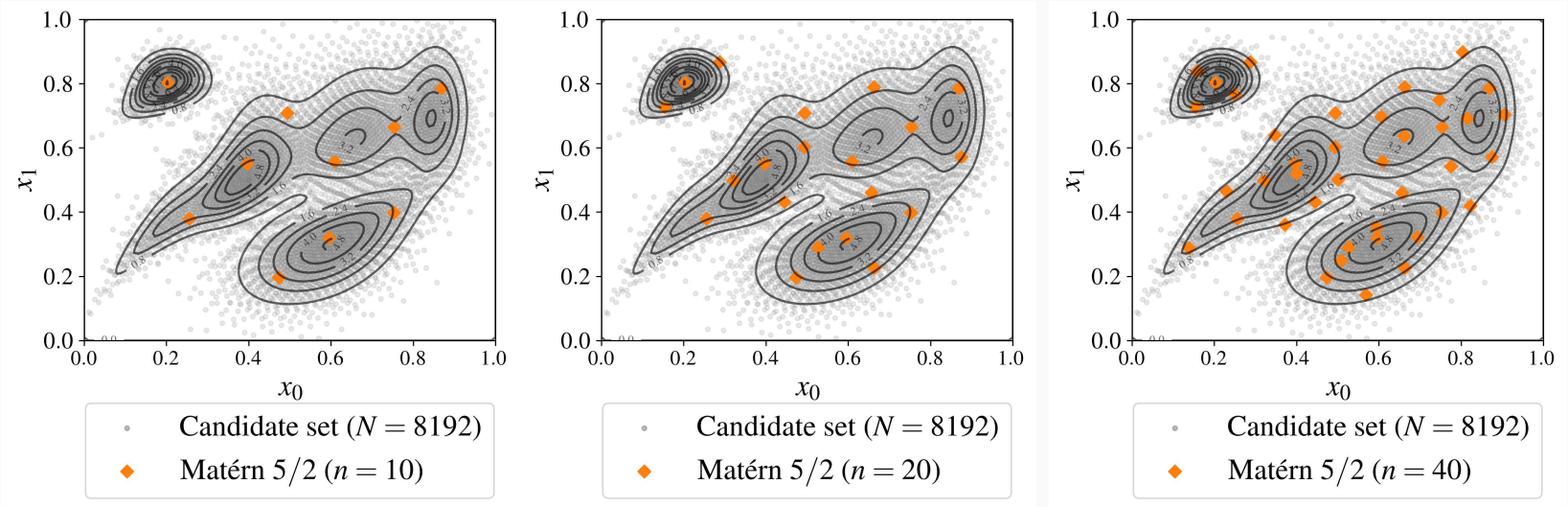

Figure 14: Kernel herding sampling on a Gaussian random mixture

Kernel herding: 2D example

Input random vector: Gaussian mixture $\mathbf{X}$ from Fig.14

Function: $g(\mathbf{x}) = x_1 + x_2$

Quantity of interest: $\mathbb{E}[g(\mathbf{X})] = \int_{\mathcal{D}_\mathbf{X}} g(\mathbf{x}) f_\mathbf{X}(\mathbf{x}) \, \mathrm{d}\mathbf{x}$

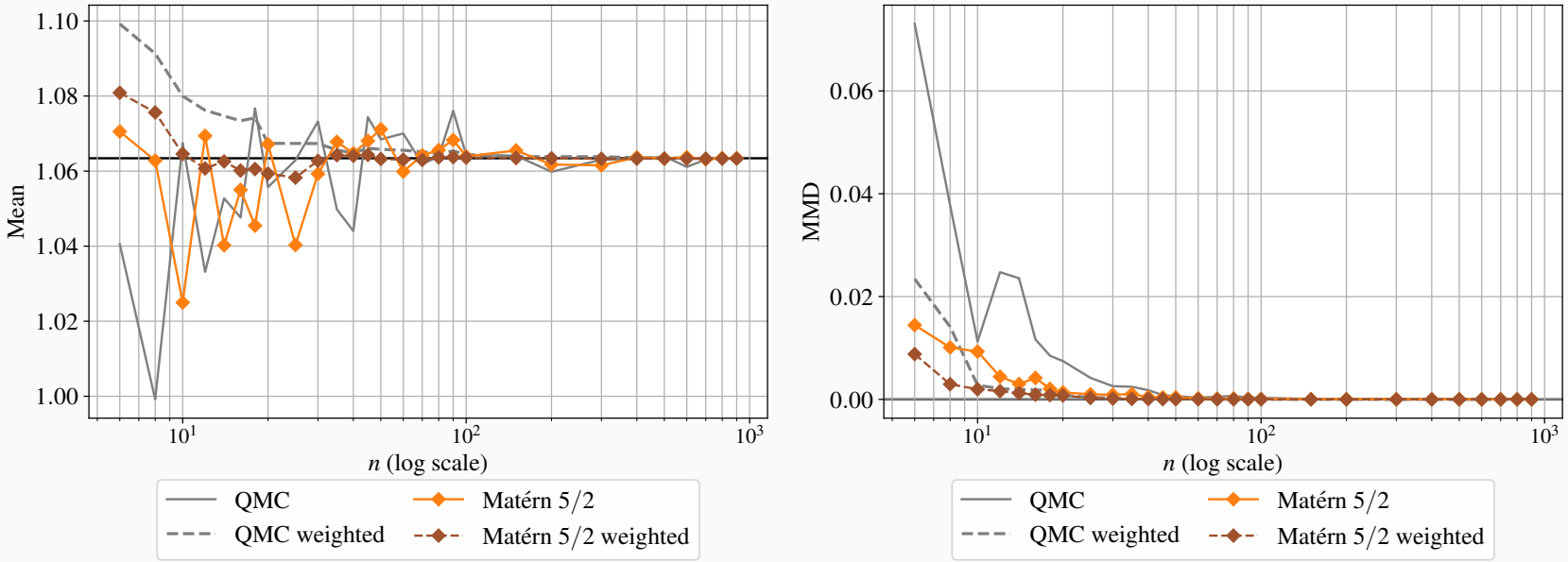

Figure 15: Analytical benchmark results on the toy-case #1

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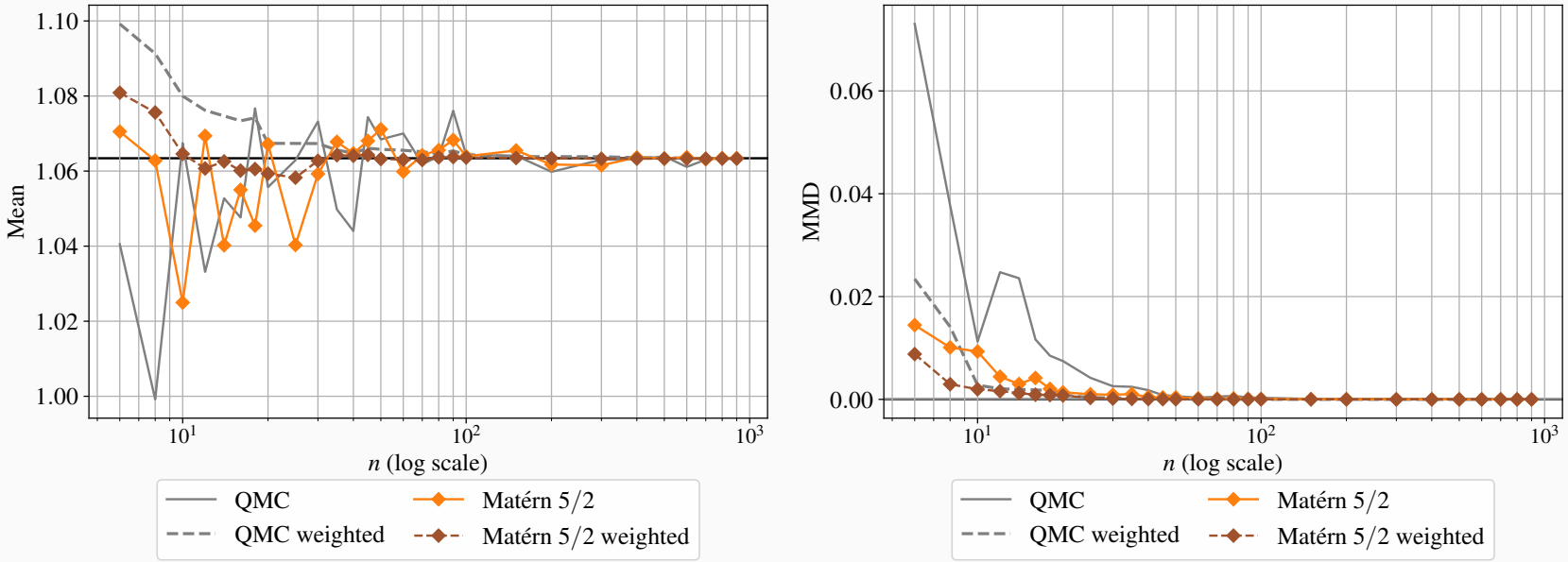


Figure 15: Analytical benchmark results on the toy-case #1

✳ **In OpenTURNS**: New dedicated Python package *otkerneldesign*

```
~$ pip install otkerneldesign
```

Kernel herding: application to probabilistic fatigue of OWT

Kernel herding extracts a representative subset from data [FCMI23]

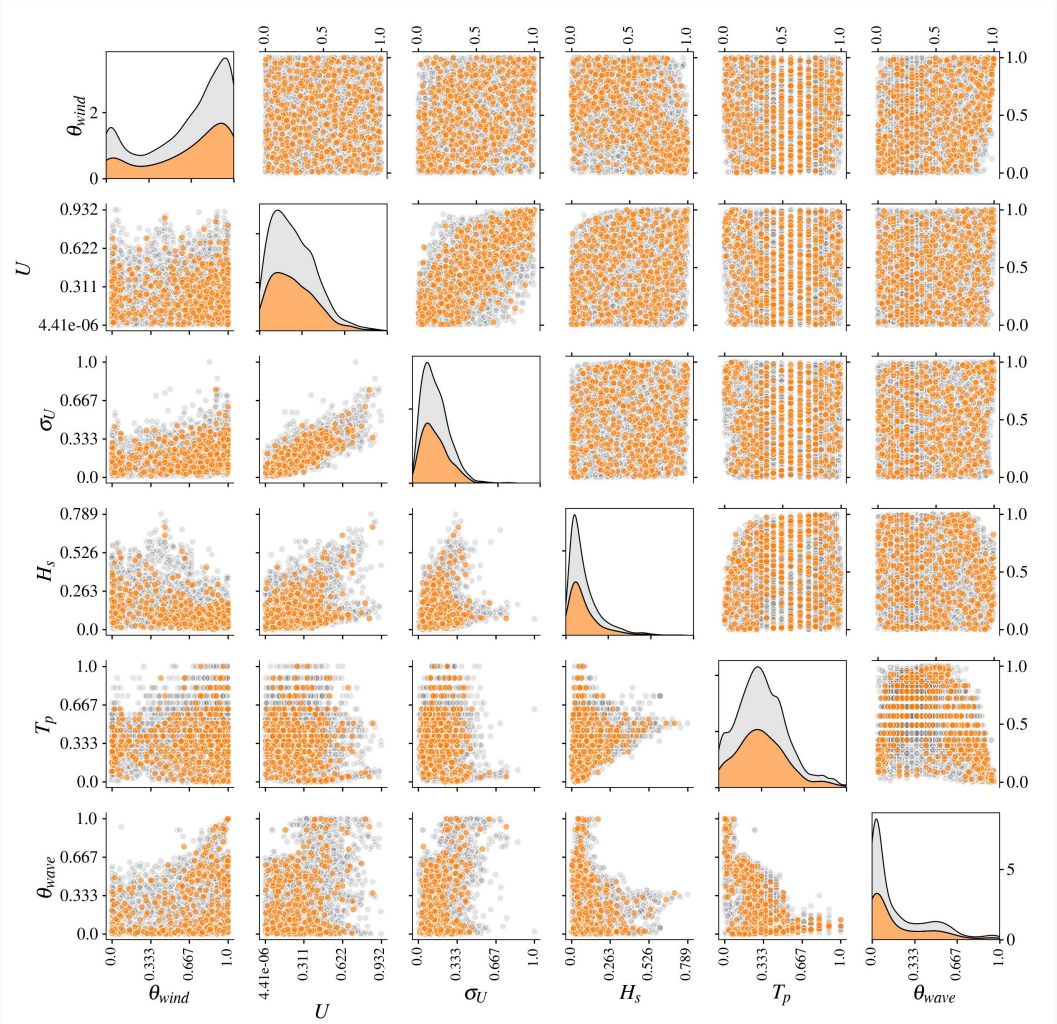


Figure 16: Teesside kernel herding design of experiments

Kernel herding: application to probabilistic fatigue of OWT

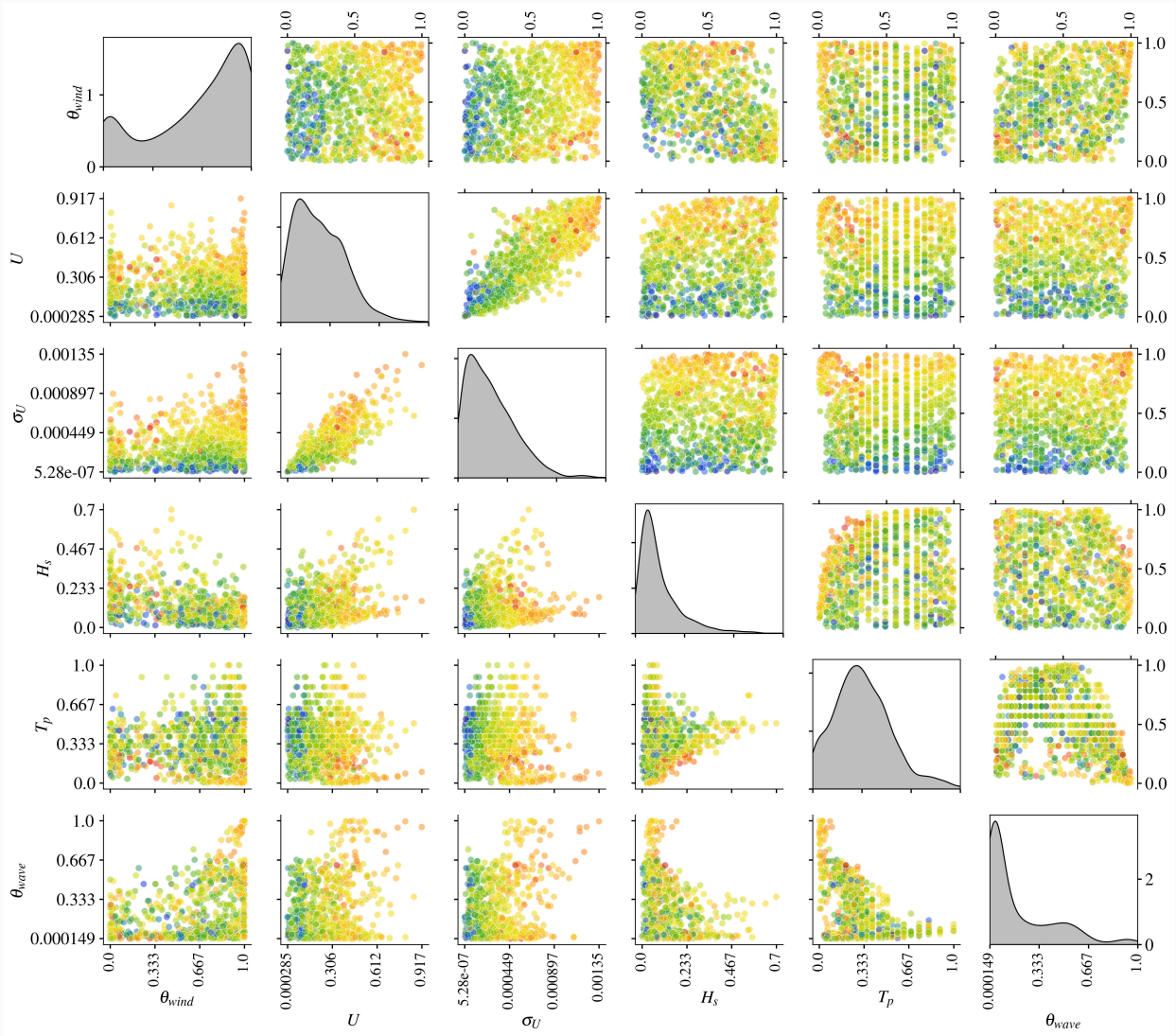


Figure 17: Teesside kernel herding with corresponding outputs (log-scale)

Kernel herding: application to probabilistic fatigue of OWT

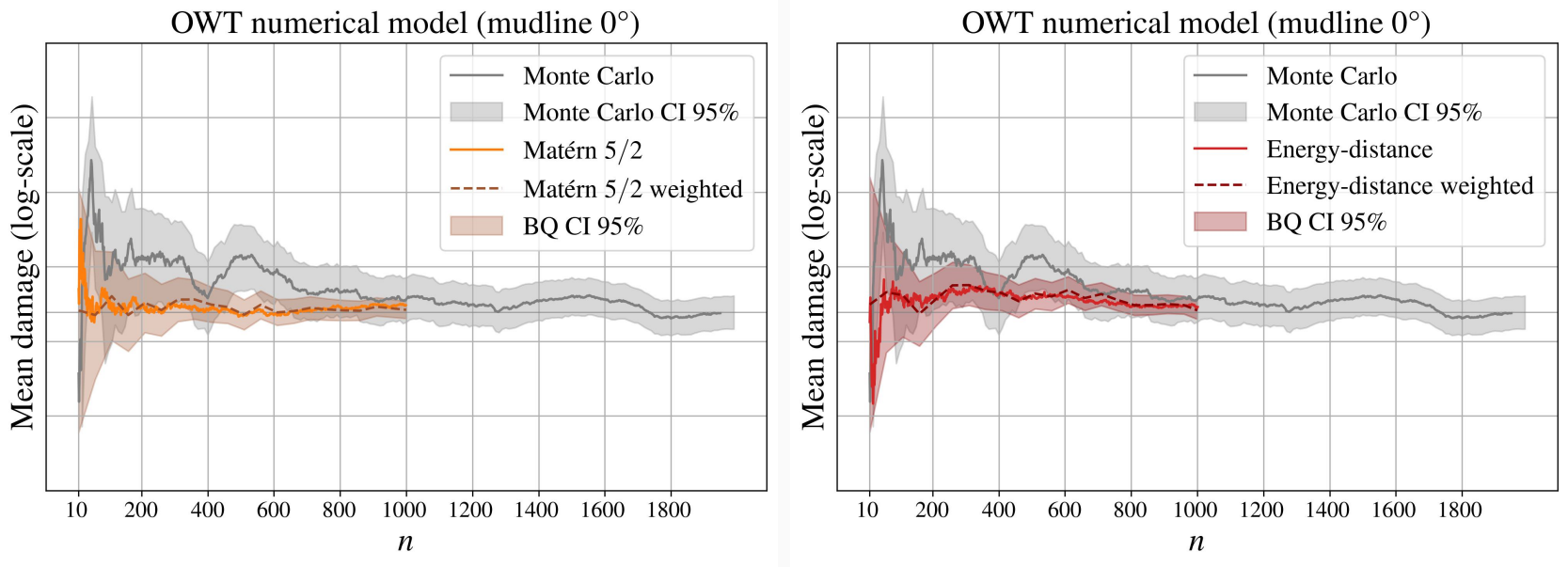


Figure 18: Kernel herding mean convergence (Matérn and energy-distance kernels) (size $n = 500$)

◆ **Remark:** The "BQ IC" is actually a prediction interval

★★ Take-home message #3 ★★

✌ To keep in mind ✌

- **Conclusions**
  - ➤ Kernel herding for quadrature offers a given-data uncertainty propagation method (i.e., without fitting a probabilistic model)
  - ➤ This method can fully exploit parallel computing (i.e., not active)
  - ➤ Possible to compute optimal Bayesian quadrature weights

★★ Take-home message #3 ★★

✌ To keep in mind ✌

- **Conclusions**
  - ➤ Kernel herding for quadrature offers a given-data uncertainty propagation method (i.e., without fitting a probabilistic model)
  - ➤ This method can fully exploit parallel computing (i.e., not active)
  - ➤ Possible to compute optimal Bayesian quadrature weights
- **Limits**
  - ➤ KH is sensitive to the chosen kernel (heuristic tuning in [FIM+23])
  - ➤ In high dimension, $\mathcal{S}$ must be larger, KH becomes costly

4. Kernel-based sensitivity analysis

Challenges in GSA

- **A few issues / challenges in standard GSA practice**
  - Output variance might not be really insightful!
  - High computational cost (e.g., 1 call $\approx$ from a few hours to a day)
  - Large number of inputs (e.g., ≈ 100 inputs)
  - Quantity of interest (QoI) possibly difficult to estimate accurately (e.g., high-order quantile, rare event probability)
  - Input and output variables may not be continuous (e.g., discrete / categorical variables, graphs, distributions)
  - (Input dependency) ➪ Another course!

GSA using the Hilbert-Schmidt Independence Criterion

◆ A few preliminary hypotheses

❑ Probabilistic modeling of d **independent** input physical variables:

$$\mathbf{X} = (X_1, X_2, \ldots, X_d)^\top \sim \mathbb{P}_{\mathbf{X}} \quad \text{over} \quad \mathcal{X} = \bigtimes_{i=1}^{d} \mathcal{X}_i \tag{14}$$

❑ Black-box model (scalar output):

$$\mathcal{M} : \left| \begin{array}{rcl} \mathcal{X} \subseteq \mathbb{R}^d & \longrightarrow & \mathcal{Y} \subseteq \mathbb{R} \\ \mathbf{X} & \longmapsto & Y = \mathcal{M}(\mathbf{X}) \end{array} \right. \tag{15}$$

❑ **Learning sample** ➪ a n-size i.i.d. sample of the couple $(\mathbf{X}, Y)$:

$$\left(\mathbf{X}^{(j)}, Y^{(j)}\right)_{(1 \leq j \leq n)} = \left(X_1^{(j)}, X_2^{(j)}, \ldots, X_d^{(j)}, Y^{(j)}\right)_{(1 \leq j \leq n)} \tag{16}$$

with $\mathbb{P}_{\mathbf{X}^{(j)}} = \mathbb{P}_{\mathbf{X}}$
and $Y^{(j)} = \mathcal{M}\left(X_1^{(j)}, X_2^{(j)}, \ldots, X_d^{(j)}\right), \forall j \in \{1, \ldots, n\}$

GSA using the Hilbert-Schmidt Independence Criterion

◆ Dependence measures for GSA

- ❑ A first idea:
  - ➤ If X_i has **no influence** on $Y \Leftrightarrow X_i$ and Y are **independent**
- ❑ Two possibilities:
  - ➤ By comparing $\mathbb{P}_Y$ and $\mathbb{P}_{Y|X_i} \Rightarrow$ **Dissimilarity measures**
  - ➤ By comparing $\mathbb{P}_{(Y,X_i)}$ and $\mathbb{P}_Y \otimes \mathbb{P}_{X_i} \Rightarrow$ **Dependence measures**
- ❑ Use of a specific dependence measure:
  - ➤ The **Hilbert-Schmidt Independence Criterion** (**HSIC**) proposed in the ML community in ~ 2005 ☞ [GHS+05]
  - ➤ Brought to the GSA community in ~ 2015 ☞ [DV15]

GSA using the Hilbert-Schmidt Independence Criterion

◆ Dependence measures for GSA (cont'd)

❑ We would like to quantify the sensitivity between X_i and Y using a dependence measure, such that:

$$S_i = d(\mathbb{P}_{(Y,X_i)}, \mathbb{P}_Y \otimes \mathbb{P}_{X_i}) \tag{17}$$

where:

- ➤ $\mathbb{P}_{(Y,X_i)}$ is the joint probability distribution
- ➤ $\mathbb{P}_Y \otimes \mathbb{P}_{X_i}$ is the product of marginals distributions

❑ Two desirable properties we are looking for:

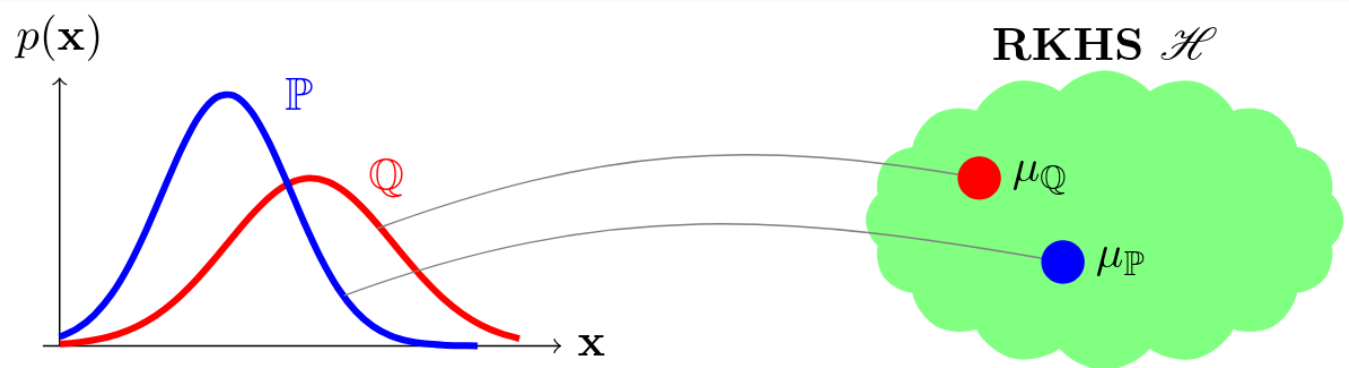
- ➤ large values of S_i imply strong dependence between X_i and Y
- ➤ $S_i = 0$ only if X_i and Y are independent

↪ How to define such a dependence measure between probability distributions?

GSA using the Hilbert-Schmidt Independence Criterion

◆ **(Recall) How to compare probability distributions?**

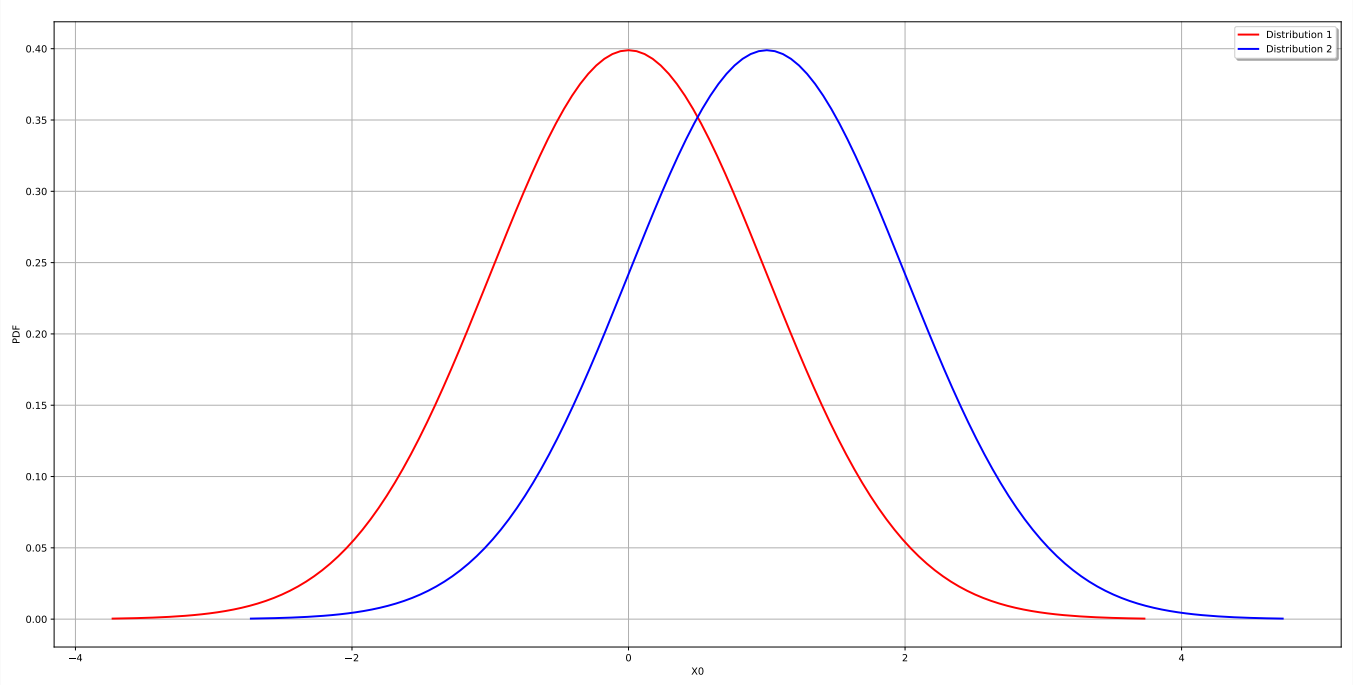
- ❑ By comparing various **features** of the distributions
- ❑ In practice, we map the distributions onto auxiliary spaces characterizing specific features
  - ➤ Feature functions $\psi(\mathbb{P}_{X_i})$, e.g., mean of the distribution $\psi(\mathbb{P}_{X_i}) = \mathbb{E}[X_i]$
- ❑ We can then compute the dependence as a function of the distance between distributions as a distance between their mappings



GSA using the Hilbert-Schmidt Independence Criterion

◆ A first example

Let us consider the following mapping: $\psi(\mathbb{P}_{X_i}) = \mathbb{E}[X_i]$

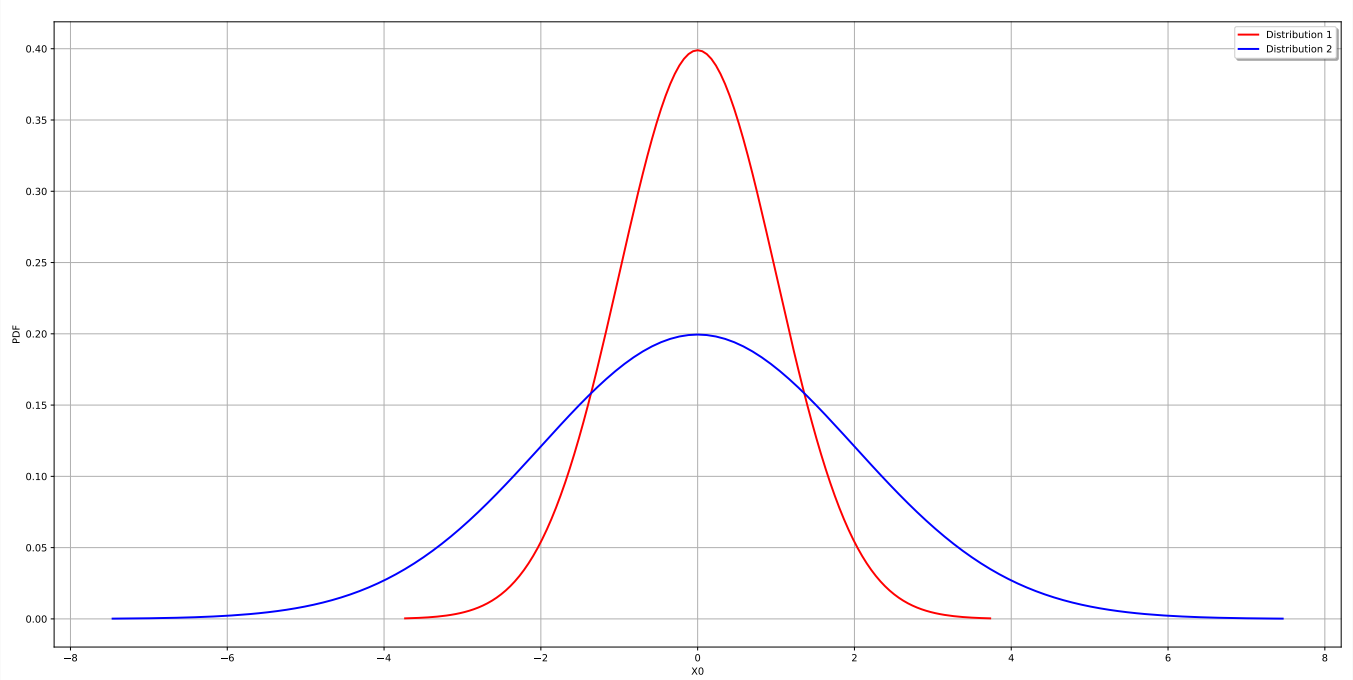


↪ Here, this approach would work ➪ we can distinguish the two distributions ✔

GSA using the Hilbert-Schmidt Independence Criterion

◆ A first example (cont'd)

Let us consider the following mapping: $\psi(\mathbb{P}_{X_i}) = \mathbb{E}[X_i]$

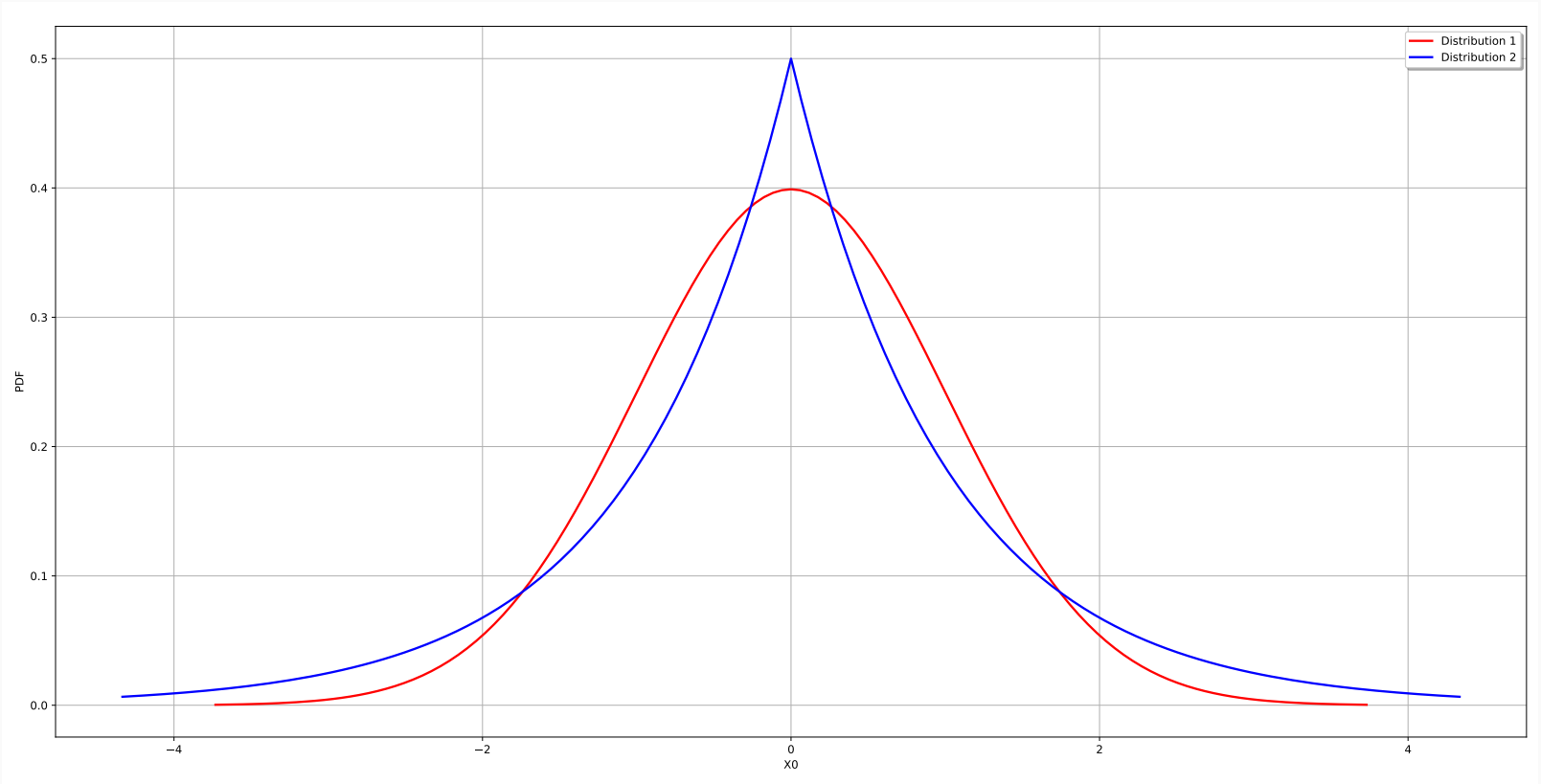


↪ Here, this approach would not work ➪ we cannot distinguish the two distributions ✘

GSA using the Hilbert-Schmidt Independence Criterion

◆ A first example (cont'd)

Let us consider the following mapping: $\psi(\mathbb{P}_{X_i}) = (\mathbb{E}[X_i], \mathrm{Var}\,(X_i))$



↪ Also in this case, we are not able to distinguish between two different distributions ✘

GSA using the Hilbert-Schmidt Independence Criterion

Limitations

For any finite number of features, there will always be, at least, 2 different distributions which appear identical with respect to the considered features!

➪ **Can we look at an infinite collection of features?**

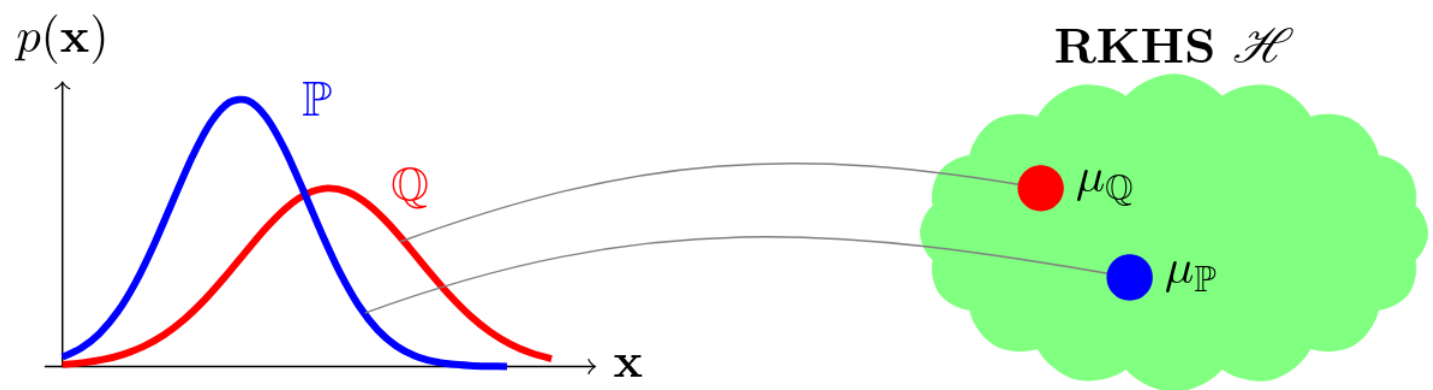
↪ **Yes, using kernel mean embedding!**

GSA using the Hilbert-Schmidt Independence Criterion

◆ Theoretical formulation

- ❑ Let us now consider $\mathcal{V}$, an RKHS over $\mathcal{X} \times \mathcal{Y}$ with kernel $V(\cdot, \cdot)$
- ❑ We consider the mean embedding of $\mathbb{P}_Y \mathbb{P}_{X_i}$ and $\mathbb{P}_{(Y, X_i)}$ in $\mathcal{V}$

$$\Delta := ||\mu_{\mathbb{P}_{(Y,X_i)}} - \mu_{\mathbb{P}_Y \mathbb{P}_{X_i}}|| \tag{18}$$



Characteristic kernels ⇒ Injective feature map

GSA using the Hilbert-Schmidt Independence Criterion

◆ **Theoretical formulation (cont'd)**

❑ Assuming $V((Y, X_i), (Y', X_i')) = K(Y, Y')K_i(X_i, X_i')$, we can show that:

$$\mathrm{HSIC}(X_i, Y)_{\mathcal{F}_i,\mathcal{G}} = \Delta^2 \tag{19}$$

$$\mathrm{HSIC}(X_i, Y)_{\mathcal{F}_i,\mathcal{G}} = \mathbb{E}\left[K_i(X_i, X_i')K(Y, Y')\right] + \mathbb{E}\left[K_i(X_i, X_i')\right]\mathbb{E}\left[K(Y, Y')\right] - 2\mathbb{E}\left[\mathbb{E}[K_i(X_i, X_i')|X_i]\,\mathbb{E}[K(Y, Y')|Y]\right]$$

where (X_i', Y') is an i.i.d. copy of (X_i, Y)

GSA using the Hilbert-Schmidt Independence Criterion

◆ Estimators

❑ A first estimator based on V-statistics ☞ [GHS+05]

$$\widehat{\mathrm{HSIC}}(X_i, Y) = \frac{1}{n^2}\mathrm{Tr}(L_i H L H) \tag{20}$$

where L_i and L are Gram matrices, and H a shift matrix

❑ A second estimator based on the distance correlation estimator ☞ [SRB07]

$$\widehat{\mathrm{HSIC}}(X_i, Y) = \frac{1}{n^2}\sum_{j_1, j_2}^{n} A_{j_1 j_2} B_{j_1 j_2} \tag{21}$$

where $A_{j_1 j_2}$ and $B_{j_1 j_2}$ are linear combinations of Gram matrices

★★ Take-home message #4 ★★

✌ To keep in mind ✌

- **A fundamental property** ➪ if **characteristic** kernels

$$\mathrm{HSIC}(X_i, Y)_{\mathcal{F}_i,\mathcal{G}} = 0 \Leftrightarrow X_i \perp Y \tag{22}$$

- **A plug-in estimator of a normalized sensitivity index** ☞ [DV15]

$$\widehat{R^2_{\mathrm{HSIC},i}} = \frac{\widehat{\mathrm{HSIC}}(X_i, Y)}{\sqrt{\widehat{\mathrm{HSIC}}(X_i, X_i)\,\widehat{\mathrm{HSIC}}(Y, Y)}} \tag{23}$$

- **Choose a characteristic kernel** $\rightarrow$ Type + Hyperparameters' estimation

$$K(z, z') = \exp\left(-\theta \|z - z'\|_2^2\right) \quad \text{(Gaussian kernel)} \tag{24}$$

with $\widehat{\theta} = 1/\widehat{\sigma^2}$ ($\widehat{\sigma^2}$ the empirical variance of the sample z)

Screening and ranking using HSIC

◆ **Screening with HSIC for high-dimensional problems**

❑ A definition of "screening":

➤ Separating the inputs between two distinct groups:
the **significantly influential** ones vs. the **non-influential** ones

❑ In the HSIC framework, one possible solution:

➤ To use some **statistical hypothesis tests** to determine whether the variables X_i and Y are independent or not ☞ [DLM16]

Screening and ranking using HSIC

◆ Statistical hypothesis testing with HSIC

❑ Due to the fundamental property of HSIC (cf. Eq. (9)):

➤ One can construct the following statistical test $\mathcal{T}$

$$\mathcal{T} : \text{Test } (H_{0,i}) : \text{HSIC}(X_i,\, Y) = 0 \quad \text{vs.} \quad (H_{1,i}) : \text{HSIC}(X_i,\, Y) > 0 \tag{25}$$

$H_{0,i}$: X_i and Y are independent

➤ And choose $\widehat{S}_{\mathcal{T}} := n \times \widehat{\text{HSIC}}(X_i,\, Y)$ as the test statistic

❑ To decide, one can use the **p-value** associated to the test $\mathcal{T}$:

➤ It is the probability, under $(\mathcal{H}_{0,i})$, that $\widehat{S}_{\mathcal{T}}$ becomes greater or equal to the observed $\widehat{S}_{\mathcal{T},\text{obs}}$ statistic on the learning sample

$$p_{\text{val}} = \mathbb{P}\left(\widehat{S}_{\mathcal{T}} \geq \widehat{S}_{\mathcal{T},\text{obs}} \mid \mathcal{H}_{0,i}\right) \tag{26}$$

Screening and ranking using HSIC

◆ Statistical hypothesis testing with HSIC

$$p_{\text{val}} = \mathbb{P}\left(\widehat{S}_{\mathcal{T}} \geq \widehat{S}_{\mathcal{T},\text{obs}} \mid H_{0,i}\right) \tag{27}$$

In other words : What is the probability of obtaining a HSIC(X_i, Y) value as large as the observed one under the assumption that Y and X_i are independent?

- ❑ To discriminate, one uses the **significance level** α (a.k.a. Type I error):
  - ➤ Typically, one can fix this level: $\alpha = 0.05$ (or $\alpha = 0.10$)
  - ➤ **Decision rule**: if $p_{\text{val}} < \alpha \Rightarrow H_{0,i}$ (i.e., independence) is rejected

  The probability of obtaining the observed HSIC(X_i, Y) value is low
  $\rightarrow$ The independence hypothesis is most likely wrong
  $\rightarrow$ X_i **has a non negligible influence on** Y

Screening and ranking using HSIC

◆ Asymptotic test for large sample size

In order to estimate how unlikely a value of $n\widehat{\mathrm{HSIC}}(X_i, Y)$ is, we can use its probability distribution

- ❑ Asymptotic results about the HSIC estimators:
  - ➤ The $n\widehat{\mathrm{HSIC}}(X_i, Y)$ estimator can be reasonably approached by a **Gamma distribution** parametrized by (γ, β) ☞ [GFT+08]
- ❑ **Asymptotic test $\mathcal{T}_{\mathrm{asymp}}$:**
  - ➤ Therefore, the p-value can be approximated as follows:

$$p_{\mathrm{val}} \approx 1 - F_{\mathrm{Ga}}\left(n \times \widehat{\mathrm{HSIC}}(X_i, Y)_{\mathrm{obs}}\right) \tag{28}$$

where $F_{\mathrm{Ga}}(\cdot)$ is the CDF of the Gamma distribution and $\widehat{\mathrm{HSIC}}(X_i, Y)_{\mathrm{obs}}$ is the observed value of the random variable $\widehat{\mathrm{HSIC}}(X_i, Y)$

Screening and ranking using HSIC

- Asymptotic test for large sample size

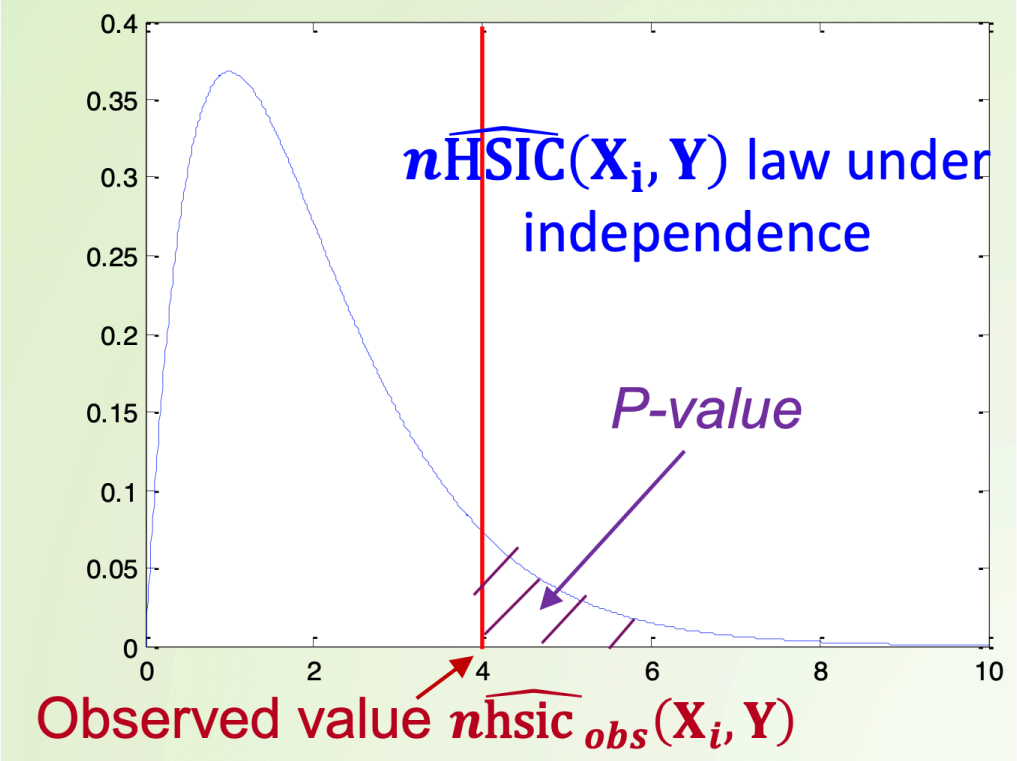


Figure 19: Asymptotic law of the HSIC estimator (source: [Mar21]).

Screening and ranking using HSIC

◆ **Non-asymptotic test for small sample size**

❑ **Permutation-based test $\mathcal{T}_{\text{perturb}}$** ☞ [DLM16]

- ➤ $Z_n := \left(X^{(j)}, Y^{(j)}\right)_{(1 \leq j \leq n)}$ an initial n-sample and $\widehat{\text{HSIC}}(Z_n)$
- ➤ $\{\tau_1, \ldots, \tau_B\}$, a set of B independent random permutations of $\{1, \ldots, n\}$
- ➤ We consider $\widehat{H}^{*b} := \widehat{\text{HSIC}}\left(X^{(j)}, Y^{(\tau_b(j))}\right)_{(1 \leq j \leq n)}$
- ➤ And the order statistic:

$$\widehat{H}^{*(1)} \leq \widehat{H}^{*(2)} \leq \cdots \leq \widehat{H}^{*(B)} \tag{29}$$

- ➤ The p-value (under $\mathcal{H}_{0,i}$) can be approximated as follows:

$$p_{\text{val}} \approx \frac{1}{B} \sum_{b=1}^{B} \mathbb{1}_{\widehat{H}^{*b} > \widehat{\text{HSIC}}(X,Y)} \tag{30}$$

If X_i and Y are independent, considering a permutation of Y should have no impact

Screening and ranking using HSIC

- **A heuristic procedure for ranking the variables**
  - Ranking the input variables w.r.t. their influence using the p-values:
    - **The lower $p_{\mathbf{val}}$ is, the stronger $(\mathcal{H}_{0,i})$ is rejected**
      $\Rightarrow$ the higher the influence of X_i
  - Rule for ranking:
    - **Increasing order of influence by decreasing order of p-values**
    - **If p-values are equal**
      $\rightarrow$ variables are ordered by increasing order of $\widehat{R^2_{\mathrm{HSIC},i}}$

★★ Take-home message #5 ★★

✌ To keep in mind ✌

- **Screening**
  - If n is large ($n > n_{\text{th}}$), $\rightarrow$ **asymptotic test**
  - If not ($n \leq n_{\text{th}}$), $\rightarrow$ **permutation-based test**
- "**Tuning parameters**"

  $n_{\text{th}} = 10^3$, $B = 200$, $\alpha = 0.05$
- **Ranking**
  - $\nearrow$ influence, $\searrow$ p-values
  - If $p_{\text{val},i} = p_{\text{val},j}$, check $\widehat{R^2_{\text{HSIC},i}}$ and $\widehat{R^2_{\text{HSIC},j}}$
- Details in this paper ☞ [DLM16]

Target SA using HSIC

◆ Target Sensitivity Analysis (TSA)

❑ Basic underlying idea of TSA:

➤ To measure the influence of the inputs on a **critical domain** of the model output, and in particular, over the **occurrence** of the critical phenomenon ☞ [RM18, MC21]

❑ **Target $\rightarrow$ critical domain/event on the model output**:

➤ $\mathcal{C} \subset \mathcal{Y}$ a critical domain such that $\mathbb{P}(Y \in \mathcal{C})$ is small

➤ Critical measure of $Y \rightarrow \mathcal{R}(Y)$ (risk measure)

➤ High-order quantile $\rightarrow \mathcal{C} := \{y \in \mathcal{Y} \mid y > \mathcal{R}(y)\}$ and $\mathcal{R}(Y) = q_{0.9}(Y)$

❑ TSA with HSIC:

➤ **Indicator function** $\mathbb{1}_{\mathcal{C}} : \mathcal{Y} \rightarrow \{0, 1\}, y \mapsto 1$ if $y \in \mathcal{C}$, 0 otherwise ☞ [DV15]

$\Rightarrow$ Use Dirac kernel

➤ **Smooth weight function** $w_{\mathcal{C}} : \mathcal{Y} \rightarrow [0, 1], y \mapsto \exp\left(-d_{\mathcal{C}}(y)/s\right)$

$\Rightarrow$ Use Gaussian kernel

★★ Take-home message #6 ★★

✌ To keep in mind ✌

❑ **Focusing on the critical domain**

- ➤ Either an indicator function or a weith function on Y
- ➤ Typical weight function "around" the binary threshold

$$w_{\mathcal{C}} : \left| \begin{array}{ccc} \mathcal{Y} & \longrightarrow & [0,1] \\ y & \longmapsto & w_{\mathcal{C}}(y) = \exp\left(-\frac{\max(c-y,\,0)}{s\,\sigma_Y}\right) \end{array} \right. \tag{31}$$

with $s = \frac{1}{5}$ a smoothness parameter and σ_Y the empirical estimation of the std of Y

❑ **A Target-HSIC index under** $w_{\mathcal{C}}(\cdot)$

$$\mathrm{T-HSIC}_{w_{\mathcal{C}}}(X_i,\, Y) = \mathrm{HSIC}(X_i,\, w_{\mathcal{C}}(\,Y)) \tag{32}$$

❑ More details in this paper ☞ [MC21]

Conditional SA using HSIC

◆ Conditional Sensitivity Analysis (CSA)

❑ Basic underlying idea of CSA:

➤ To measure the influence of the inputs within a **critical domain** of the model output, ignoring what happens outside ☞ [MC21]

❑ **Conditional $\rightarrow$ conditional to a critical event**:

➤ Consider $P_{Y|\, Y\in\mathcal{C}}$ with $\{\, Y \in \mathcal{C}\}$ characterized either by $\not\Vdash_{\mathcal{C}}$ (hard thresholding) or by $w_{\mathcal{C}}$ (smooth)

➤ Implicitly, $P_{\mathbf{X}|\, Y\in\mathcal{C}}$ is no more equal to the product of marginals

★★ Take-home message #7 ★★

✌ To keep in mind ✌

- **Characterize the critical domain**
  - Either with a hard conditioning (indicator function) or a smooth one
  - Introduction of a weight matrix W
- **A Conditional-HSIC index**

$$\mathrm{C}-\widehat{\mathrm{HSIC}}_{w_C}(X_i,\, Y) = \frac{1}{n^2}\mathrm{Tr}(\, WL_i\, WH_1\, LH_2) \tag{33}$$

- More details in this paper ☞ [MC21]

In practice: the proposed methodology

◆ The cooking recipe

1. Define the goal of the study:
   - ➤ Screening vs. Ranking
   - ➤ Type of analysis: Global / Target / Conditional
   - ➤ Maximum allowable budget (sample size)
2. Generate input samples such that $\mathbf{X} \sim P_{\mathbf{X}}$ according to $P_{\mathbf{X}}$ and get corresponding output samples (e.g., by crude Monte Carlo sampling)
3. Perform the analysis:
   - ➤ Choose kernels for inputs and output
   - ➤ Choose an estimator (U-stat vs. V-stat)
   - ➤ If necessary (TSA / CSA): define a weight function
   - ➤ Choose a test strategy (asymptotic vs. permutation-based)
   - ➤ Get HSIC & R^2_{HSIC} indices and p-values
4. Aggregate results from several analyses (e.g., GSA and TSA)
   - ➤ Use p-values first
   - ➤ Then, use R^2_{HSIC} indices

Thank your for your attention!

Any question?

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