# New Perspectives for Sensitivity Analysis

Sebastien Da Veiga – Safran Tech

ETICS 2016

# OUTLINE

- **Context**

- **Part I: Screening methods**
  - Model-based approaches
  - Model-free distances

- **Part II: Generalized GSA**
  - Distances between probability distributions
  - RKHS embedding
  - Orthogonal decompositions

# CONTEXT

## ➔ Sensitivity Analysis

- Goal : identify and rank the input parameters according to their impact on the output of a computer code

- Why ?
  - Reduce the output uncertainty efficiently by reducing the uncertainty of the main contributors
  - Improve the knowledge of the physical phenomenon,
  - Simplify the model

- Notations

Computer code

$$Y = \eta(X_1, \ldots, X_d)$$

Output

Input parameters

# CONTEXT

## ➔ Two points of view

- Local Sensitivity: studies the behavior of the output locally around a nominal value of the inputs

$$S_i = \frac{\sigma^2_{X_i}}{\mathrm{Var}(Y)} \left( \frac{\partial \eta(X)}{\partial X_i} |_{X=X_0} \right)^2$$

  - *Easy to compute and apprehend*
  - *But local approach, turns global only if the model is linear*

- Global sensitivity: all input parameters vary in their uncertain domain and we analyze the output variations

There are links between the viewpoints when local sensitivity is repeated (DGSM, Lamboni et al. 2013)

# CONTEXT

## ➔ Global Sensivity Analysis (GSA) – 2 families of methods

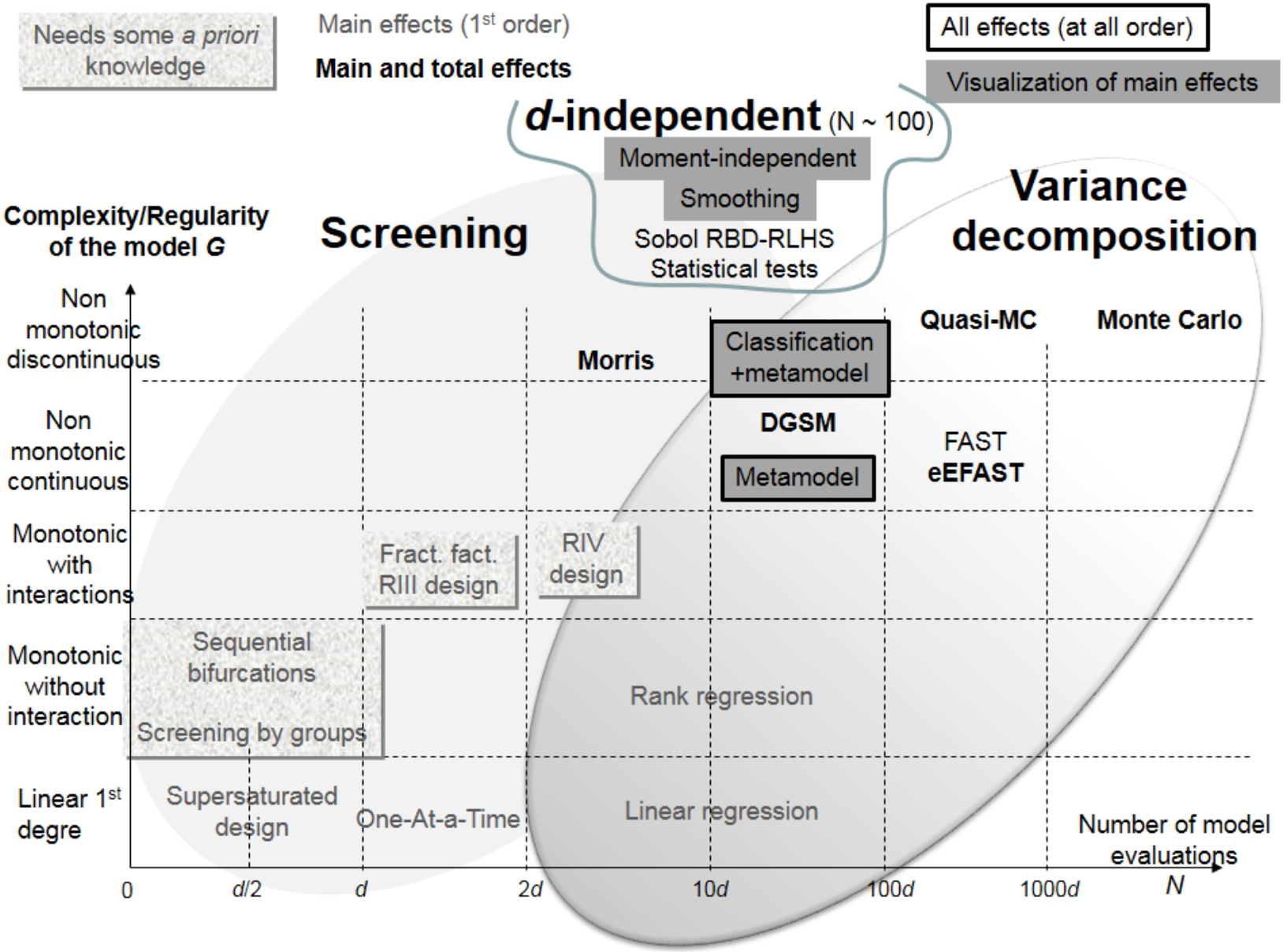
- Screening methods
  - Standard DOEs
  - Sequential bifurcation, …
  - Morris

$$n \approx d/2 - 10d$$

- Quantitative methods based on a variance decomposition
  - Linear regression, SRC, …
  - Sobol indices

$$n \approx 2d - 10^4 d$$

# CONTEXT




Iooss & Saltelli 2015

# CONTEXT

## ➔ Goal of this course: alternative methods outside GSA literature

- Screening methods ➔ Feature selection
  - Model-based
  - Model-free

- Quantitative methods based on a variance decomposition ➔ Going beyond the variance
  - Density-based indices
  - Generalized decompositions
  - Link with feature selection

# OUTLINE

➔ Context

➔ Part I: Screening methods
- Model-based approaches
- Model-free distances

➔ **Part II: Generalized GSA**
- Distances between probability distributions
- RKHS embedding
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# CONTEXT

## ➔ GSA – Focus on Sobol indices

- Sobol-Hoeffding decomposition for independent input parameters

$$\eta(X) = \eta_0 + \sum_{i=1}^{d} \eta_i(X_i) + \sum_{1 \leq i < j \leq d} \eta_{i,j}(X_i, X_j) + \ldots + \eta_{1,\ldots,d}(X_1, \ldots, X_d)$$

- Functions are centered and orthogonal
- Formulas with conditional expectations:

$$\begin{aligned}
\eta_0 &= \mathbb{E}(Y) \\
\eta_i(X_i) &= \mathbb{E}(Y|X_i) - \mathbb{E}(Y) \\
\eta_{i,j}(X_i, X_j) &= \mathbb{E}(Y|X_i, X_j) - \mathbb{E}(Y|X_i) - \mathbb{E}(Y|X_j) + \mathbb{E}(Y) \\
&\ldots
\end{aligned}$$

# CONTEXT

## ➔ GSA – Focus on Sobol indices

- By orthogonality

$$\mathrm{Var}(\eta(X)) = \sum_{i=1}^{d} \mathrm{Var}(\eta_i(X_i)) + \sum_{1 \le i < j \le d} \mathrm{Var}(\eta_{i,j}(X_i, X_j)) + \ldots + \mathrm{Var}(\eta_{1,\ldots,d}(X_1, \ldots, X_d))$$

- The total variance is decomposed into pieces involving main effects, 2nd order interactions, and so on
- => Possibility to define the sensitivity index of a groupt of input parameters

$$S_I(X_I) = \frac{\mathrm{Var}(\eta_I(X_I))}{\mathrm{Var}(\eta(X))}$$

$$S_i(X_i) = \frac{\mathrm{Var}(\mathbb{E}(Y|X_i))}{\mathrm{Var}(Y)}$$ Main effect

$$S_i^T(X_i) = \sum_{I \supseteq i} S_I$$ Total effect

# CONTEXT

## ➔ Limitations

- Variance decomposition is just a particular (and limited) analysis of the output variation
- The numerical code is expensive to evaluate
  - Usually rely on surrogate model to estimate Sobol indices
- The number of input parameters may be large (100 – 1000)
  - In practive, a first screening step is necessary
- Inputs & outputs may not be scalars (curves, …)

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*Take Home Message I*
*Generalized GSA*

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*Links between generalized GSA and feature selection …*

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*Take Home Message II*
*Links between generalized GSA and feature selection …*

*… which can accommodate structured objects*

# OUTLINE

➔ Context

➔ **Generalized GSA**

- Distances between probability distributions
- RKHS embedding
- Orthogonal decompositions

➔ Conclusion & Perspectives

# GENERALIZED GSA

## ➔ Going beyond the variance decomposition

- « Jitter » the input probability distributions (Lemaître et al. 2015)
- Indices based on contrast functions (Fort et al. 2014)

$$S_i^{\psi} = \mathbb{E}\psi(Y;\theta^*) - \mathbb{E}_{(X_i,Y)}\psi(Y;\theta_i(X_i))$$

$$\theta^* = \arg\min_{\theta} \mathbb{E}\psi(Y;\theta)$$

$$\theta_i(x) = \arg\min_{\theta} \mathbb{E}(\psi(Y;\theta)|X_i = x)$$

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- Quantify the impact of an input parameter on the **probability distribution of the output**

$$S_i^{TV} = \int |p_Y(y) - p_{Y|X_i=x}(y)| p_{X_i}(x) dxdy$$

Borgonovo 2007

$$S_i^{KL} = \int p_{Y|X_i=x}(y) \ln\left(\frac{p_{Y|X_i=x}(y)}{p_Y(y)}\right) p_{X_i}(x) dxdy$$

Kraskov et al. 2001

# GENERALIZED GSA

## ➔ General framework for distributional indices

- From a broad perspective, the impact of an input parameter may be defined through the choice of a similarity measure between probability distributions

$$S_i = \mathbb{E}_{X_i}\left(d(P_Y, P_{Y|X_i})\right)$$

Baucells and Borgonovo 2013
D. 2014

  - If the input probability distribution and the conditional one are « close », the input parameter has little influence

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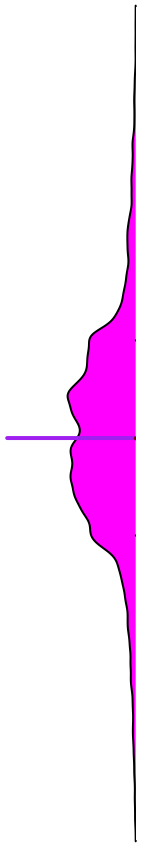
- Toy example

$$Y = \sin(X_1) + 5\sin^2(X_2) + 0.1X_3^4\sin(X_1)$$

$$X_1, X_2, X_3, X_4 \sim U(-\pi, \pi)$$

Ishigami function with dummy variable

# GENERALIZED GSA



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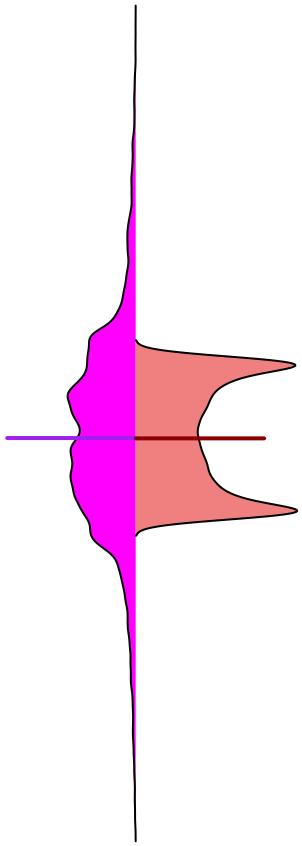

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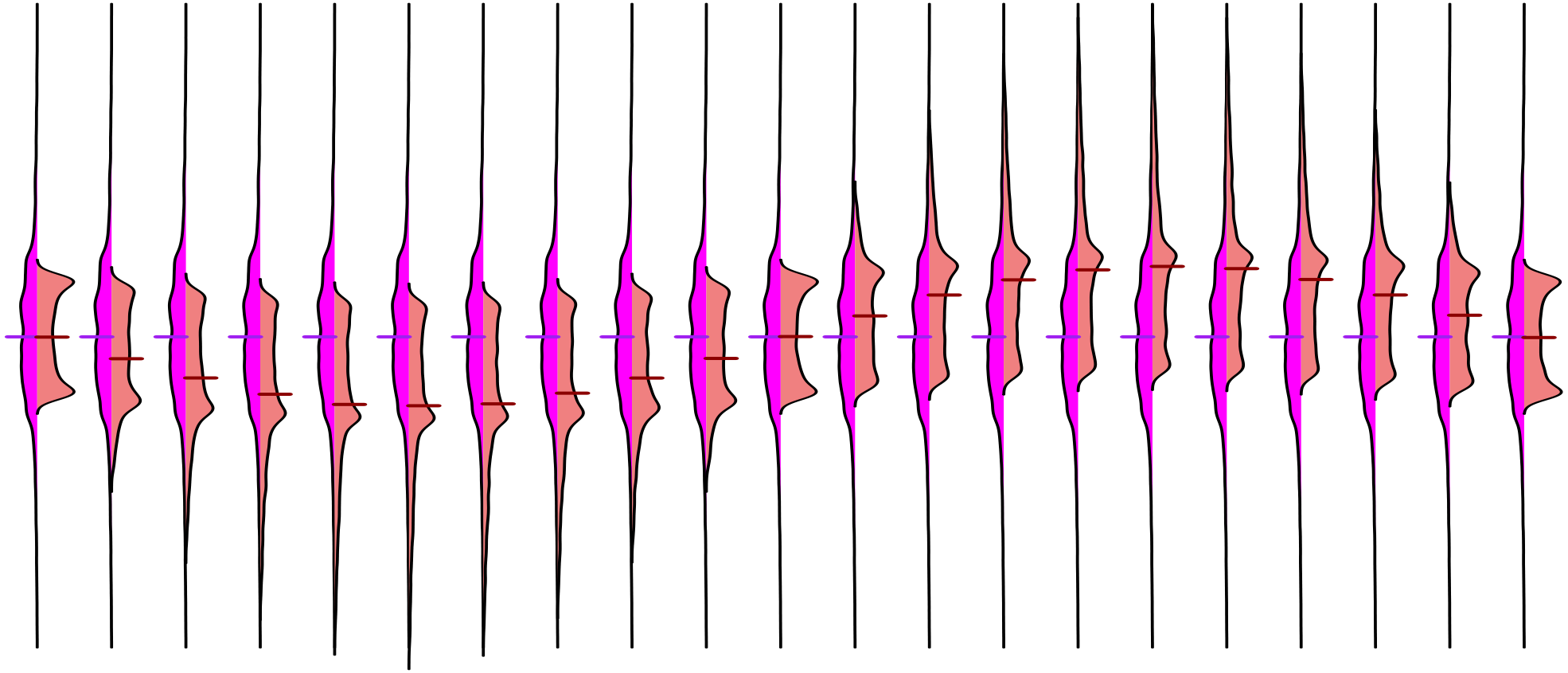

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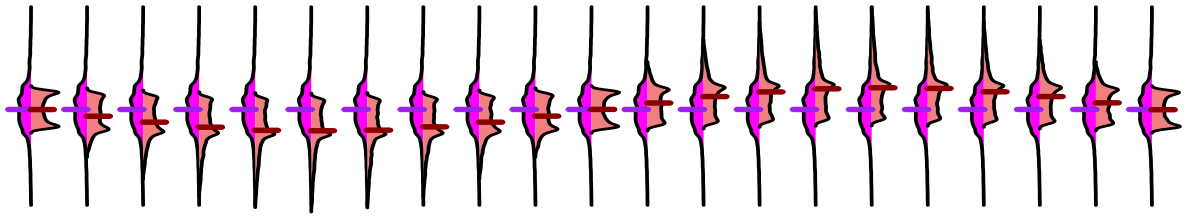
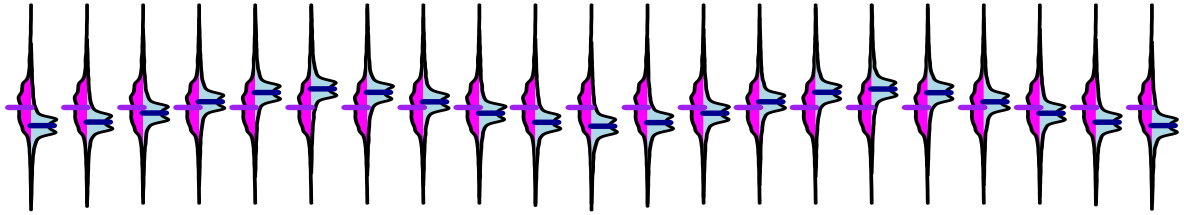
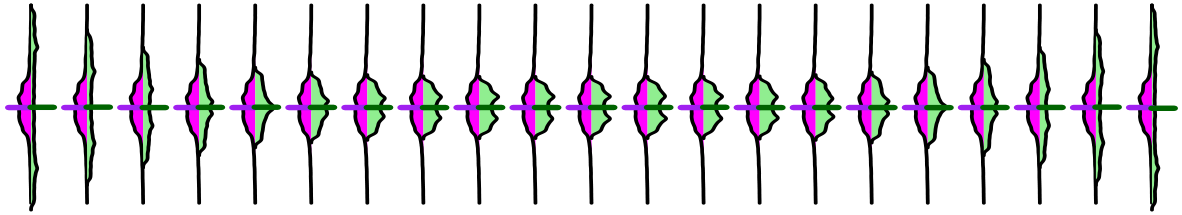


X2 fixed



X3 fixed



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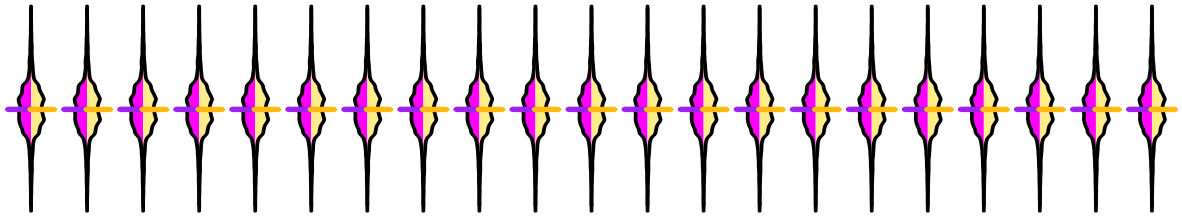

What do you think ?

# GENERALIZED GSA

## ➔ How can we compare probability distributions ?

- The basics

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  - Compare their means

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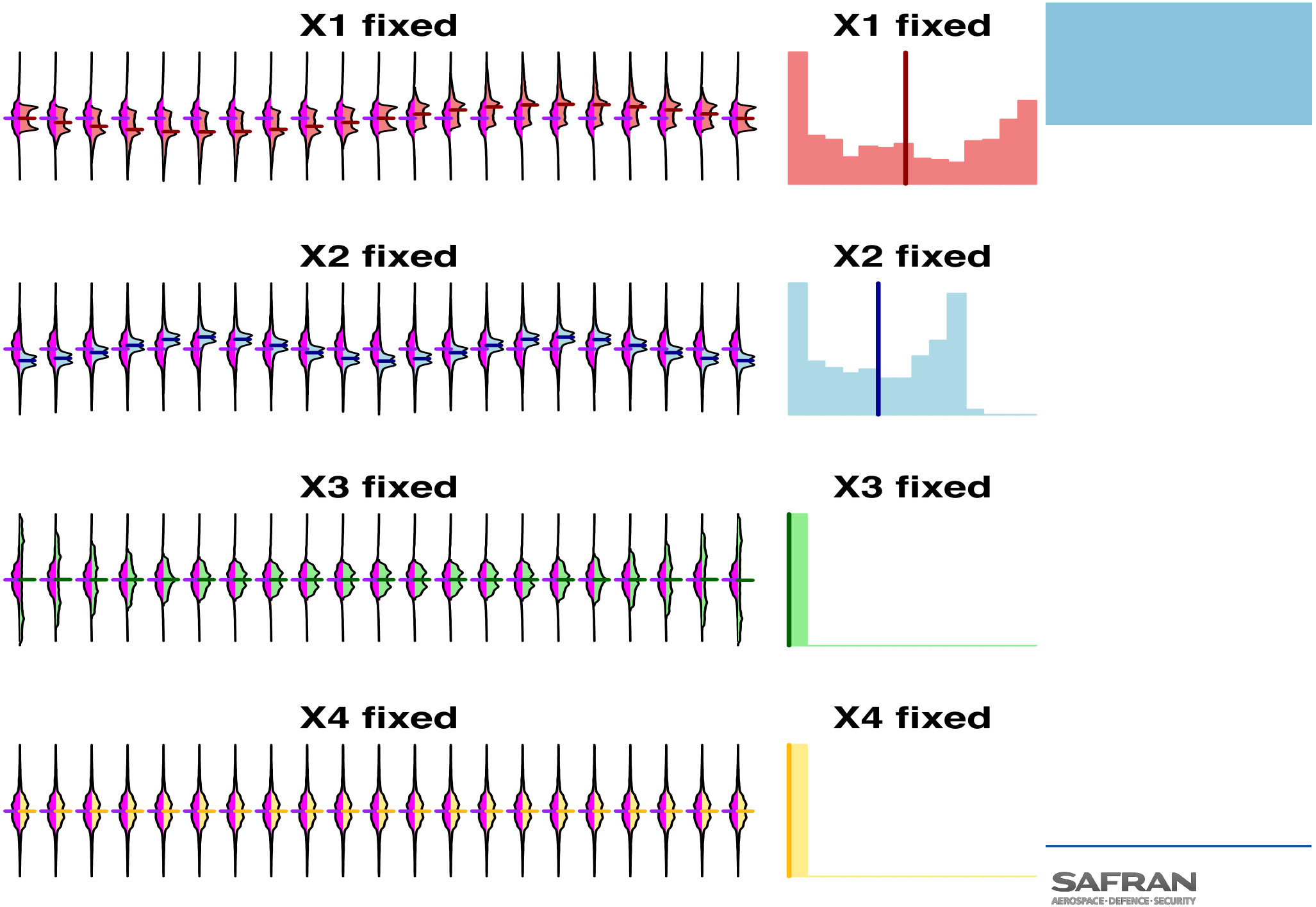
X1 fixed
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X2 fixed
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- The f-divergence family

$$d_f(P_Y||P_{Y|X_i}) = \int f\left(\frac{p_Y(y)}{p_{Y|X_i}(y)}\right) p_{Y|X_i}(y)dy$$

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$$S_i^f = \int f\left(\frac{p_Y(y)p_{X_i}(x)}{p_{X_i,Y}(x,y)}\right) p_{X_i,Y}(x,y)dxdy$$ D. 2014

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  - Includes as particular cases

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- Maximum Mean Discrepancy (MMD) or Integral Probability Metrics (IPMs)

# GENERALIZED GSA

## ➔ Maximum Mean Discrepancy

$$\mathrm{MMD}(P, Q; F) := \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(x) \right]$$

## ➔ The distance is zero iif the probability distributions are equal

- F = bounded continuous functions (Dudley metric)
- F = functions with bounded variations (Kolmogorov metric)
- F = Lipschitz bounded functions (Earth mover's distance – Wasserstein metric)

# GENERALIZED GSA

## ➔ Distributional indices: advantages

- Account for the whole effect of a parameter on the output distribution and not only on the mean
- Density-based, which means
  - Many methods and codes for estimation
  - As we have seen, several distances can be investigated without any additional cost

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## ➔ Limitations

- Density estimation suffers from the curse of dimensionality
  - If we want to consider outputs which are not scalars, this will be a bottleneck
  - Impossible to compute a total index equivalent in this setting
    - Even low order interactions
- Estimation bias

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  - Interpretation is problematic

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- A possible point of view: RKHS embedding of probability distributions

# OUTLINE

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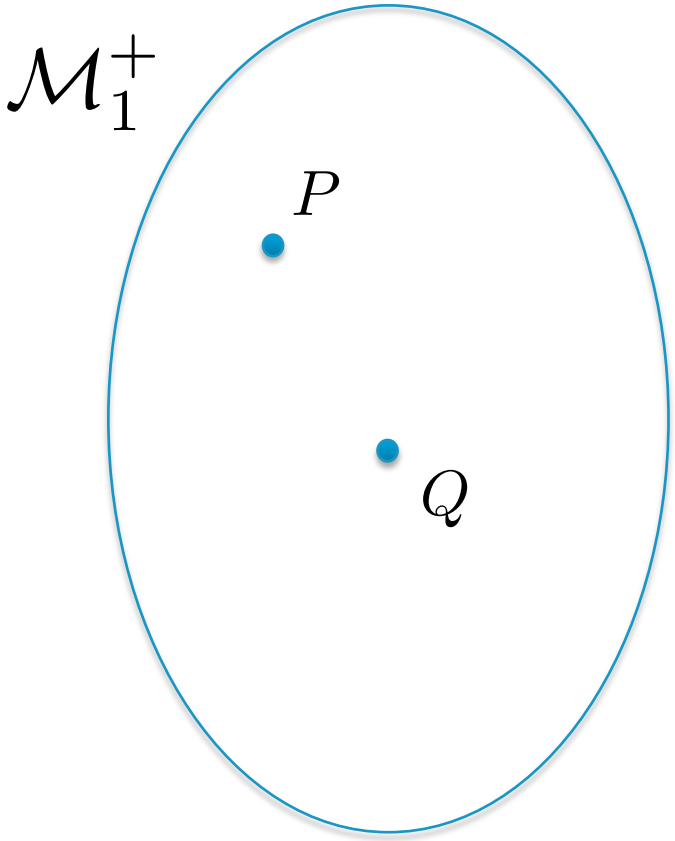
➔ **Generalized GSA**

- Distances between probability distributions
- RKHS embedding
- Orthogonal decompositions

➔ Conclusion & Perspectives

# RKHS EMBEDDING



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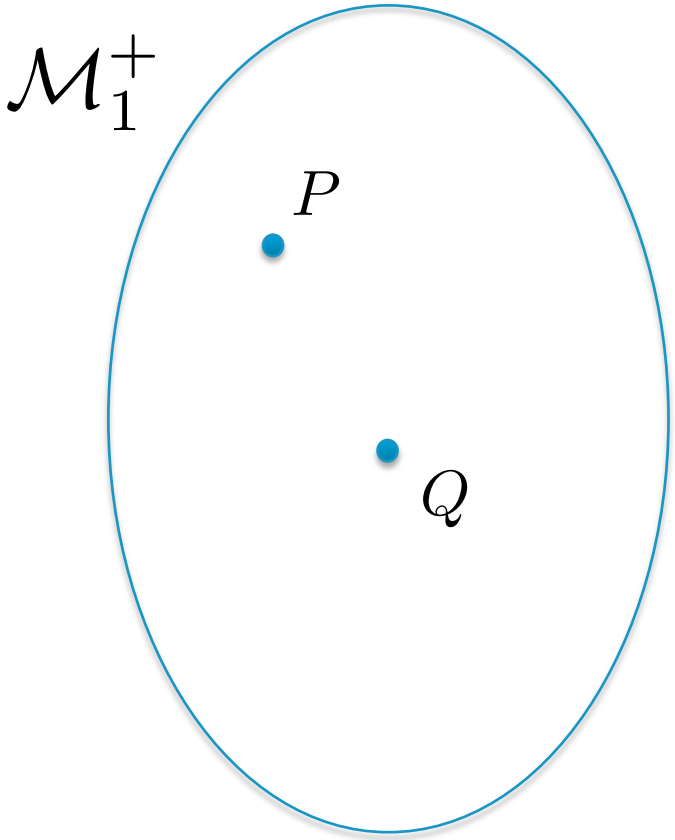
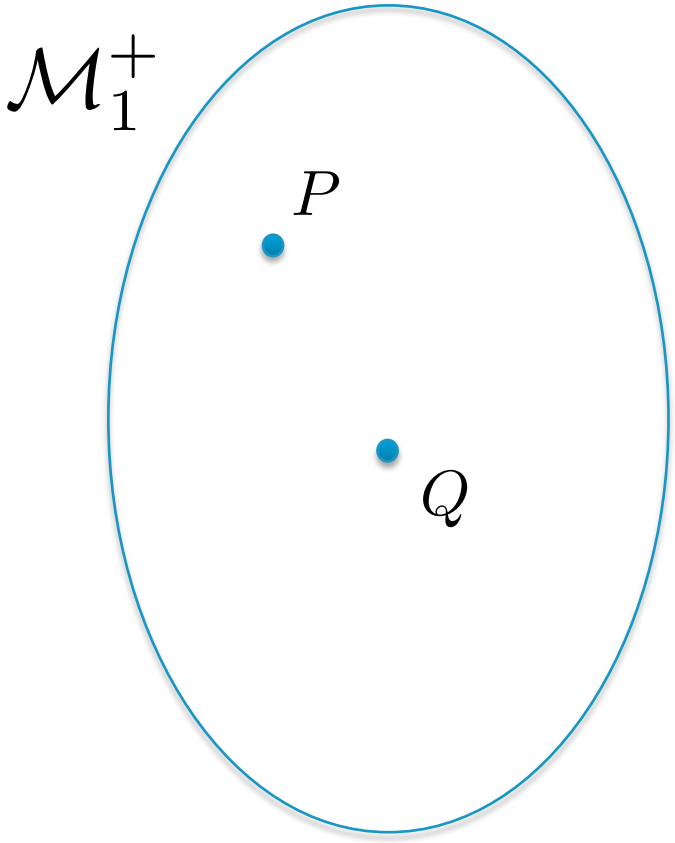



$$d(P,Q) = \sup_{A \in \Sigma} |P(A) - Q(A)|$$

$$\text{TV} \qquad = \frac{1}{2} \int_{\Omega} |f_P - f_Q| d\mu$$

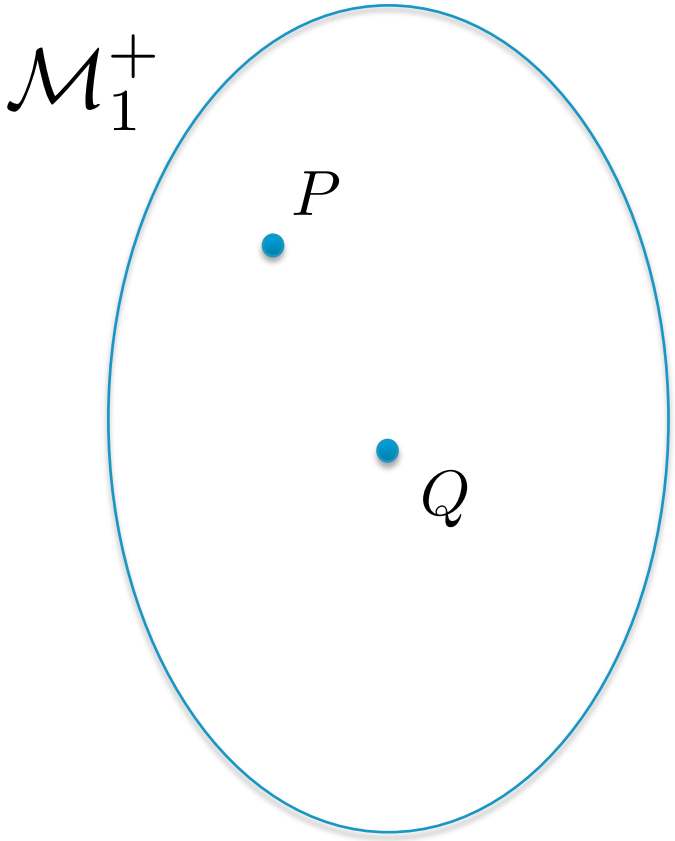
# RKHS EMBEDDING




$$d(P,Q) = \int_\Omega f_P log(f_P/f_Q) d\mu$$

KL

# RKHS EMBEDDING




Other point of view: represent a probability distribution with some features

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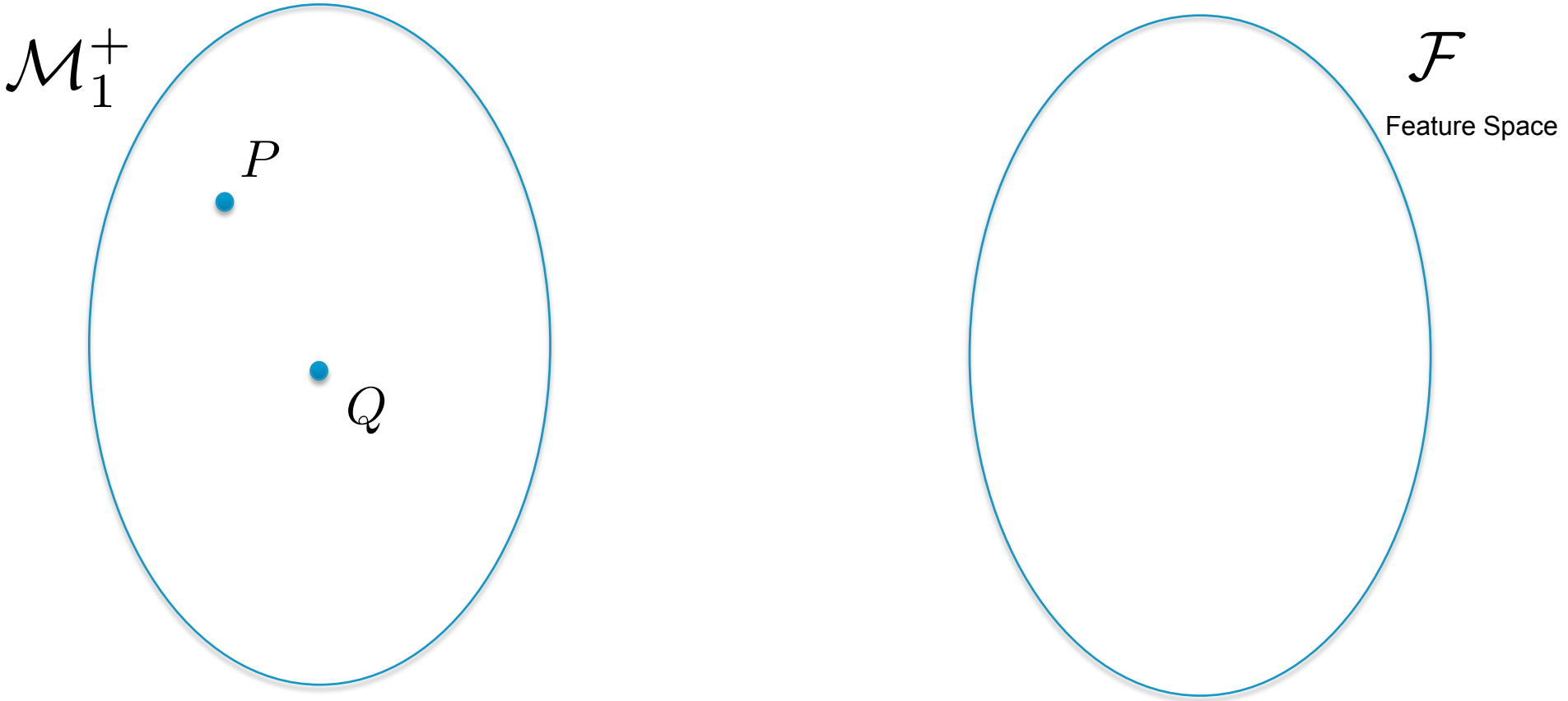


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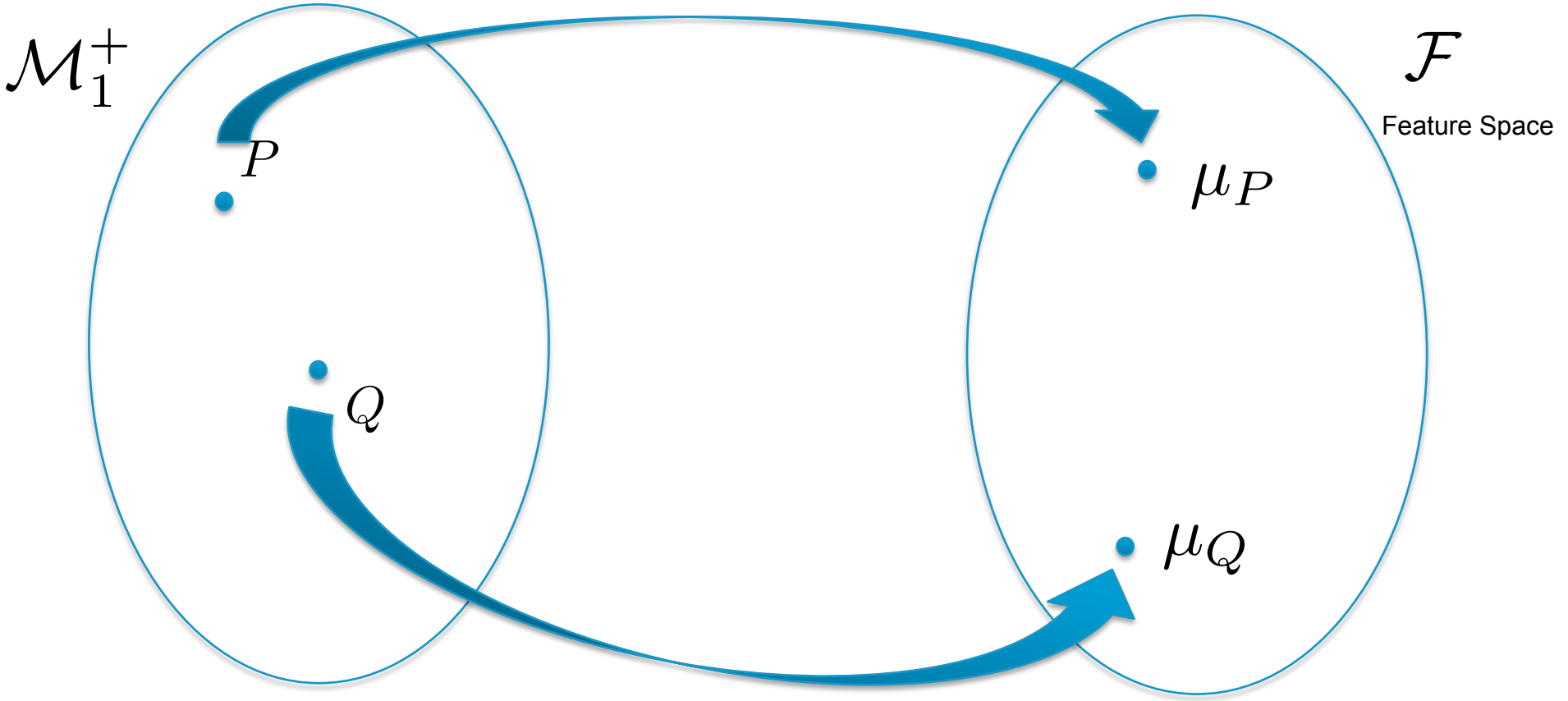


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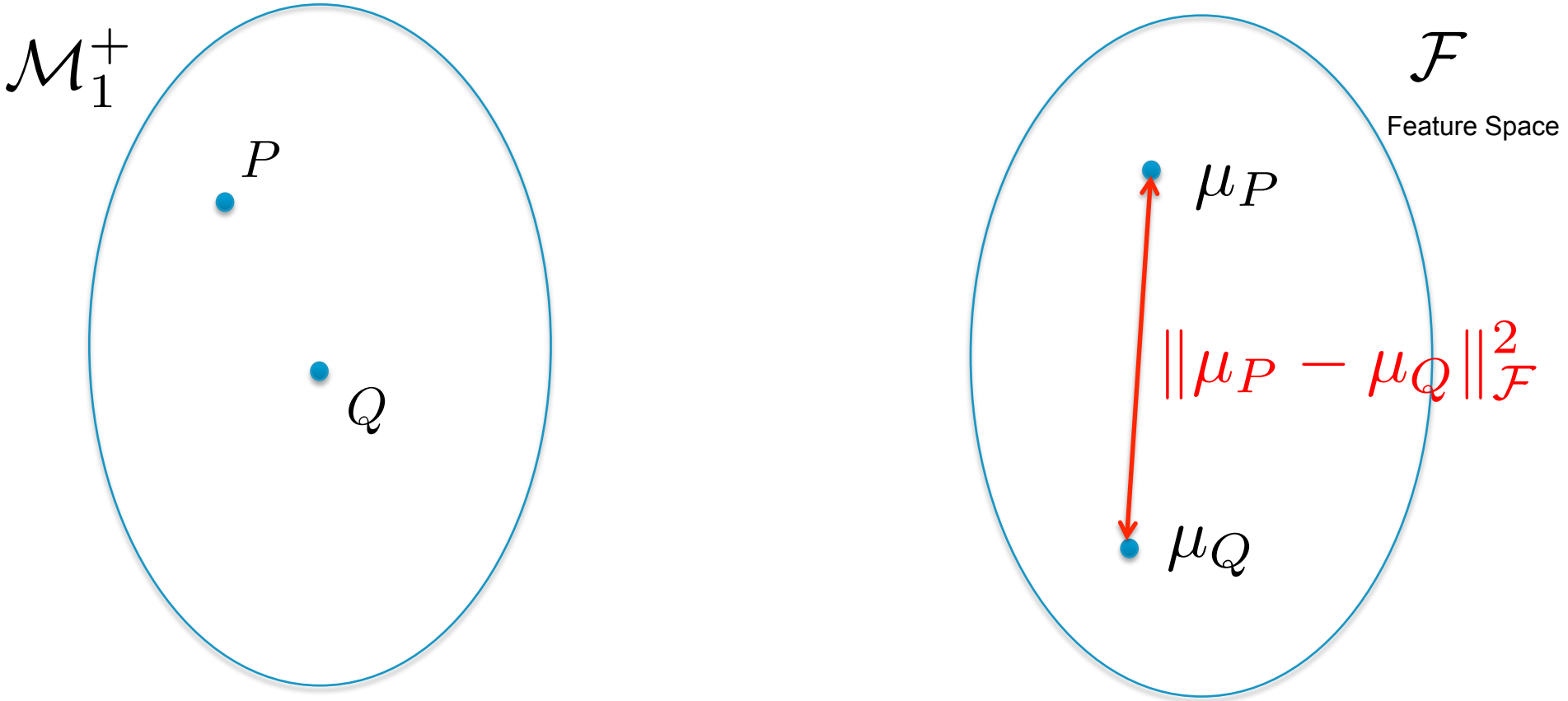
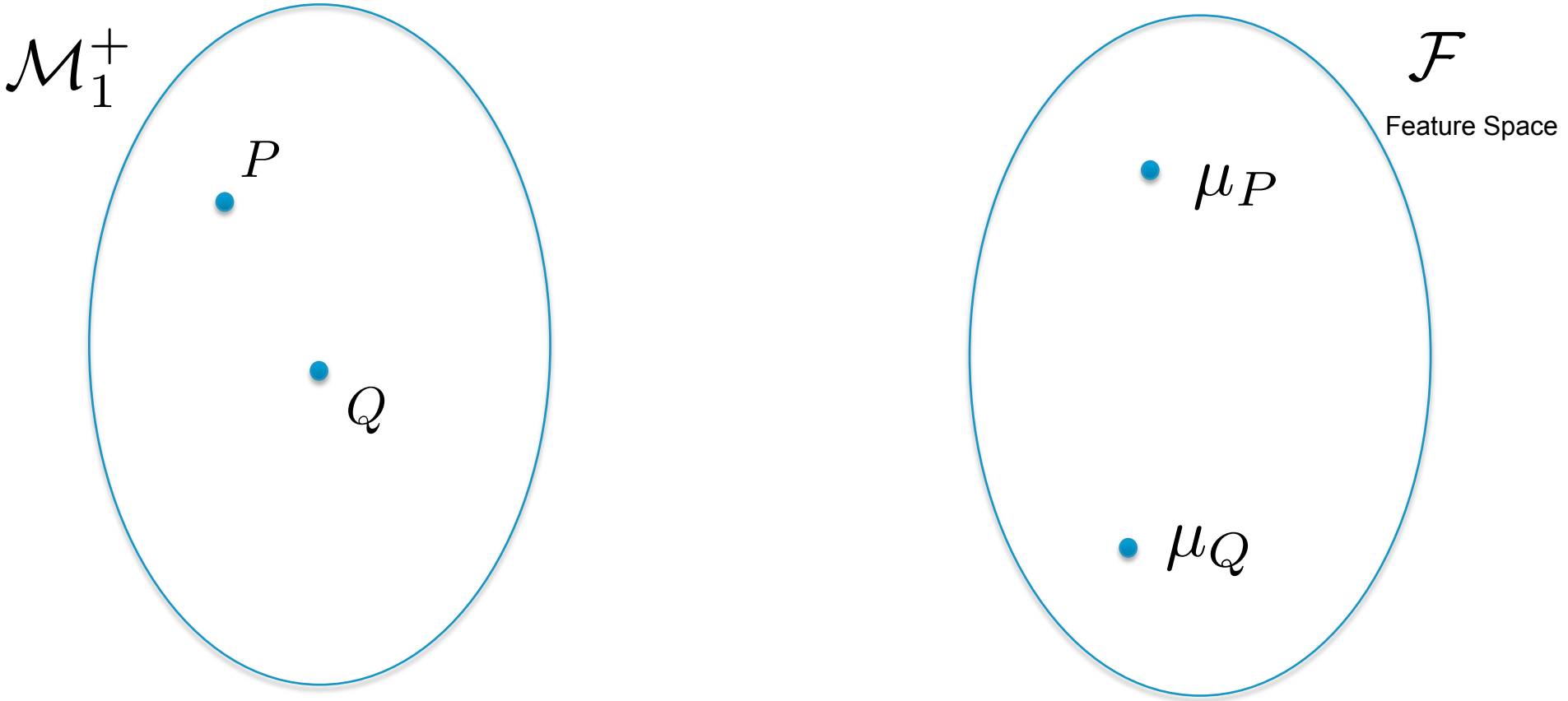


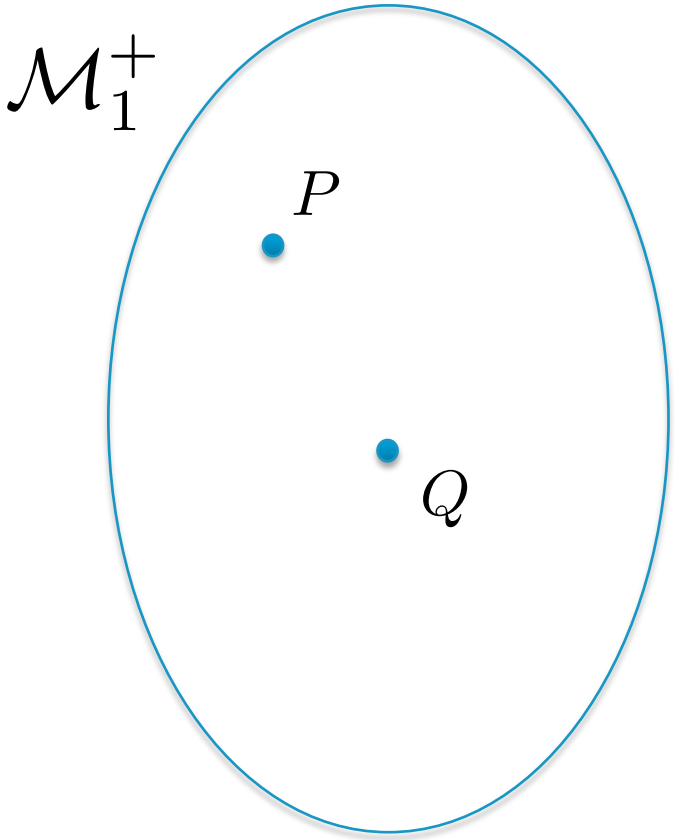

The dissimilarity between probability distributions is measured through the distance between their representation in the feature space

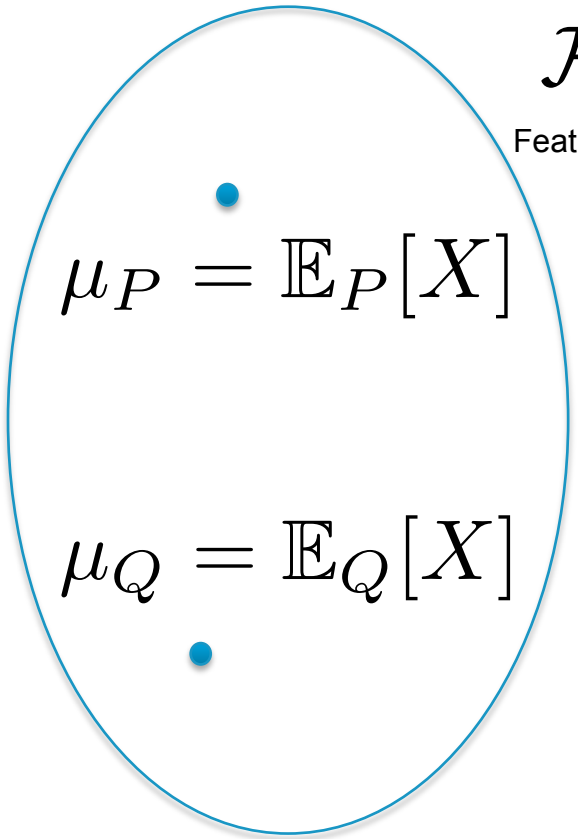
# RKHS EMBEDDING




Question: which feature ?

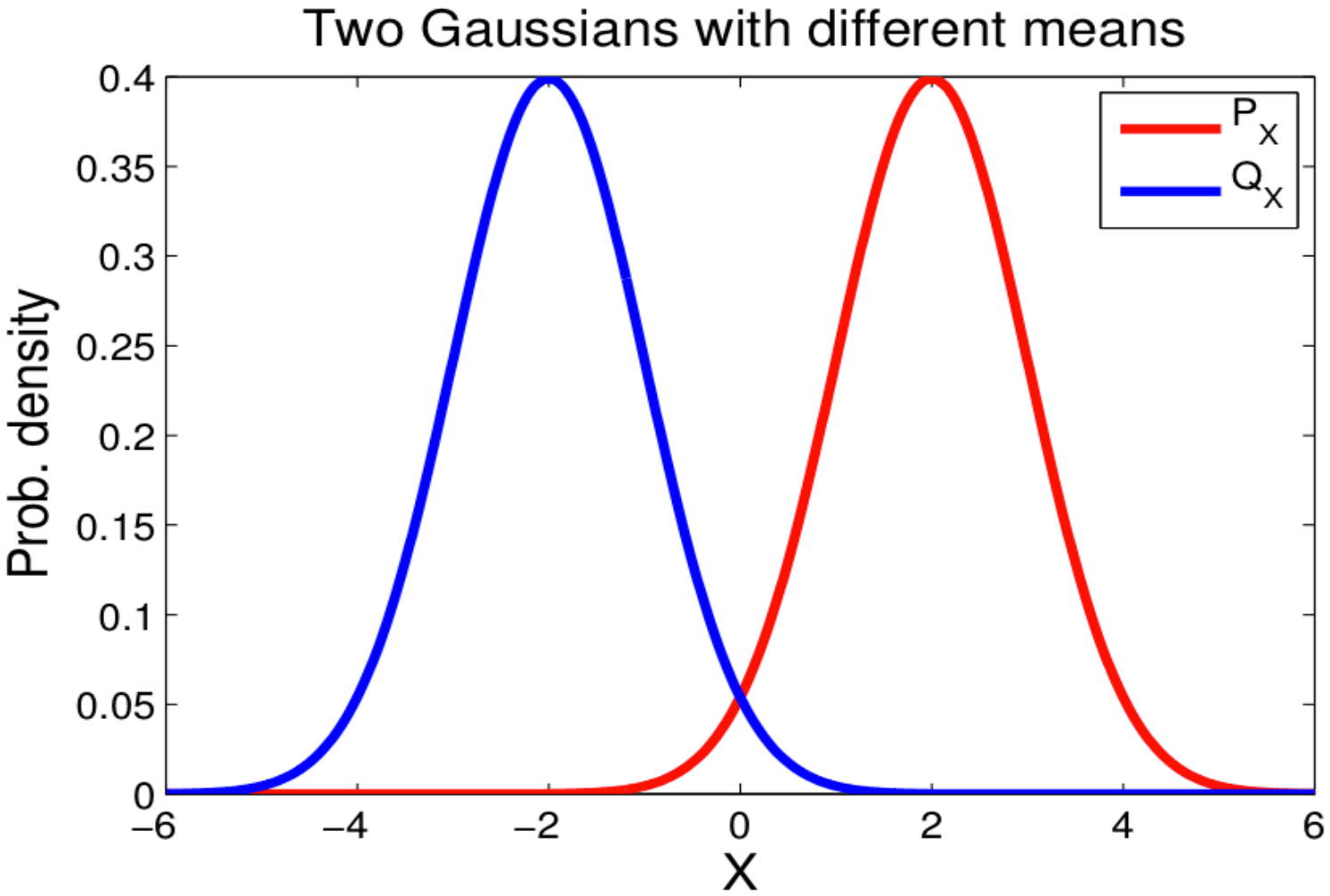
# RKHS EMBEDDING




Dissimilarity measured only through the means

# RKHS EMBEDDING




**OK**

✓

Gretton 2012

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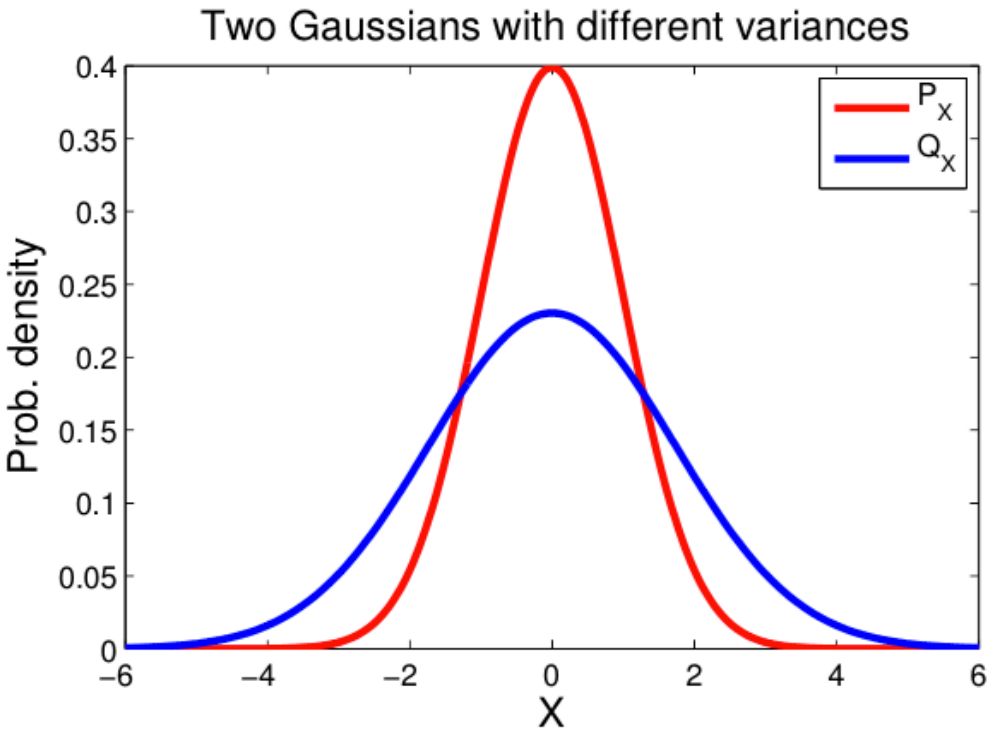


**NOK**

✗

Gretton 2012

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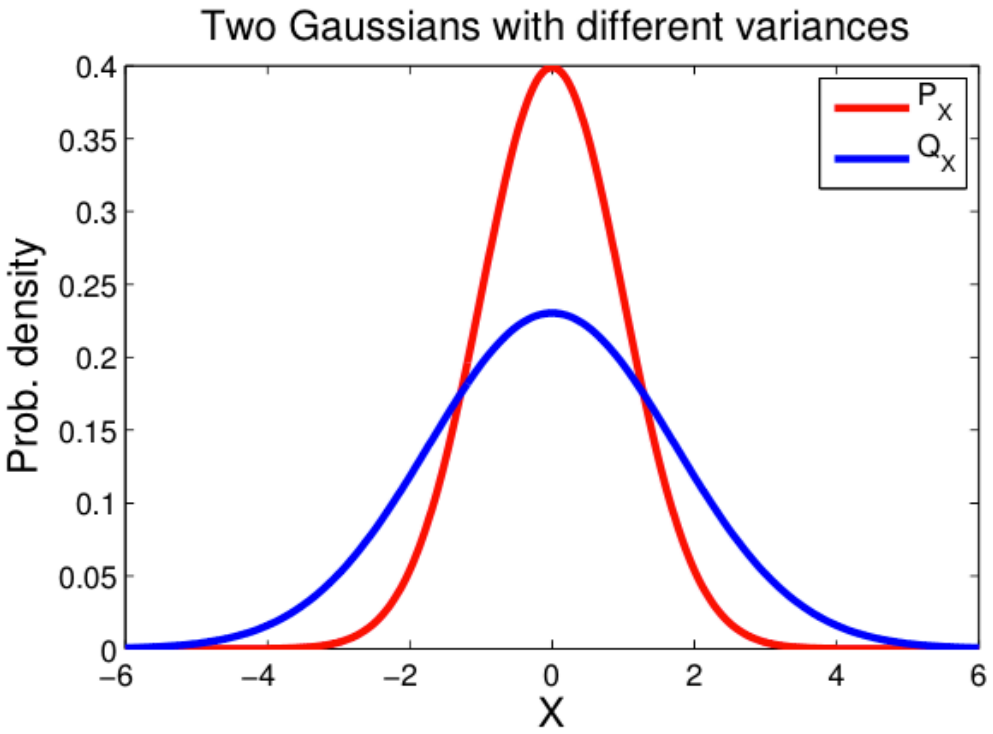


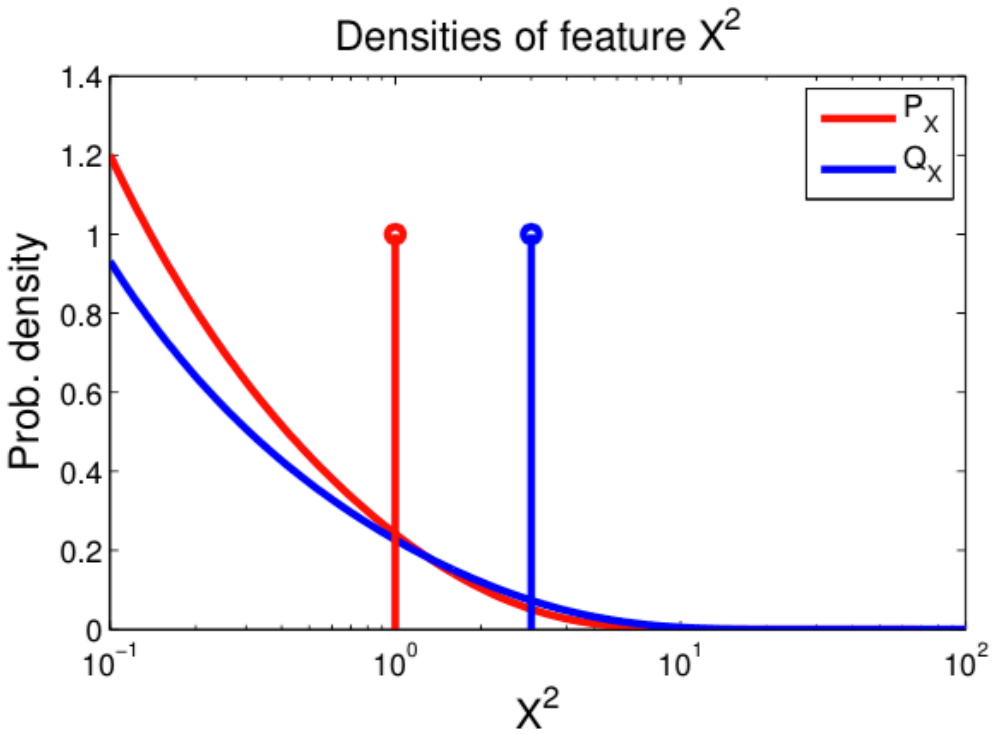


**NOK**

✗

**OK**

✓

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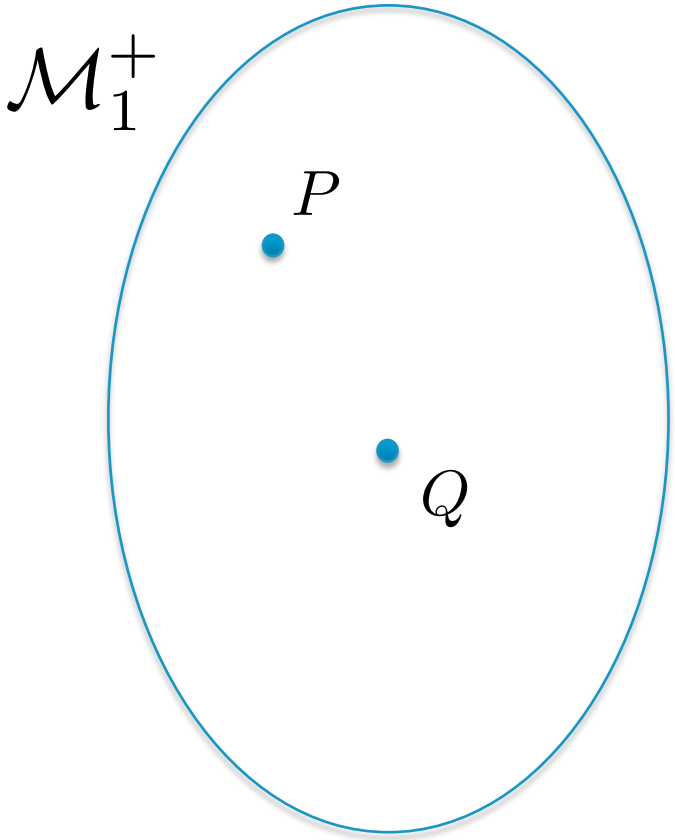
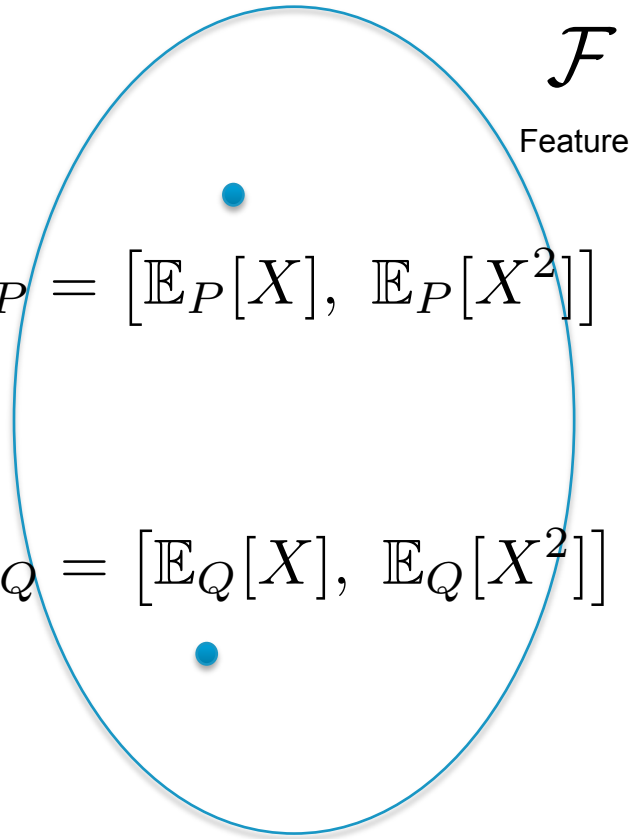
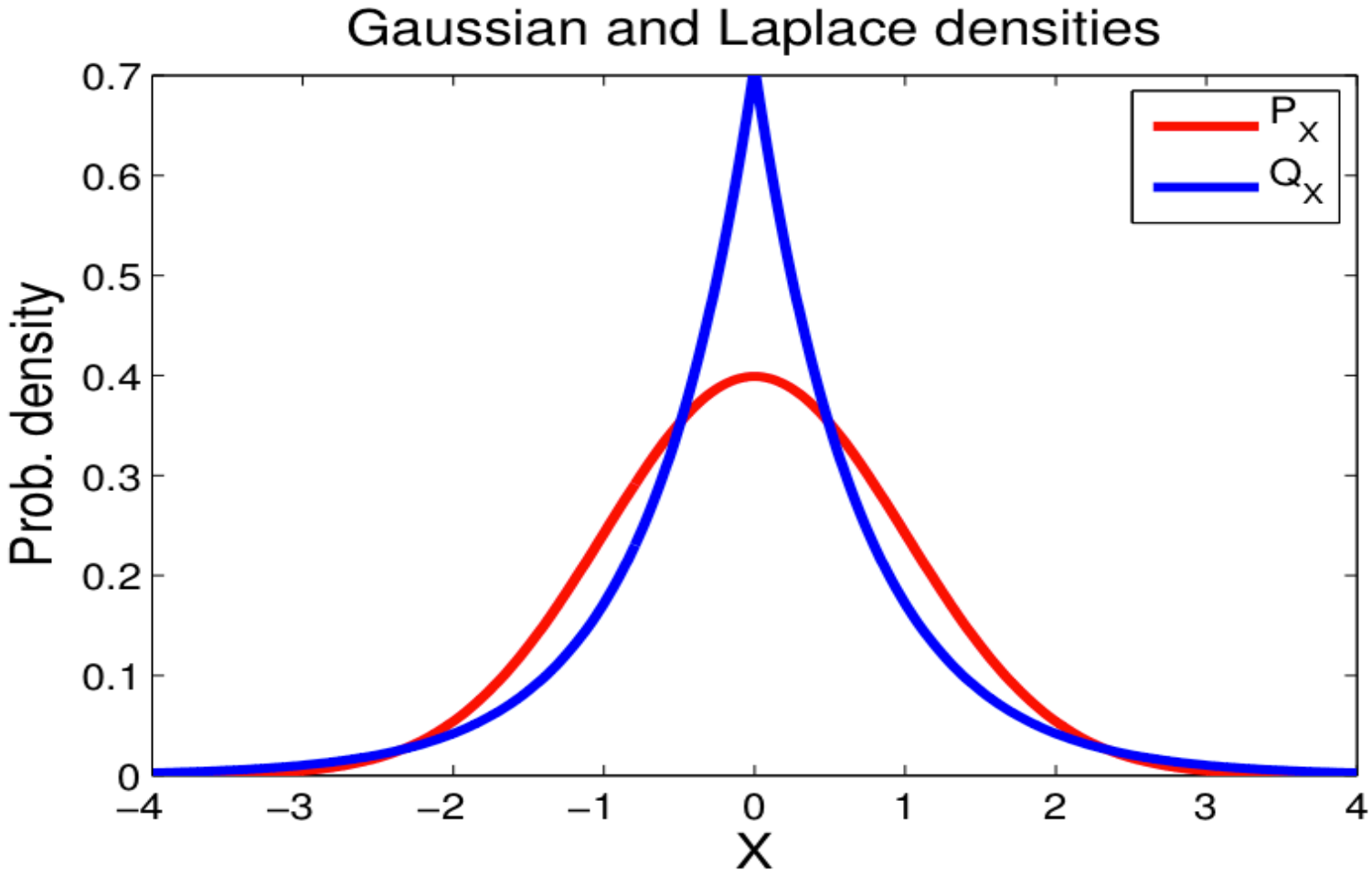



Dissimilarity measured only through means & variances

# RKHS EMBEDDING

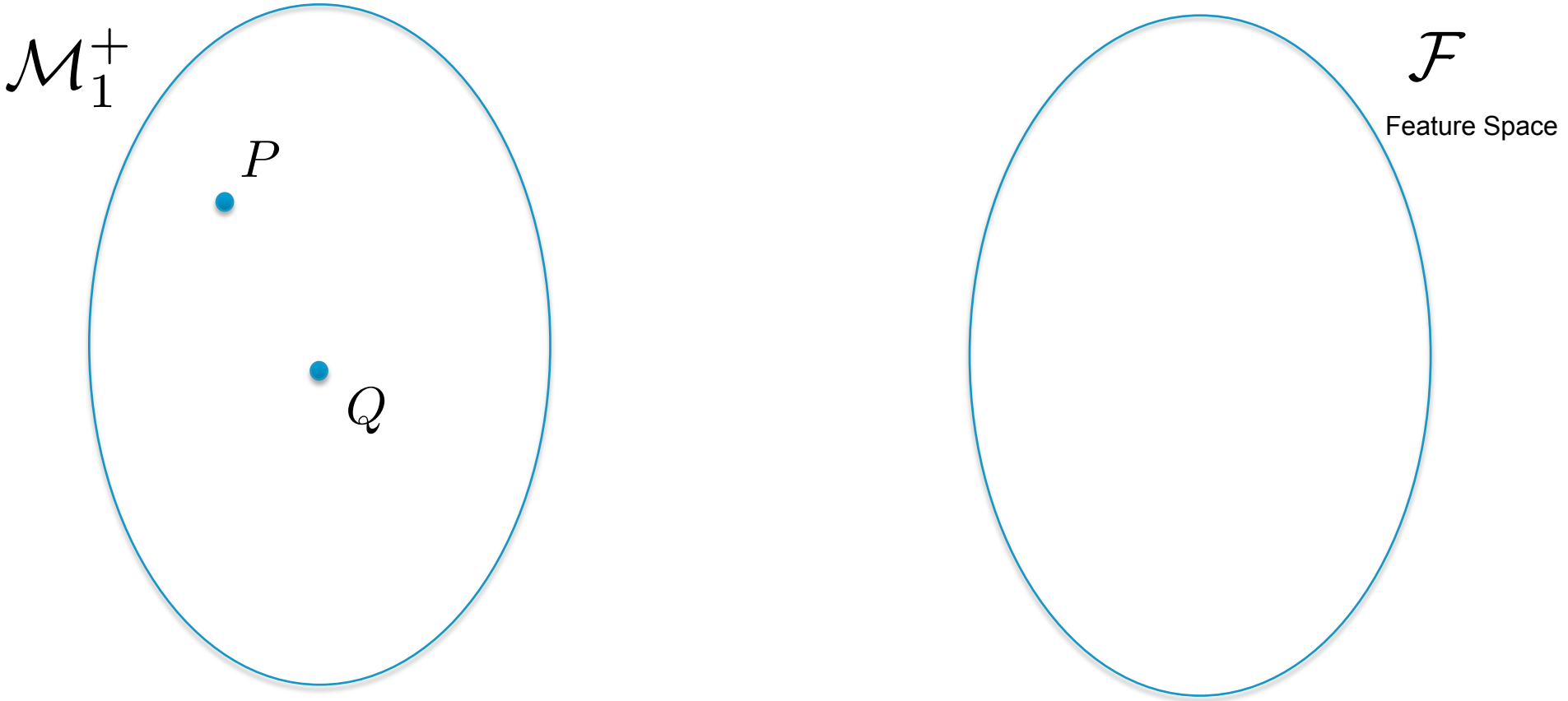



**NOK**

✗

Gretton 2012

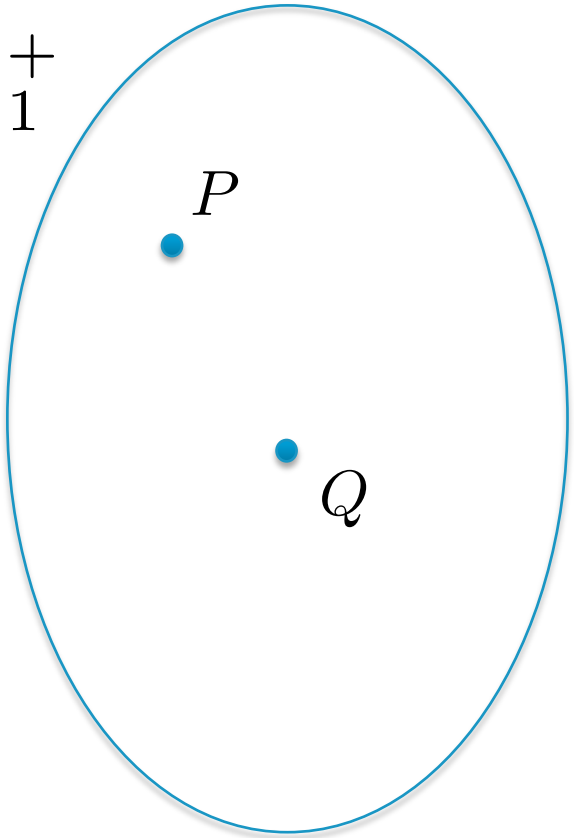
# RKHS EMBEDDING

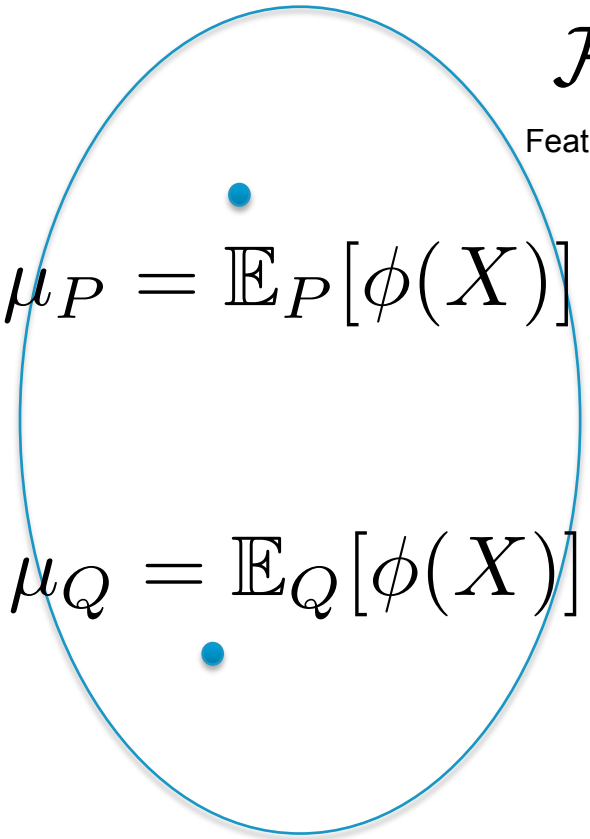



General setting: take a feature map

$$\phi : \Omega \to \mathcal{F}$$

# RKHS EMBEDDING

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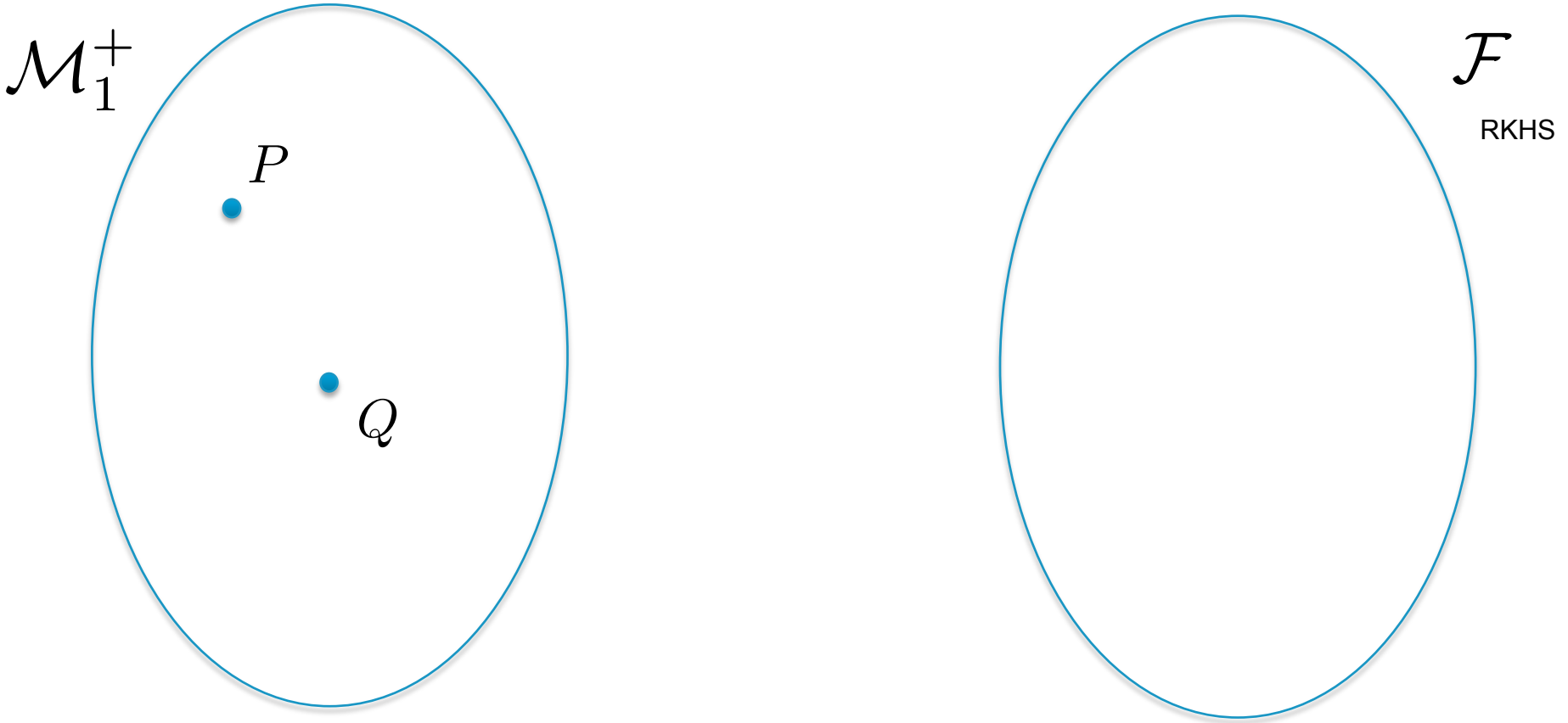
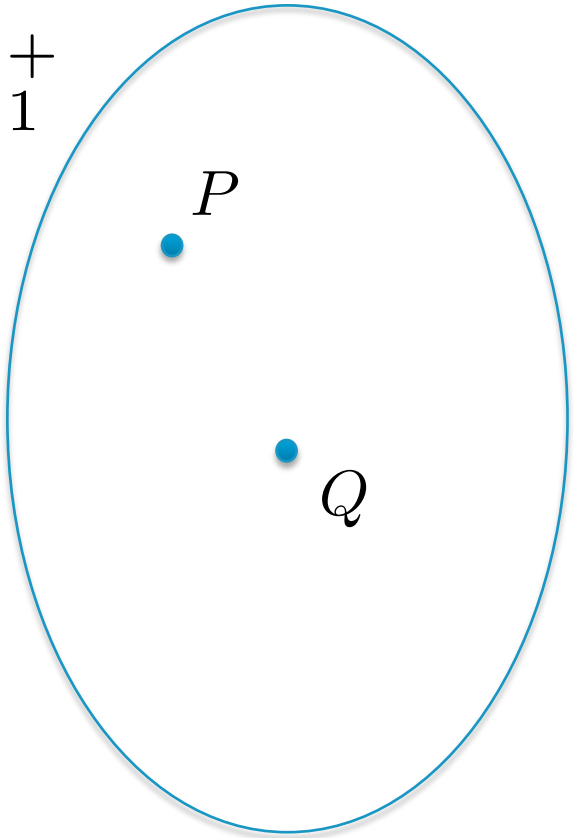
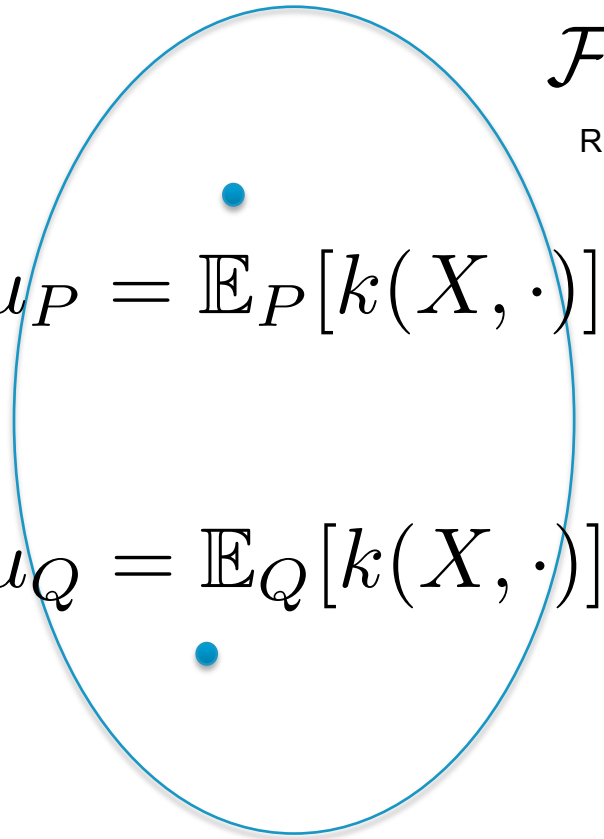



Instead of choosing the feature map, make it implicit and assume that the feature space is a RKHS with a given kernel

$$k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{F}}$$

# RKHS EMBEDDING

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# RKHS EMBEDDING

## ➔ In practice

- Choose the kernel
- How can the distance be computed in the feature space ?

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- How can the distance be computed in the feature space ?

$$\begin{aligned}\|\mu_P - \mu_Q\|_{\mathcal{F}}^2 &= \langle \mu_P, \mu_P \rangle_{\mathcal{F}}^2 + \langle \mu_Q, \mu_Q \rangle_{\mathcal{F}}^2 - 2\langle \mu_P, \mu_Q \rangle_{\mathcal{F}} \\ &= \dots \\ &= \mathbb{E}_{X \sim P, X' \sim P}[k(X, X')] + \mathbb{E}_{Y \sim Q, Y' \sim Q}[k(Y, Y')] - 2\mathbb{E}_{X \sim P, Y \sim Q}[k(X, Y)]\end{aligned}$$

Standard reproducing RKHS property

- Distance which involves only the kernel
  - Kernel trick in action
- Several nice papers on the subject
  - Smola et al. 2007, Song 2008, Song et al. 2009

# RKHS EMBEDDING: REMEMBER MMD ?

➔ **Maximum Mean Discrepancy**

$$\mathrm{MMD}(P, Q; F) := \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(x) \right]$$

➔ **The distance is zero iif the probability distributions are equal**

- F = bounded continuous functions (Dudley metric)
- F = functions with bounded variations (Kolmogorov metric)
- F = Lipschitz bounded functions (Earth mover's distance – Wasserstein metric)

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- F = Lipschitz bounded functions (Earth mover's distance – Wasserstein metric)
- **F = unit ball in a characteristic RKHS** (Sriperumbudur et al. 2008)

# RKHS EMBEDDING: REMEMBER MMD ?

## ➔ Maximum Mean Discrepancy in a RKHS

$$\begin{aligned}
\mathrm{MMD}^2(P,Q;F) &= \left( \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(x) \right] \right)^2 \\
&= \left( \sup_{f \in F} \left\langle f, \mu_P - \mu_Q \right\rangle_{\mathcal{F}} \right)^2 \\
&= \left\| \mu_P - \mu_Q \right\|_{\mathcal{F}}^2
\end{aligned}$$

$$\|h\|_{\mathcal{F}} = \sup_{f \in F} \langle f, h \rangle_{\mathcal{F}}$$

**MMD point of view and feature space point of view are equivalent**

# RKHS EMBEDDING: TOWARDS GSA

➔ **General framework**

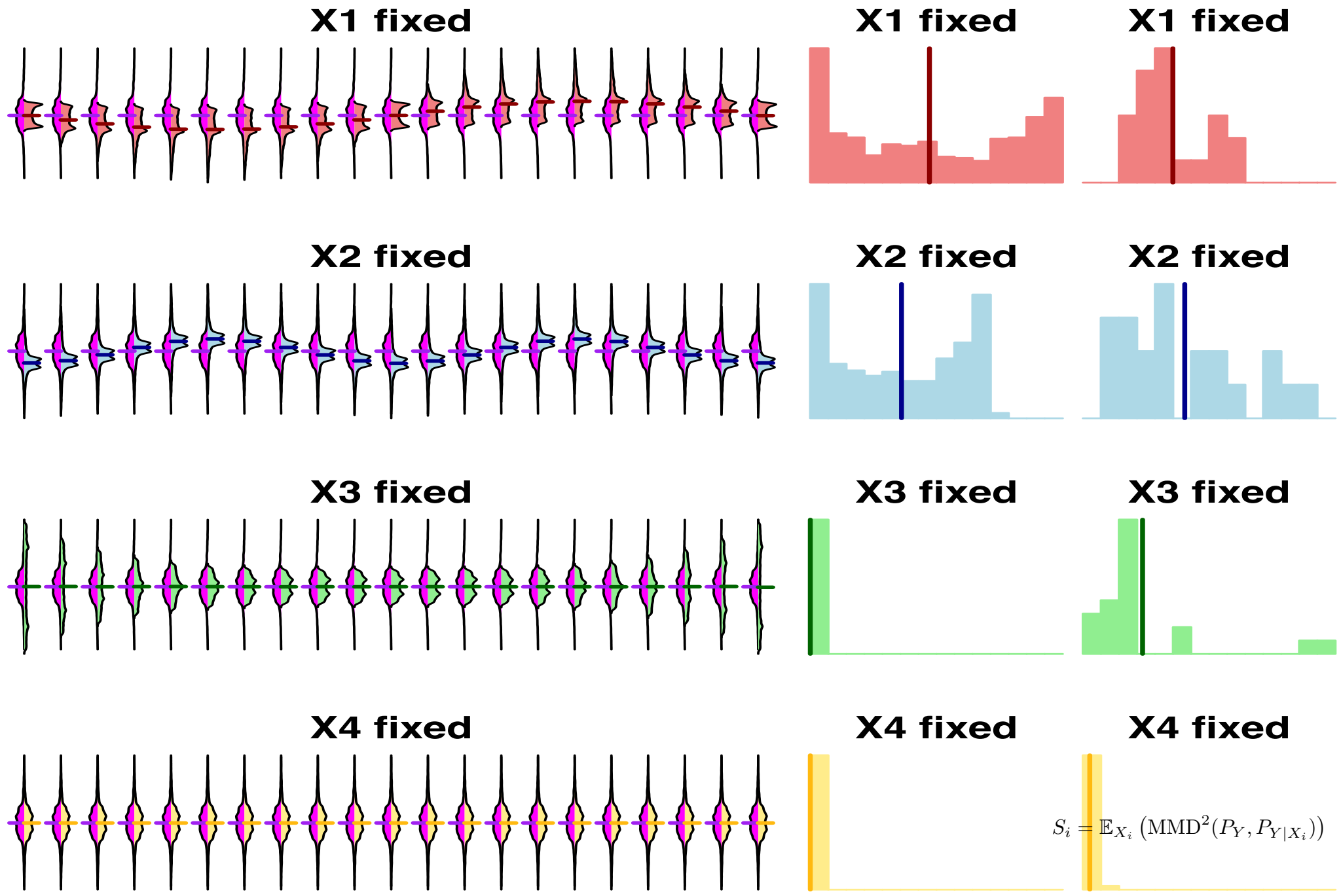
$$S_i = \mathbb{E}_{X_i}\left(d(P_Y, P_{Y|X_i})\right)$$

➔ **If we use the MMD distance**

$$d(P_Y, P_{Y|X_i}) = \mathrm{MMD}^2(P_Y, P_{Y|X_i})$$

$$\boxed{S_i = \mathbb{E}_{X_i}\left(\mathrm{MMD}^2(P_Y, P_{Y|X_i})\right)}$$

$$S_i = \int_\Omega k(y,y')\left[p_Y(y) - p_{Y|X_i=x_i}(y)\right]\left[p_Y(y') - p_{Y|X_i=x_i}(y')\right] p_{X_i}(x_i) dy dy' dx_i$$


X1 fixed
X1 fixed
X1 fixed
X2 fixed
X2 fixed
X2 fixed
X3 fixed
X3 fixed
X3 fixed
X4 fixed
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# RKHS EMBEDDING: TOWARDS GSA

## ➔ A few remarks

- You can choose any kernel
- **If we want to distinguish probability distributions, we must use a characteristic kernel**
  - e.g. Gaussian, exponential

Fukumizu et al. (2008)
Sriperumbudur et al. (2008)

- But in practice you can choose any kernel, including

$$k(y, y') = \langle y, y' \rangle \overset{\text{1D}}{=} yy'$$

Feature map is identity
Comparison through means only

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$$\mathbb{E}\left(\mathrm{MMD}^2(P_Y, P_{Y|X_i})\right) = \mathrm{Var}(\mathbb{E}(Y|X_i))$$

Unnormalized Sobol index

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- This is thus a natural extension of Sobol
- Question: where does the normalizing constant come from ?
  - Sobol-Hoeffding decomposition !
  - **Can we have the same ?**

# RKHS EMBEDDING: DECOMPOSITION I

➔ **Re-write the Sobol-Hoeffding decomposition**

$$\mathrm{Var}(Y) = \sum_{u \subseteq \{1,\dots,d\}, u \neq \emptyset} g_u$$

$$g_u = \sum_{v \subseteq u} (-1)^{|u|-|v|} \mathrm{Var}\left(\mathbb{E}(Y|X_v)\right)$$

# RKHS EMBEDDING: DECOMPOSITION I

➔ **Theorem (D. 2016)**

$$\mathbb{E}\left(\mathrm{MMD}^2\left(P_{Y|X_{1:d}}, P_Y\right)\right) = \sum_{u \subseteq \{1,\ldots,p\}, u \neq \emptyset} g_u$$

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➔ **MMD sensitivity indices**

$$S_u^{\mathrm{MMD}} = \frac{\sum_{v\subseteq u}(-1)^{|u|-|v|}\mathbb{E}\left(\mathrm{MMD}^2\left(P_{Y|X_v}, P_Y\right)\right)}{\mathbb{E}\left(\mathrm{MMD}^2\left(P_{Y|X_{1:d}}, P_Y\right)\right)}$$

# RKHS EMBEDDING: DECOMPOSITION I

## ➔ Alternate interpretation of MMD indices

- If we use a Mercer kernel,

$$k(y, y') = \sum_{j=1}^{\infty} \Phi_j(y)\Phi_j(y')$$

- As a result, 1st order MMD indices are given by

$$S_i^{\mathrm{MMD}} = \frac{\sum_{j=1}^{\infty} \mathrm{Var}(\mathbb{E}(\Phi_j(Y)|X_i))}{\sum_{j=1}^{\infty} \mathrm{Var}(\Phi_j(Y))} = \sum_{j=1}^{\infty} \alpha_j S_i^{\mathrm{Sobol}}\left[\phi_j(Y)\right]$$

*Linear combination of the Sobol index for a (potential) infinity of transformations of the output (i.e. features)*

# RKHS EMBEDDING: ESTIMATION

## ➔ Standard MMD estimation

$$\widehat{\mathrm{MMD}}^2 = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} \left[ k(x_i, x_j) - k(x_i, x'_j) - k(x'_i, x_j) + k(x'_i, x'_j) \right]$$

$$\{x_i\}_{i=1}^n \sim P, \ \{x'_i\}_{i=1}^n \sim Q$$

# RKHS EMBEDDING: ESTIMATION

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## ➔ What about the MMD sensitivity index ?

$$S_i = \mathbb{E}_{X_i} \left( \mathrm{MMD}^2(P_Y, P_{Y|X_i}) \right)$$

- Brute-force Monte-Carlo very expensive
- Possible to use Pick & Freeze estimation
- Ongoing investigation of replicated designs to get rid of the input dimension

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*If you want to use a surrogate model bsaed on kriging, ask me the question at the end of the talk !*

- Brute-force Monte-Carlo very expensive
- Possible to use Pick & Freeze estimation
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# RKHS EMBEDDING: FEATURE SELECTION

➔ **We can go even further !**

# RKHS EMBEDDING: FEATURE SELECTION

- We can go even further !
- Remember the density-based index

$$S_i^{KL} = \int p_{Y|X_i=x}(y) \ln \left( \frac{p_{Y|X_i=x}(y)}{p_Y(y)} \right) p_{X_i}(x) dx dy$$

# RKHS EMBEDDING: FEATURE SELECTION

- **We can go even further !**
- **Remember the density-based index**

$$
\begin{aligned}
S_i^{KL} &= \int p_{Y|X_i=x}(y) \ln \left( \frac{p_{Y|X_i=x}(y)}{p_Y(y)} \right) p_{X_i}(x) dx dy \\
&= \int p_{Y,X_i}(y,x) \ln \left( \frac{p_{Y,X_i}(y,x)}{p_Y(y) p_{X_i}(x)} \right) dx dy = I(X_i;Y)
\end{aligned}
$$

*Mutual Information*

- **In this case, the sensitivity index is a dependence measure between random variables**

# RKHS EMBEDDING: FEATURE SELECTION

- **From a broad perspective, a dependence measure compares the joint distribution and the product of the marginals**
  - If close, the variables are dependent
  - How do we compare the joint distribution and the product of the marginals ?

# RKHS EMBEDDING: FEATURE SELECTION

- **From a broad perspective, a dependence measure compares the joint distribution and the product of the marginals**
  - If close, the variables are dependent
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$$\begin{aligned}
\mathrm{MMD}^2\left(P_{Y,X}, P_Y P_X\right) &= \left(\sup_{f \in F}\left[\mathbb{E}_{P_{XY}} f(x,y) - \mathbb{E}_{P_X P_Y} f(x,y)\right]\right)^2 \\
&= \|\mu_{P_{XY}} - \mu_{P_X P_Y}\|^2_{\mathcal{F}\times\mathcal{G}} \\
&= \mathrm{HSIC}(X,Y)
\end{aligned}$$

Hilbert-Schmidt Independence Criterion
Gretton 2005

# RKHS EMBEDDING: FEATURE SELECTION

➔ **HSIC estimation from a sample of the joint distribution**

$$\widehat{\mathrm{HSIC}}(X,Y) = \frac{1}{n^2}\mathrm{trace}\left(KHLH\right)$$

$$[K]_{ij} = k_{\mathcal{X}}(x_i, x_j) \qquad [L]_{ij} = k_{\mathcal{Y}}(y_i, y_j) \qquad [H]_{ij} = \delta_{ij} - \frac{1}{n}$$

$$\{(x_i, y_i)\}_{i=1}^{n} \sim P_{XY}$$

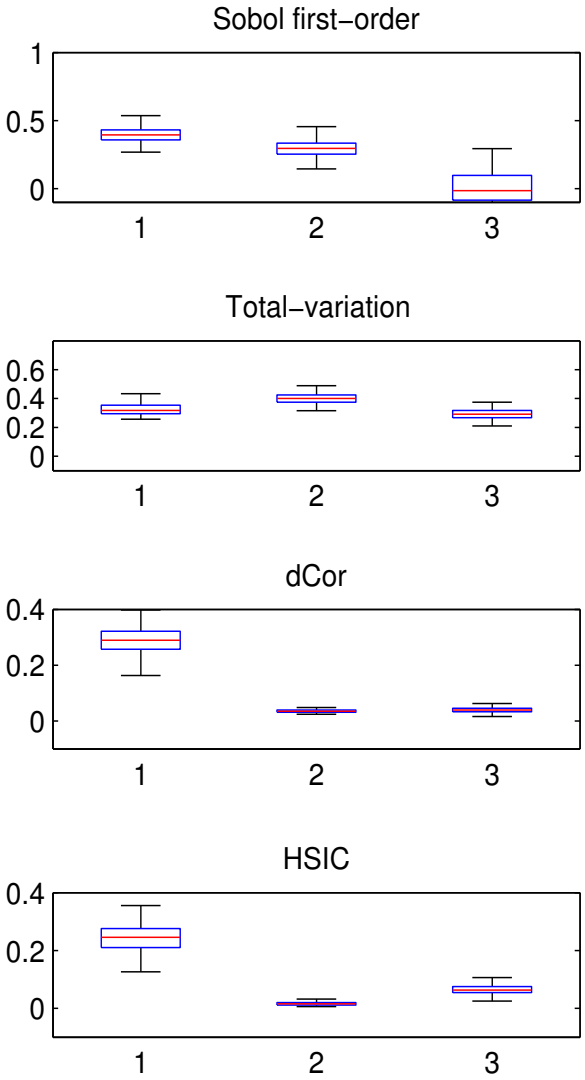
➔ **Several feature selection techniques based on this measure**

- Song et al. (2007a,b,c), Balasubramanian et al. (2013), Yamada et al. 2013

# RKHS EMBEDDING: FEATURE SELECTION

- **In a GSA context, just rank the input parameters according to their HSIC value with the output**
  - A normalization inspired by SRC is proposed in D. (2014)

- **Good screening properties**
  - At a very low computational cost (~ 100, independent of the input dimension)



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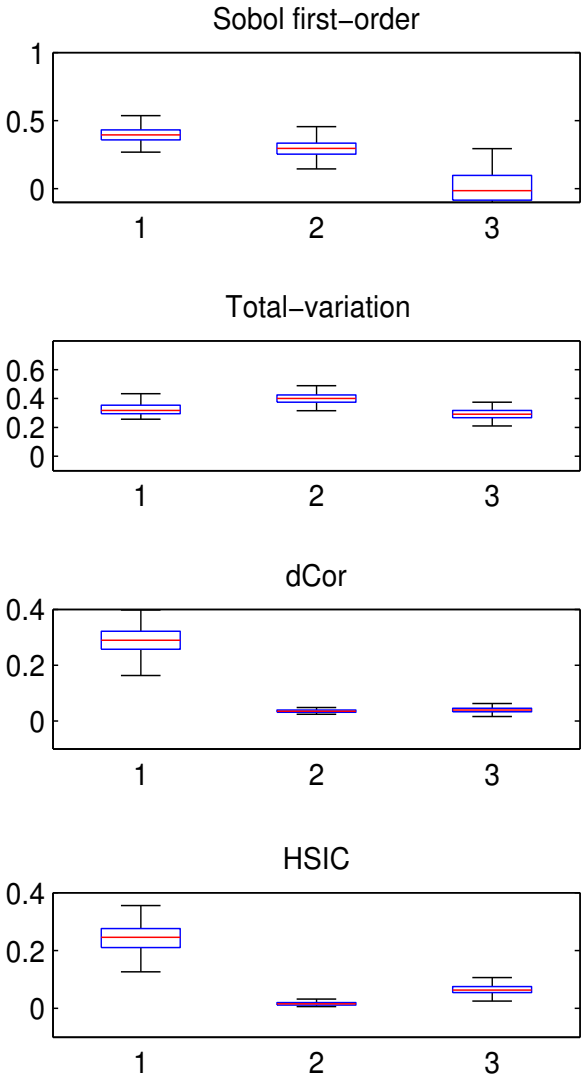
  - A normalization inspired by SRC is proposed in D. (2014)
- **Good screening properties**
  - At a very low computational cost (~ 100, independent of the input dimension)
- **Would be great if we could use this measure as a sensitivity index**
  - With particular case the MMD indices
  - With a decomposition
  - **Link between feature selection and GSA**



# RKHS EMBEDDING: DECOMPOSITION II

➔ **Theorem (D. 2016)**

$$\mathrm{HSIC}\left(Y, X_{1:d}\right) = \sum_{u \subseteq \{1,\ldots,p\}, u \neq \emptyset} g_u$$

$$g_u = \sum_{v \subseteq u} (-1)^{|u|-|v|} \mathrm{HSIC}\left(Y, X_v\right)$$

If the kernel on each input satisfies

$$\int_{\mathcal{X}} k_{\mathcal{X}}(x, x') dP_X(x) = 1$$

$$\begin{aligned}
k_{\mathcal{X}} &= 1 + k^0_{\mathcal{X}} \\
k^0_{\mathcal{X}}(x, x') &= k(x, x') - \frac{\int_{\mathcal{X}} k(x, x') dP_X(x') \int_{\mathcal{X}} k(x, x') dP_X(x)}{\iint_{\mathcal{X} \times \mathcal{X}} k(x, x') dP_X(x) dP_X(x')} \\
k^0_{\mathcal{X}}(x, x') &= k(x, x') - \int_{\mathcal{X}} k(x, x') dP_X(x') - \int_{\mathcal{X}} k(x, x') dP_X(x) \\
&\quad + \iint_{\mathcal{X} \times \mathcal{X}} k(x, x') dP_X(x) dP_X(x')
\end{aligned}$$

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$$S_u^{\mathrm{HSIC}} = \frac{\sum_{v \subseteq u} (-1)^{|u|-|v|} \mathrm{HSIC}\left(Y, X_v\right)}{\mathrm{HSIC}\left(Y, X_{1:d}\right)}$$

# RKHS EMBEDDING: DECOMPOSITION II

## ➔ More remarks

- You have to choose a kernel for each input and output
- **If we want to detect independence, we must use a characteristic kernel**
  - e.g. Gaussian, exponential
- The decomposition holds for a centered-like kernel
  - Actually same assumption for the ANOVA-kernel of Durrande et al. (2013)

Fukumizu et al. (2008)
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Uniform inputs $k_{\mathcal{X}}(x, x') \rightarrow \delta(x, x')$

ex: $k_{\mathcal{X}}(x, x') = \frac{1}{\sqrt{2\pi a^2}} \exp\left(\frac{1}{2a^2}(x - x')^2\right), \quad a \rightarrow 0$

$$S_u^{\mathrm{HSIC}} \longrightarrow S_u^{\mathrm{MMD}}$$

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$$S_u^{\text{HSIC}} \longrightarrow S_u^{\text{MMD}}$$

$k_{\mathcal{Y}}(y, y') = yy'$

$$S_u^{\text{MMD}} = S_u^{\text{Sobol}}$$

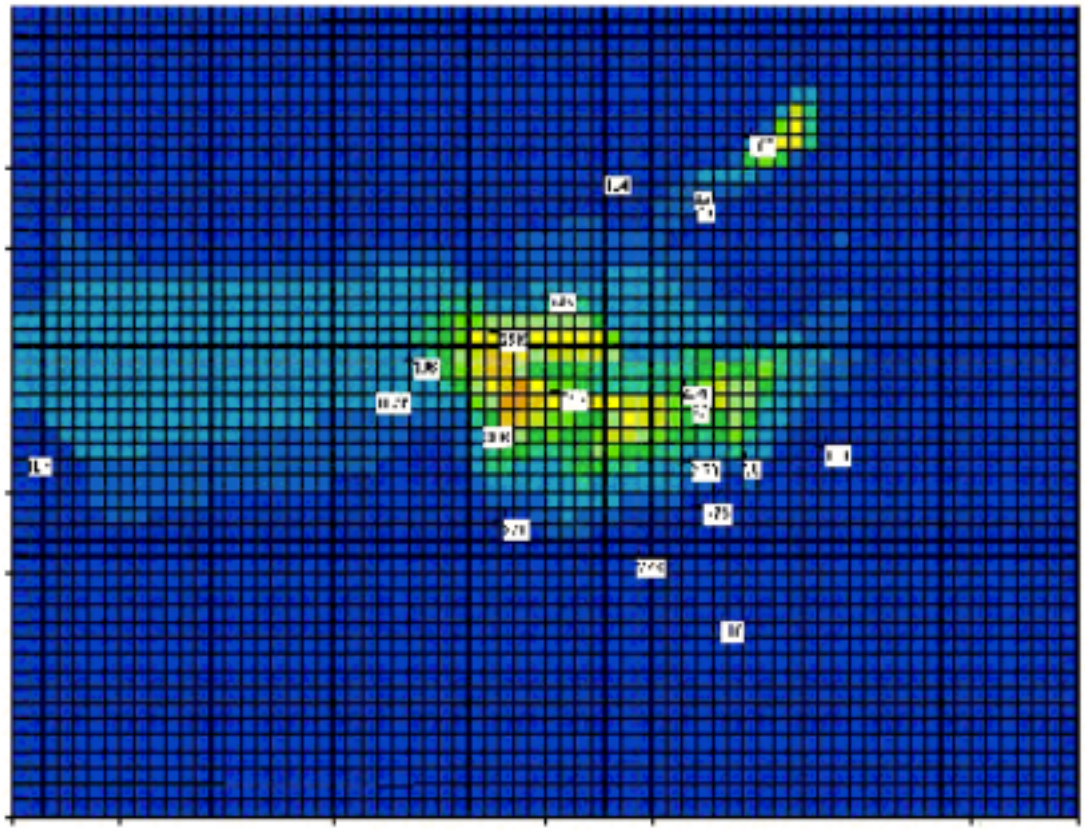
# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

- **The RKHS point of view comes with a huge literature and dedicated kernels**
  - If your inputs or outputs are vectors, curves, texts, images, timeseries, DNA sequences, probability distributions, … there is a kernel available
    - **We then have a generic GSA framework which can handle them, with a decomposition into main effects and interactions**

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

## ➔ Example 1: migration of strontium 90 in a storage site (Marthe testcase CEA)

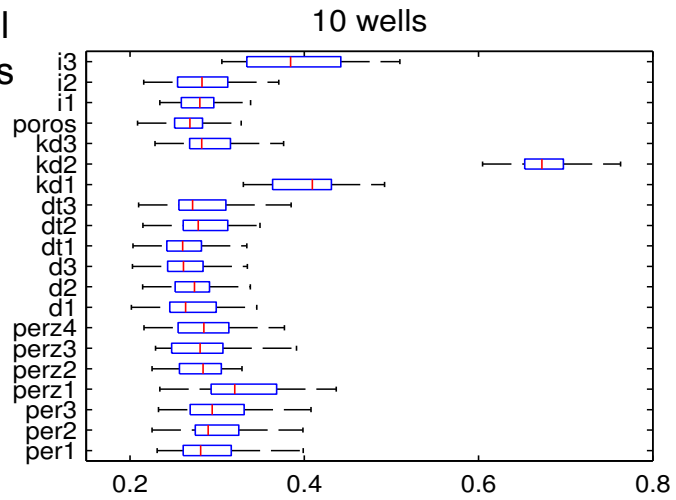
- Inputs
  - 20 geological parameters
- Outputs
  - Strontium concentration at 10 observation wells
  - 2D maps of concentration (64x64=4096 pixels)

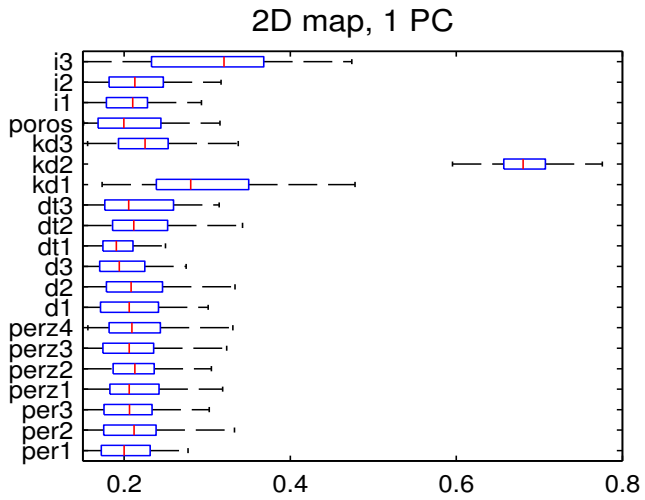


Marrel et al. 2011

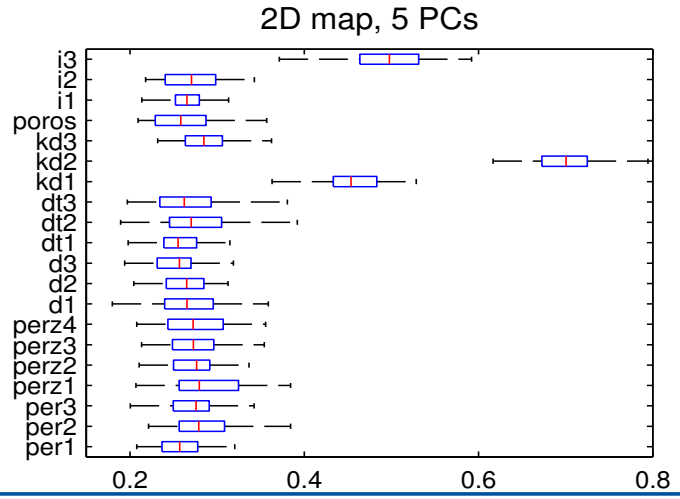
# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

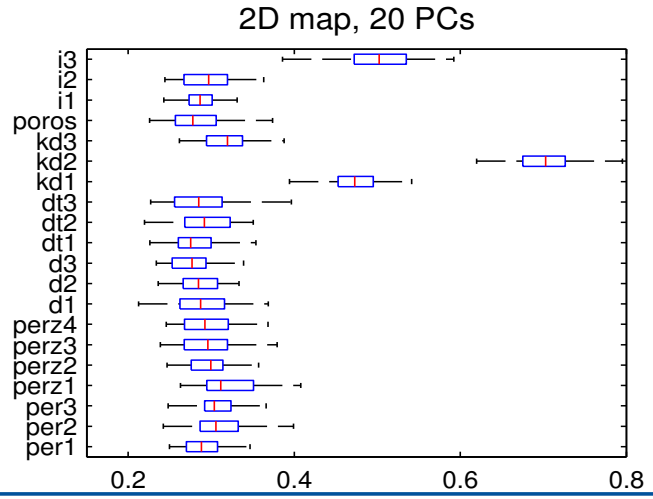
Gaussian kernel in 10 dimensions (wells)




PCA kernel on 2D maps




D. 2014

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

- **Example 2: uncertainty on the distribution assigned to the input parameters**
  - Fact: in practice it may be hard to model the uncertainty on the input parameters
    - Diverging expert judgments, no available data,…
  - Question : is it a concern for some of the inputs ?
    - In other words, if we change the probability distribution of an input, does this change the result of the sensitivity analysis ?

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

## ➔ Example 2: uncertainty on the distribution assigned to the input parameters

- Fact: in practice it may be hard to model the uncertainty on the input parameters
  - Diverging expert judgments, no available data,…

- Question : is it a concern for some of the inputs ?
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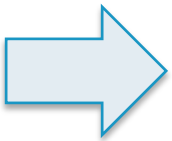
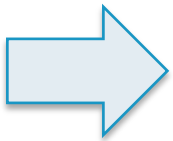
## ➔ Usual problem

$$X_1, \ldots, X_d$$

$$\mathbb{P}_{X_1}, \ldots, \mathbb{P}_{X_d}$$



**Model**
For a given value of the inputs, we compute the value of the output



$$Y$$

$$\mathbb{P}_Y$$

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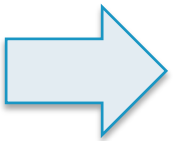
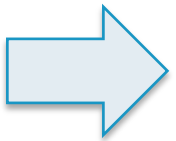
## ➔ Higher-level problem

$$\mathbb{P}_{X_1}, \ldots, \mathbb{P}_{X_d}$$

$$\mathbb{P}_{\mathbb{P}_{X_1}}, \ldots, \mathbb{P}_{\mathbb{P}_{X_d}}$$



**Model**
For a given combination of input distributions, we report the result of the sensitivity analysis



$$S_1, \ldots, S_d$$

$$\mathbb{P}_{S_1,\ldots,S_d}$$

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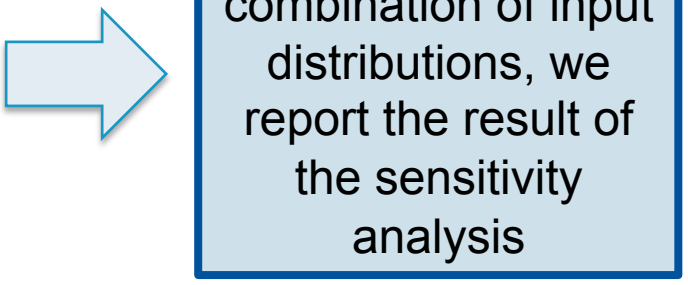


$$\ldots, S_d$$

$$\mathbb{P}_{S_1,\ldots}$$

Not necessarily what is interesting
Idea : ranking of variables

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

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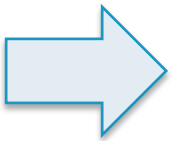

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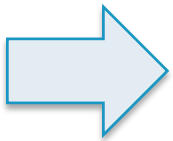

Rank of the input variables

$$R_1, \ldots, R_d$$

$$\mathbb{P}_{R_1,\ldots,R_d}$$

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

## ➔ Higher-level problem

- Goal: for each input variable, compute the HSIC index between its probability distribution and the list containing the rankings

## ➔ Is it possible ? Which kernels ?

- Kernel on the « inputs »
  - Kernel for probability distributions

- Kernel on the « output »
  - Kernel for ranking lists

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  - Kernel for probability distributions

$$k(\mathbb{P}, \mathbb{Q}) = \exp\left(-\gamma \mathrm{MMD}^2(\mathbb{P}, \mathbb{Q})\right)$$

Sriperumbudur 2010

- Kernel on the « output »
  - Kernel for ranking lists

$$k(\{R_i\}, \{R'_i\}) = \exp\left(-\gamma K(\{R_i\}, \{R'_i\})\right)$$

Jiao & Vert 2015

Kendall's Tau Distance

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

## ➔ Example 2: Ishigami function

$$Y = \sin(X_1) + 3\sin^2(X_2) + 0.1X_3^4\sin(X_1)$$

## ➔ Uncertainty on the input distributions

- With probability 1/3, uniform distribution on [0,1]
- With probability 1/3, triangular distribution on [0,1] with mode chosen uniformly in [0,1]
- With probability 1/3, truncated Gaussian distribution on [0,1] with mean chosen uniformly in [0.25,0.75] and standard deviation equal to 0.1

## ➔ Question : does the uncertainty on the input distribution have an impact on the ranking of the most influential variables

- The ranking here is performed according to 1st order Sobol indices, which are computed by Pick & Freeze with a sample of size 1000

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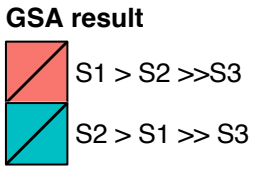


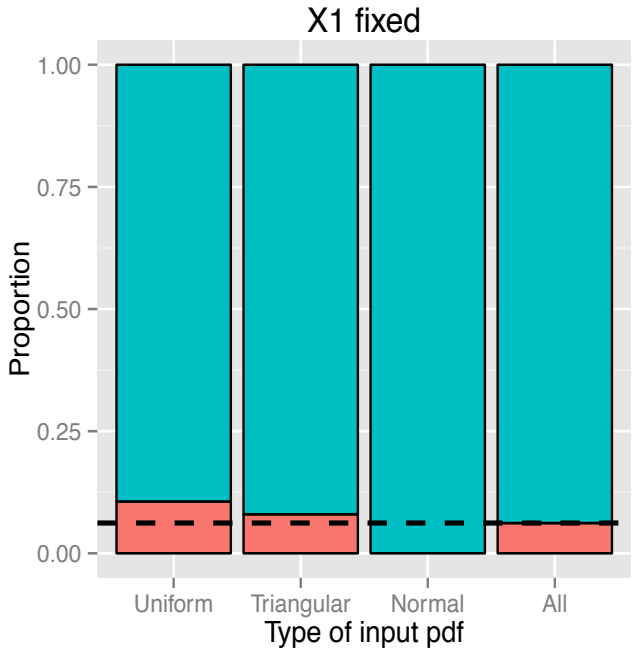


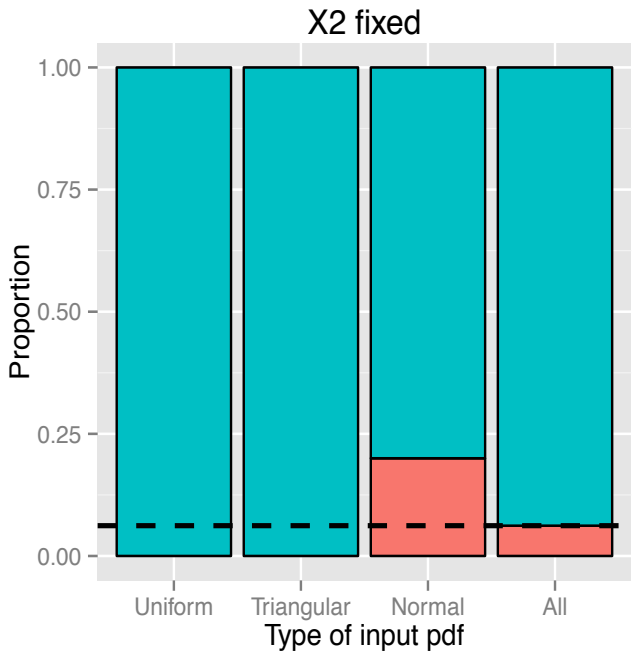


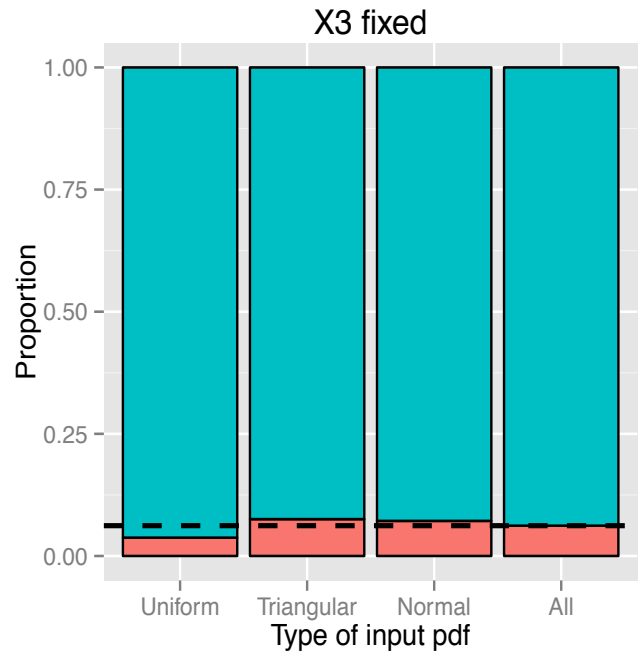

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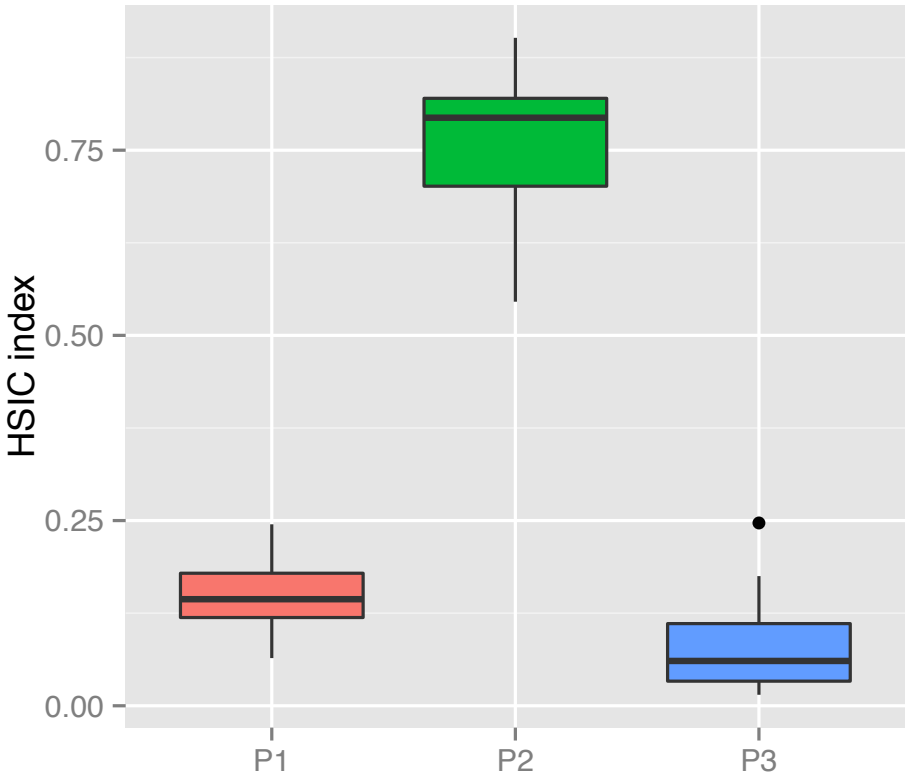


20 repetitions, 100 combinations of input distribution

- The choice of the distribution X3 does not influence the ranking
- The distribution of X2 has the highest impact: it may be interested to invest time & money to improve the knowledge of this distribution

# RKHS EMBEDDING: LET'S PLAY WITH KERNELS

- **The RKHS point of view comes with a huge literature and dedicated kernels**
  - If your inputs or outputs are vectors, curves, texts, images, timeseries, DNA sequences, probability distributions, … there is a kernel available
    - **We then have a generic GSA framework which can handle them, with a decomposition into main effects and interactions**
  - And you can recover previously studied sensitivity indices with particular kernels

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$$k_{\mathcal{X}}(x, x') \to \delta(x, x')$$

$$\text{ex: } k_{\mathcal{X}}(x, x') = \frac{1}{\sqrt{2\pi a^2}} \exp\left(\frac{1}{2a^2}(x - x')^2\right), \quad a \to 0$$

$$S_u^{\text{HSIC}} \longrightarrow S_u^{\text{MMD}}$$

$$k_{\mathcal{Y}}(y, y') = yy'$$

$$S_u^{\text{MMD}} = S_u^{\text{Sobol}}$$

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$$S_i^{\mathrm{HSIC}} \to \int_{\Omega} \left( \frac{\partial \eta(x)}{\partial x_i} \right)^2 dx$$

We recover the 1st order DGSM indices !

# CONCLUSION

➔ **New sensitivity index which generalizes GSA through the use of kernels**

$$S_u^{\mathrm{HSIC}} = \frac{\sum_{v \subseteq u} (-1)^{|u|-|v|} \mathrm{HSIC}\left(Y, X_v\right)}{\mathrm{HSIC}\left(Y, X_{1:d}\right)}$$

- In theory, this is a density-based index: better measure of the influence than a mere mean
- Limiting cases include Sobol & DGSM
- Decomposition into main effects & interactions: interpretation is possible
- Built upon a feature selection technique: the frontier between screening methods and quantitative approaches may disappear

# CONCLUSION

- **I honestly think there is potentiel there, but**
  - Extensive benchmark studies are still needed
    - In particular kernels for curves, 3D objects, …

- **From a theoretical perspective**
  - Investigate the links with ANOVA-kernels
  - See if we can recover other sensitivity indices as particular cases
  - Use replicated designs for MMD indices estimation

- **Should be soon available in the R package sensitivity**

# PRACTICAL SESSION

## ➔ Play with MMD & HSIC indices

- Try different kernels
- Investigate convergence towards Sobol
- (Play with probability measures as inputs !)
- (Play with outputs beyond scalars !)