Painless embeddings of distributions: the function space view

Part 1 - introduction to embeddings

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A Very Short Introduction to Kernels

- Hilbert space of functions $\mathcal{F}$ from $\mathcal{X}$ to $\mathbb{R}$
- RKHS: evaluation operator $\delta_x \ : \ \mathcal{F} \to \mathbb{R}, \ f \mapsto f(x)$ bounded

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$$f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{F}}$$

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- Moore-Aronszajn: Every RKHS has a UNIQUE positive definite kernel
  - ...and vice versa

Introduction to distribution embeddings

Talk Outline

- How to define a metric on the space of probability measures
  - Function revealing differences in distributions
  - Distance between means in space of features (RKHS)
  - Same thing: the MMD [Gretton et al., 2007, Borgwardt et al., 2006]

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- Related problem: independence [Gretton et al., 2008]

Function Showing Difference in Distributions (1)

- Idea: avoid density estimation when comparing distributions $\mathbf{P}$ and $\mathbf{Q}$

  [Fortet and Mourier, 1953]

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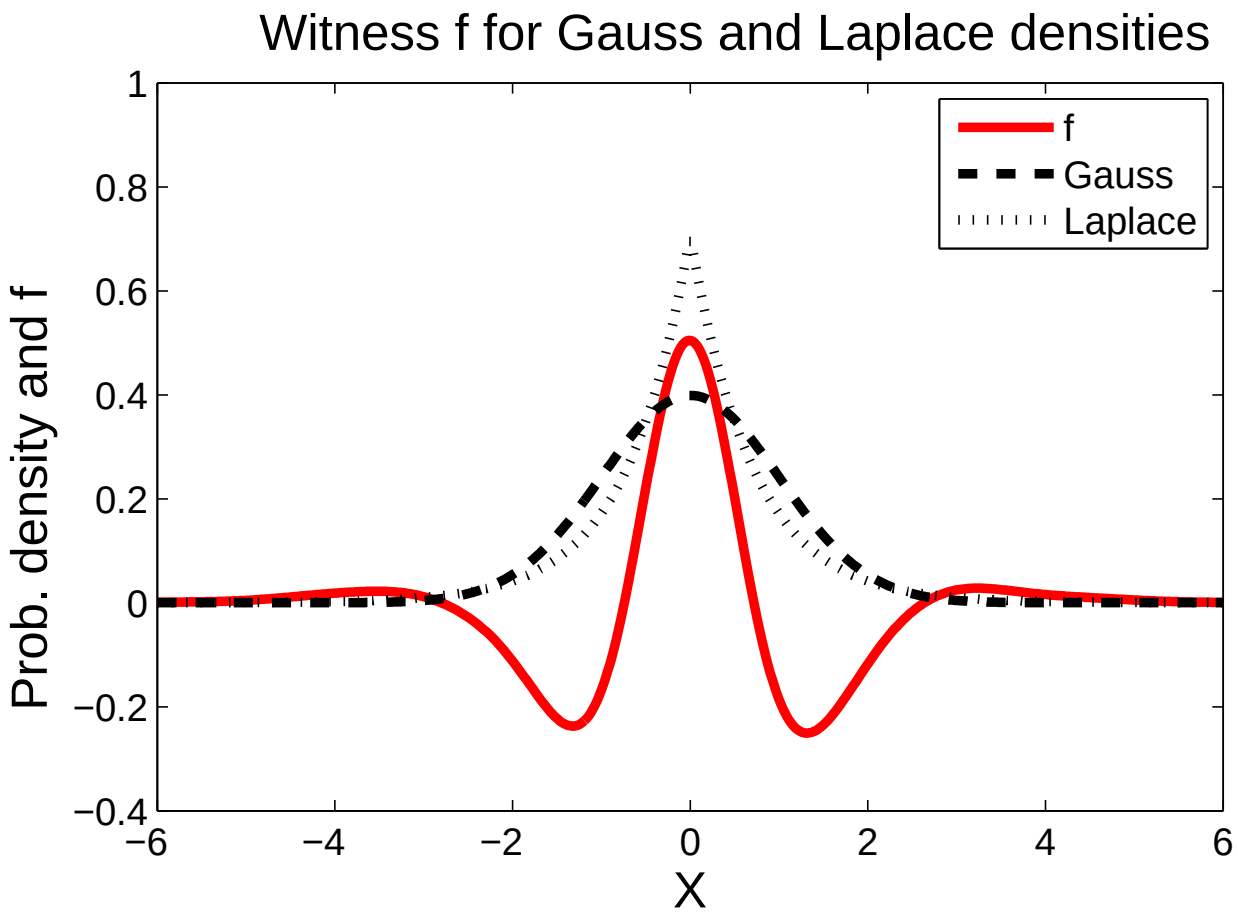
  - Examples: Gaussian, Laplace, ...

Function Showing Difference in Distributions (2)

- Gauss **P** vs Laplace **Q**



Function Showing Difference in Distributions (3)

- The (kernel) MMD:

$$\mathrm{MMD}^2(\mathbf{P}, \mathbf{Q}; F)$$

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- Reminder:

$$\mu_x := \int k(\cdot, x)\, d\mathbf{P}(x)$$

Characteristic kernels

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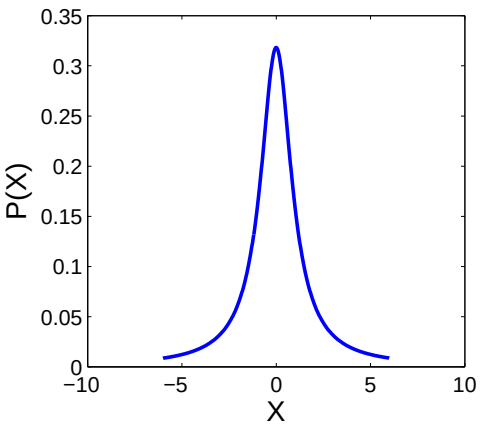
- Fourier representation of MMD:

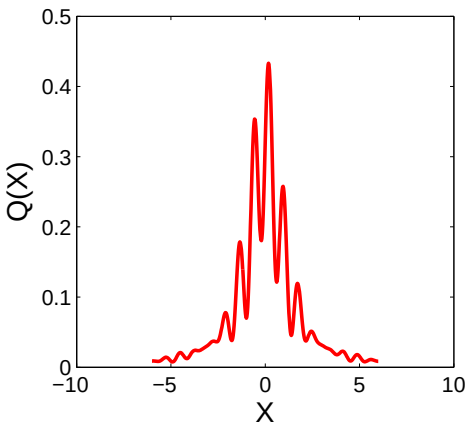
$$\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) := \left\| \left[\left(\bar{\phi}_{\mathbf{P}} - \bar{\phi}_{\mathbf{Q}} \right) \Lambda \right]^\vee \right\|_{\mathcal{F}}$$

  - $\phi_{\mathbf{P}}$ characteristic function of $\mathbf{P}$
  - $f^\wedge$ is Fourier transform, $f^\vee$ is inverse fourier transform

Characteristic Kernels (2)

- Example: **P** differs from **Q** at (roughly) one frequency





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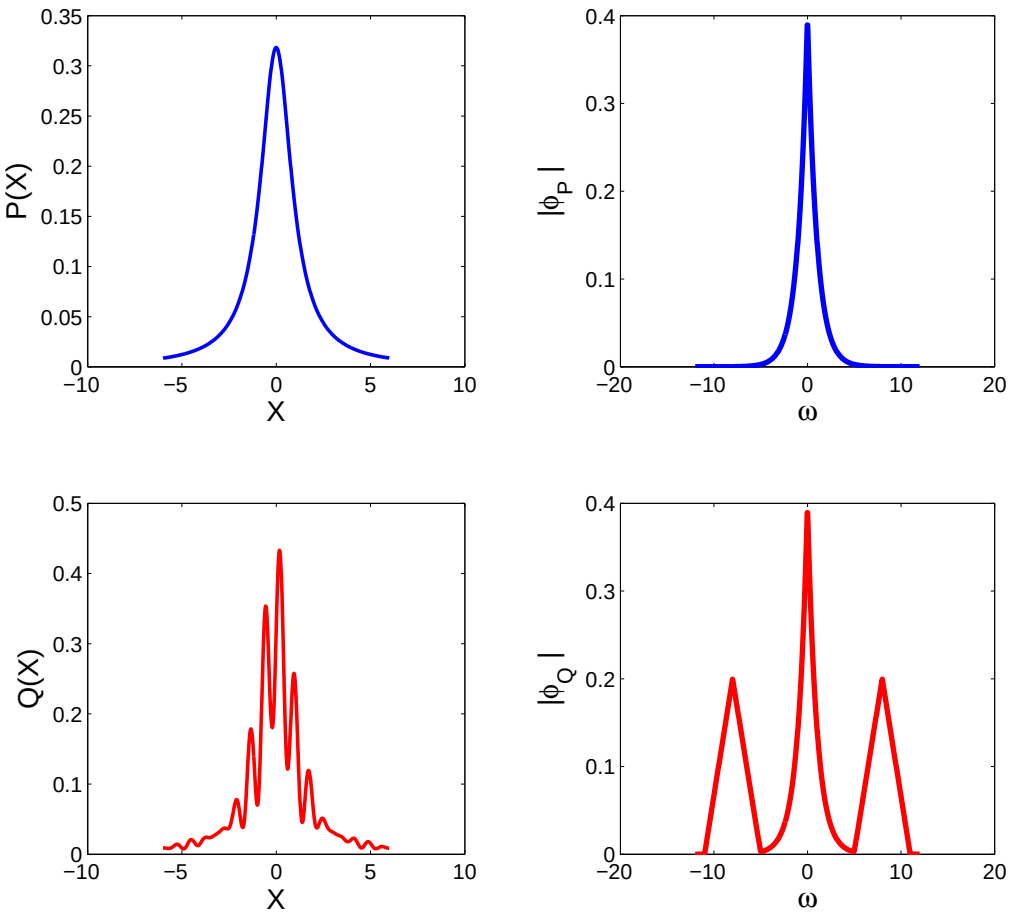

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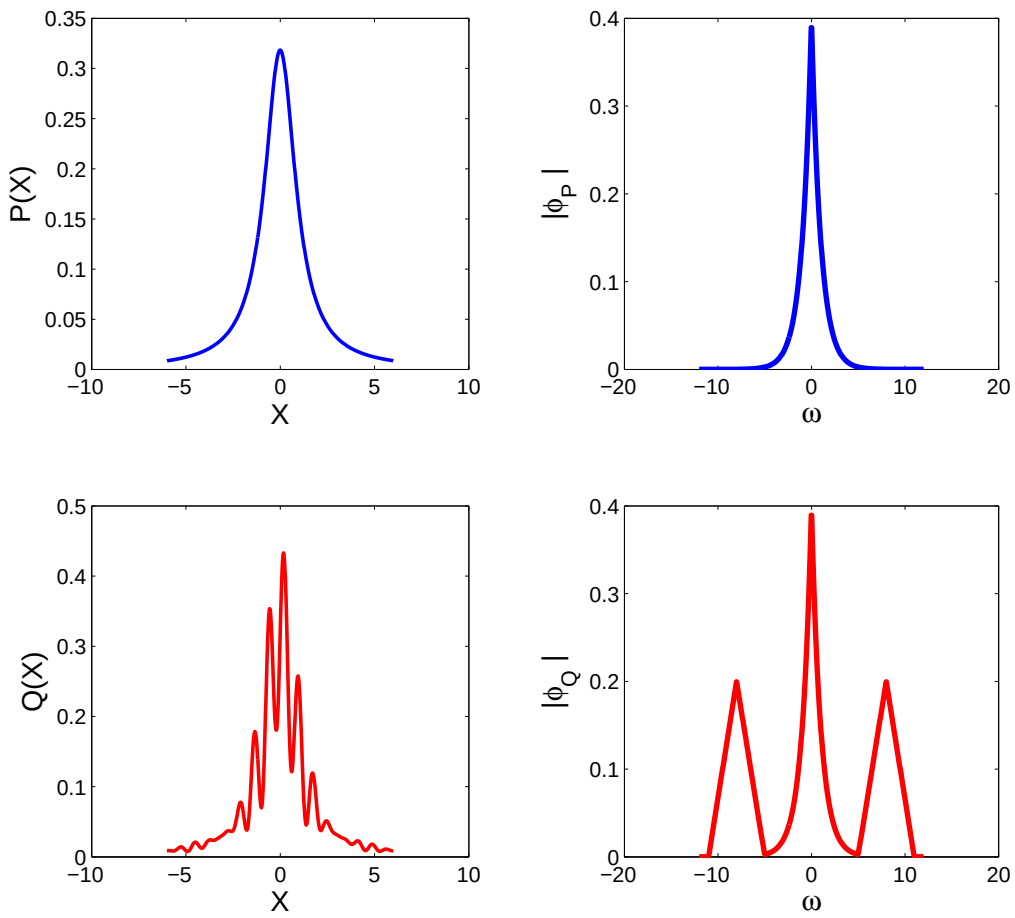
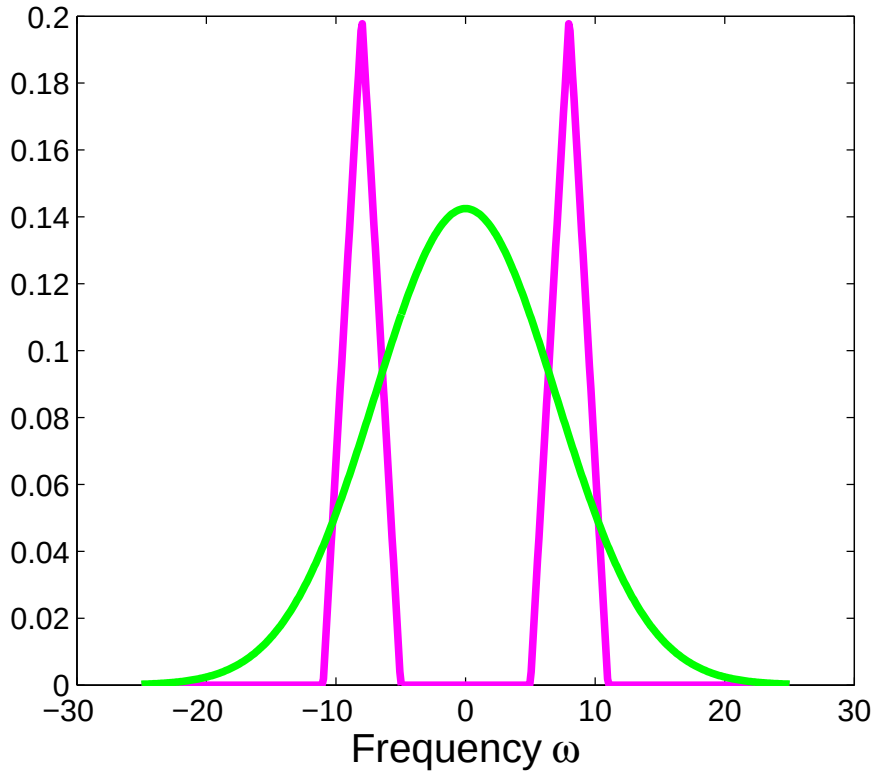


- **Gaussian** kernel
- Difference in distribution spectra



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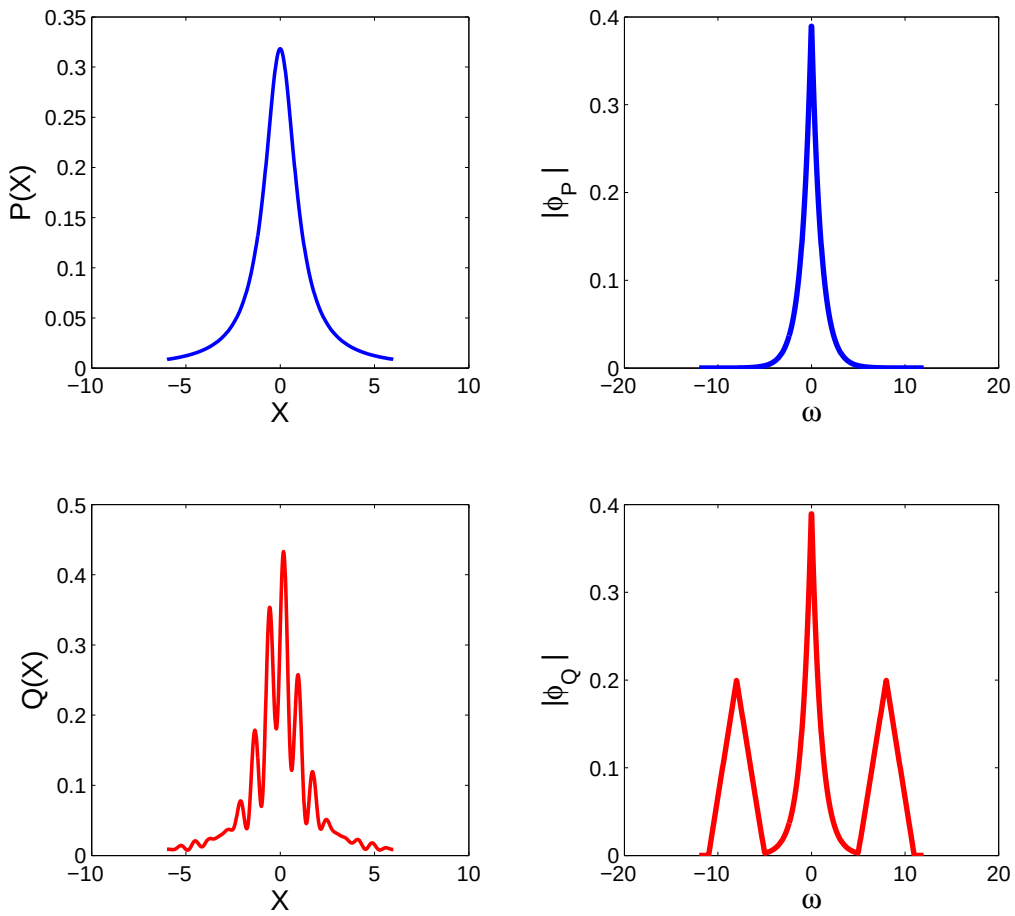

- **Gaussian** kernel characteristic
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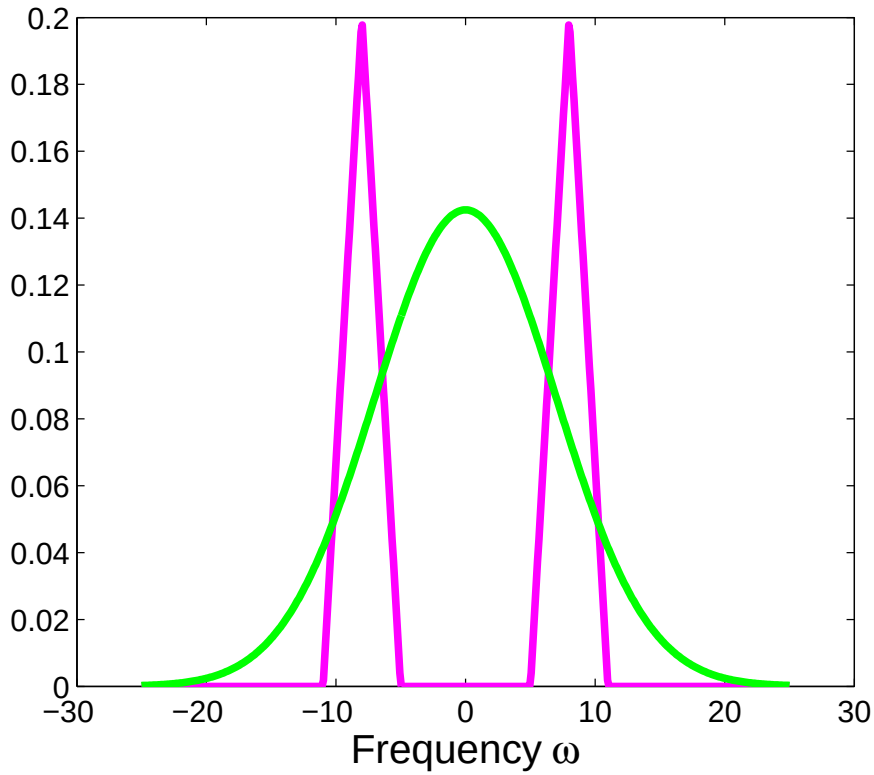

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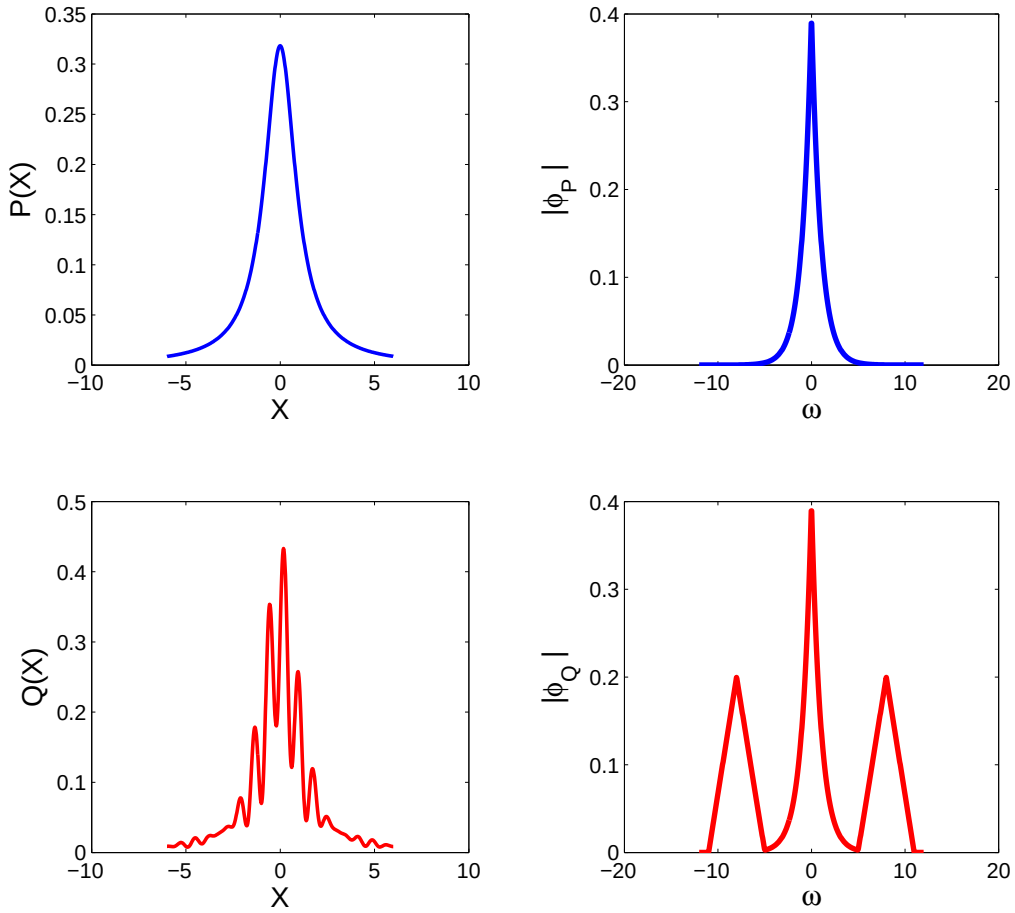
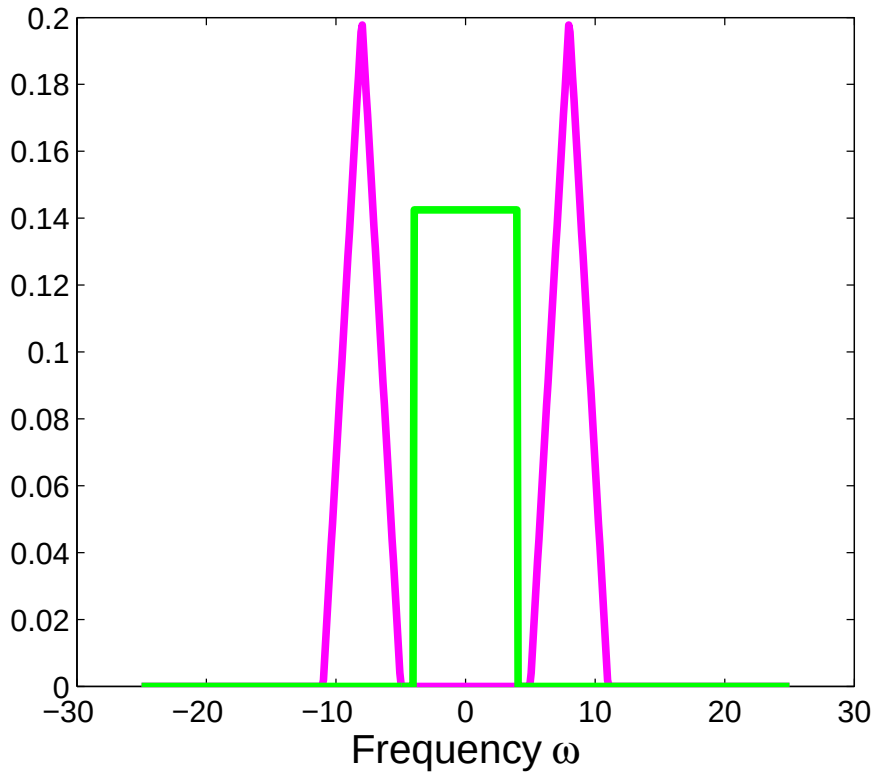


- **Sinc** kernel NOT characteristic
- Difference in distribution spectra



Characteristic Kernels (4)

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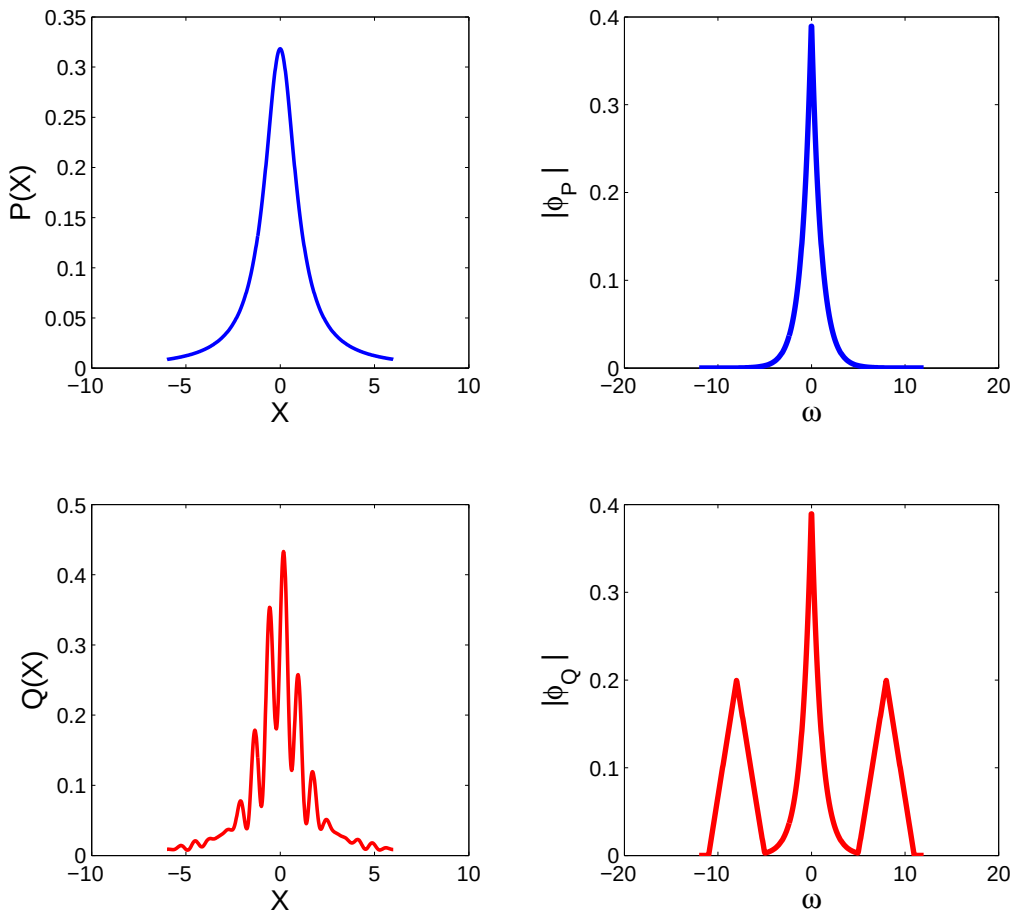
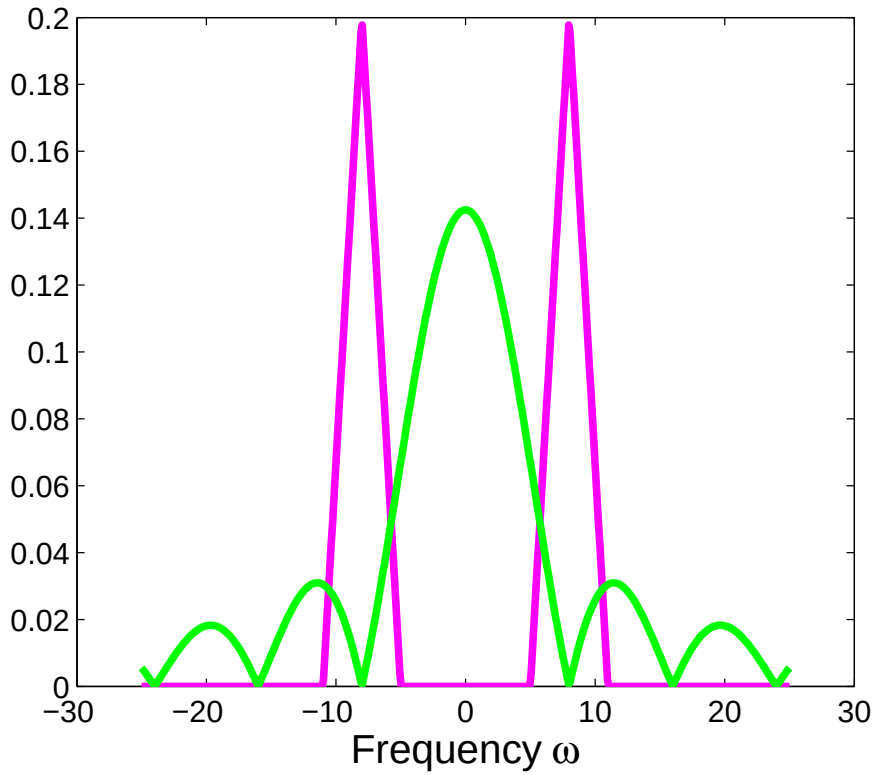


- **B-Spline** kernel ???
- Difference in distribution spectra



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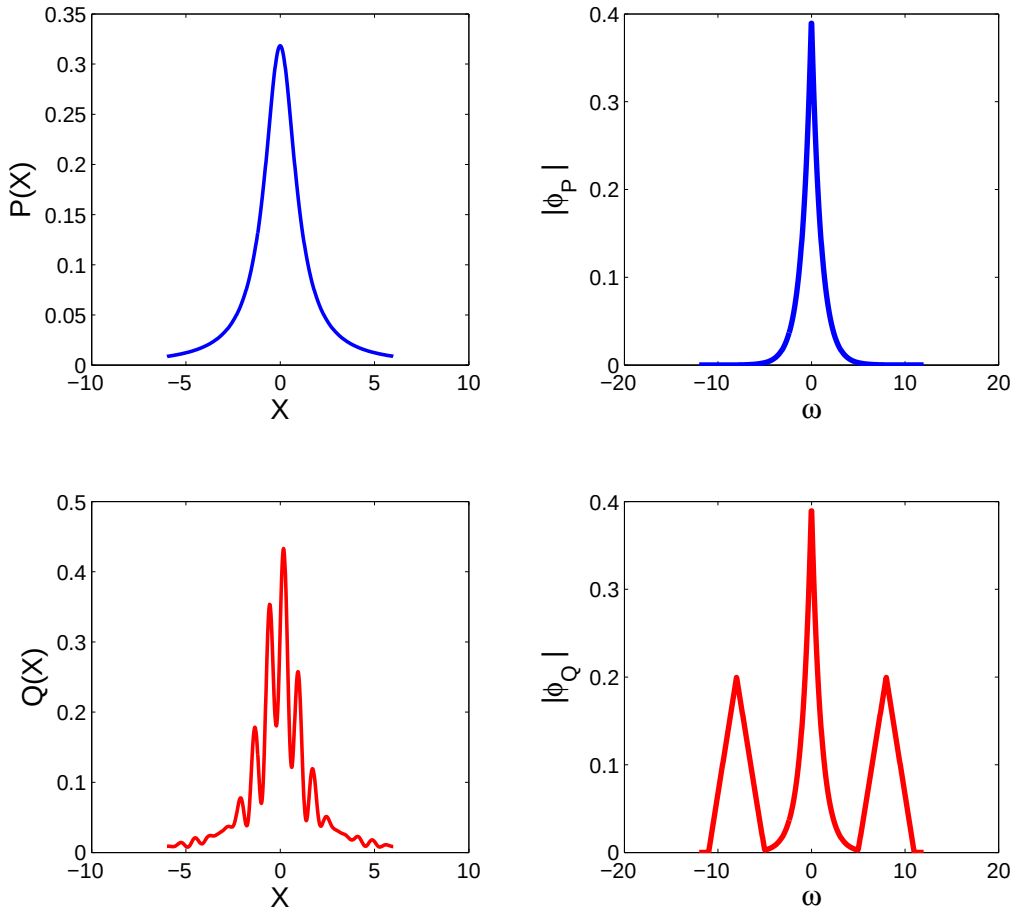

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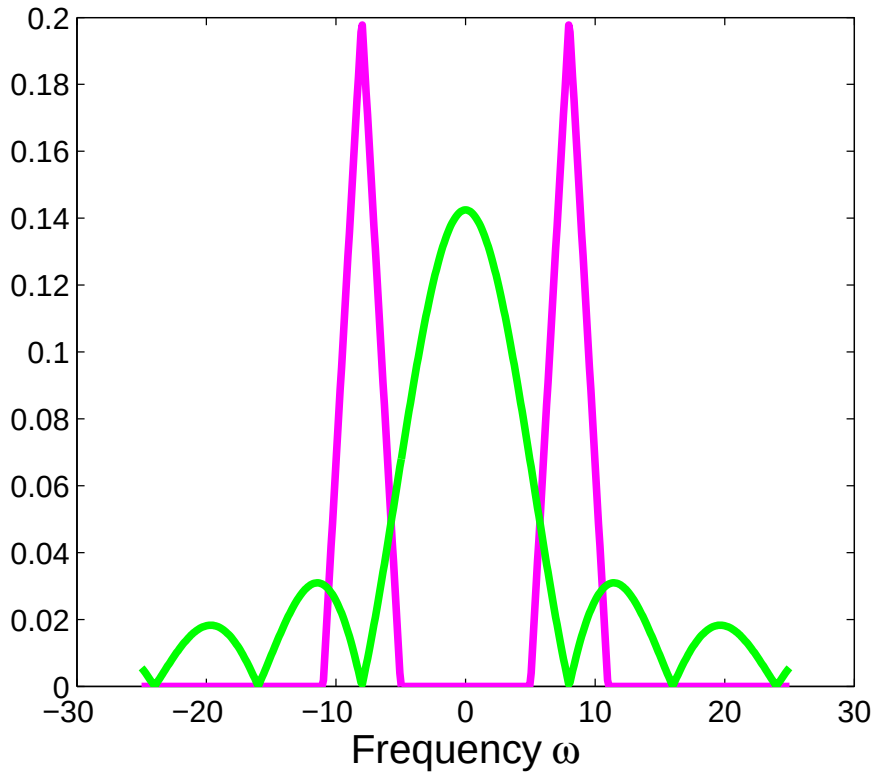

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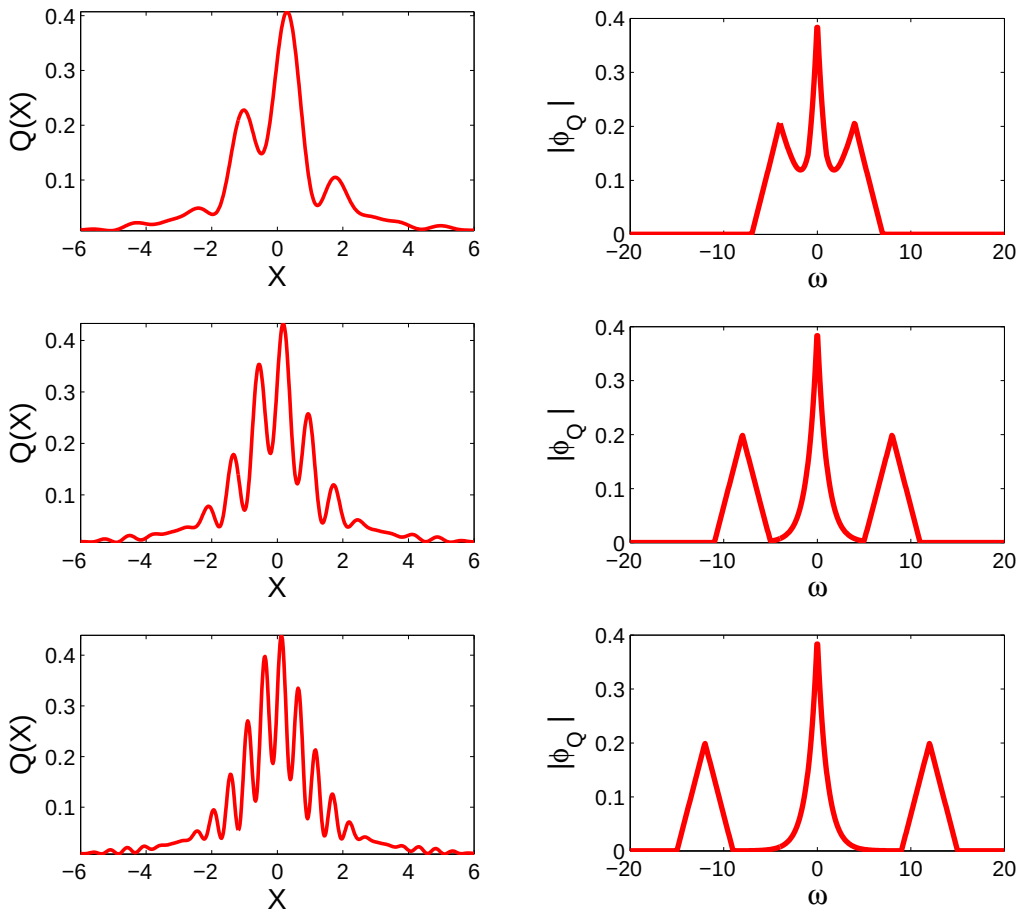
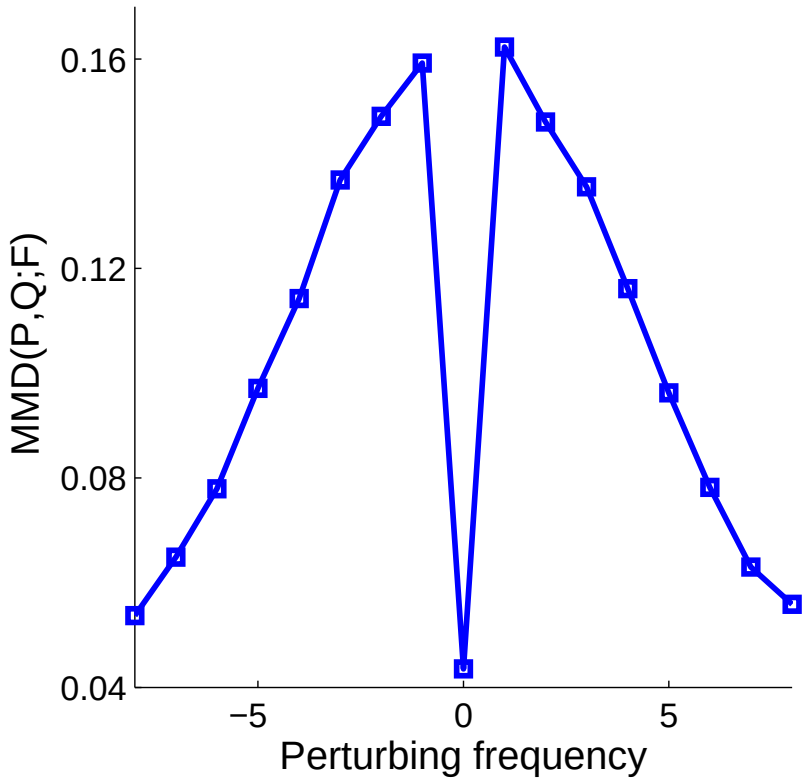
- Another example: universal kernels on compact domains, includes NON-translation invariant [Steinwart, 2001]
- Similar reasoning wherever extensions of Bochner's theorem exist:
  - Locally compact Abelian groups (periodic domains)
  - Compact, non-Abelian groups (orthogonal matrices)
  - The semigroup $\mathbb{R}_n^+$ (histograms)

Kernel Choice (1)

- Gaussian kernel example



- MMD vs frequency of perturbation to **P**



Kernel Choice (2)

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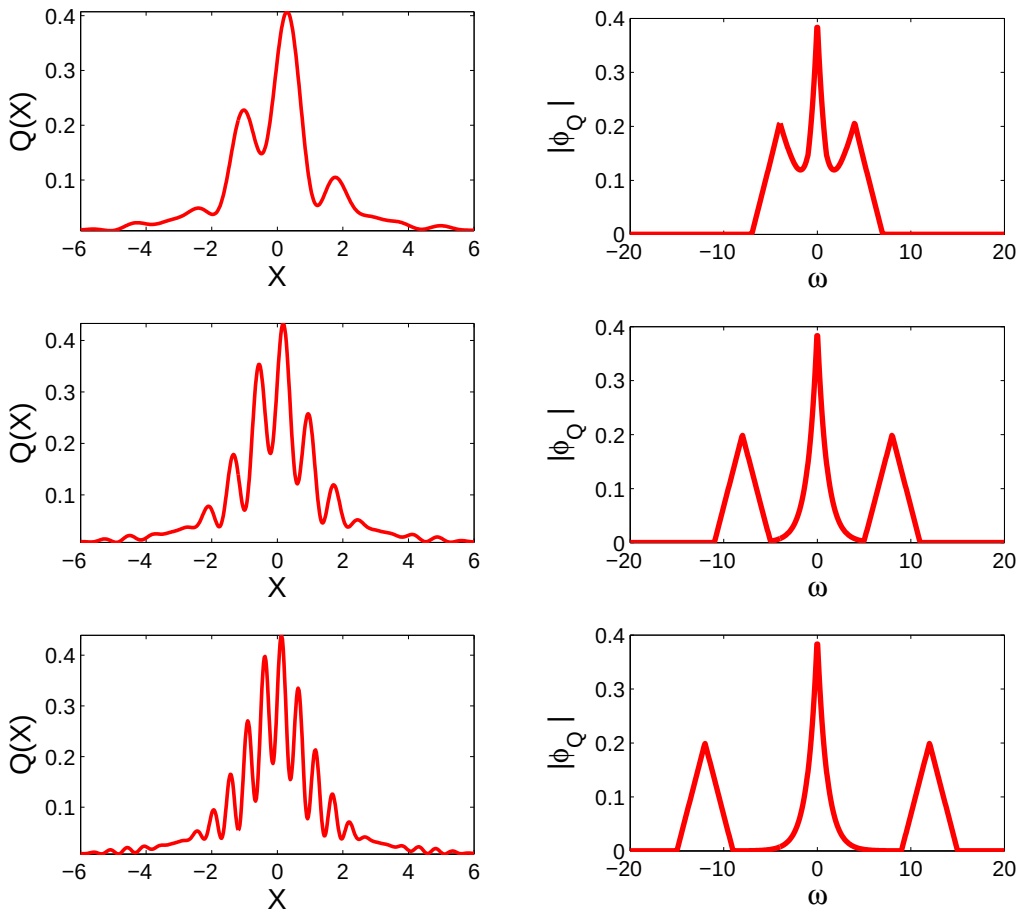

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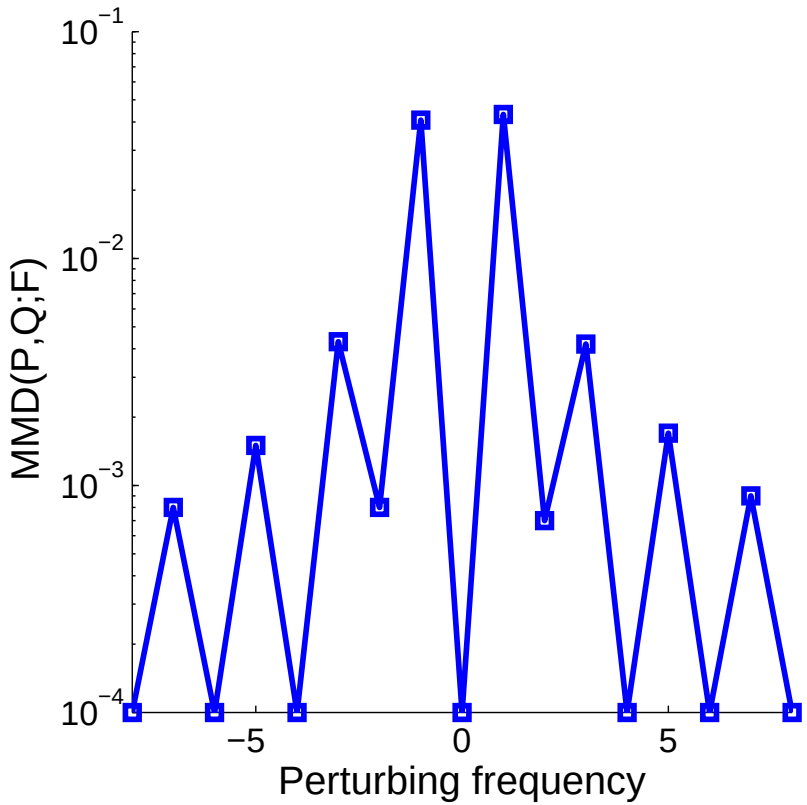

Dependence detection using MMD

MMD for Independence (1)

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- MMD between mapping of $\mathbf{P}$ and mapping of $\mathbf{P}_x\mathbf{P}_y$
- Covariance operators in spaces of features
  - Spectral norm (COCO) [Gretton et al., 2005b,c]
  - Hilbert-Schmidt norm (HSIC) [Gretton et al., 2005a]

MMD for Independence (2)

- $\mathcal{F}$ with kernel $k(x, x')$, $\mathcal{G}$ with kernel $l(y, y')$
- Define the product space $\mathcal{F} \times \mathcal{G}$ with kernel

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and

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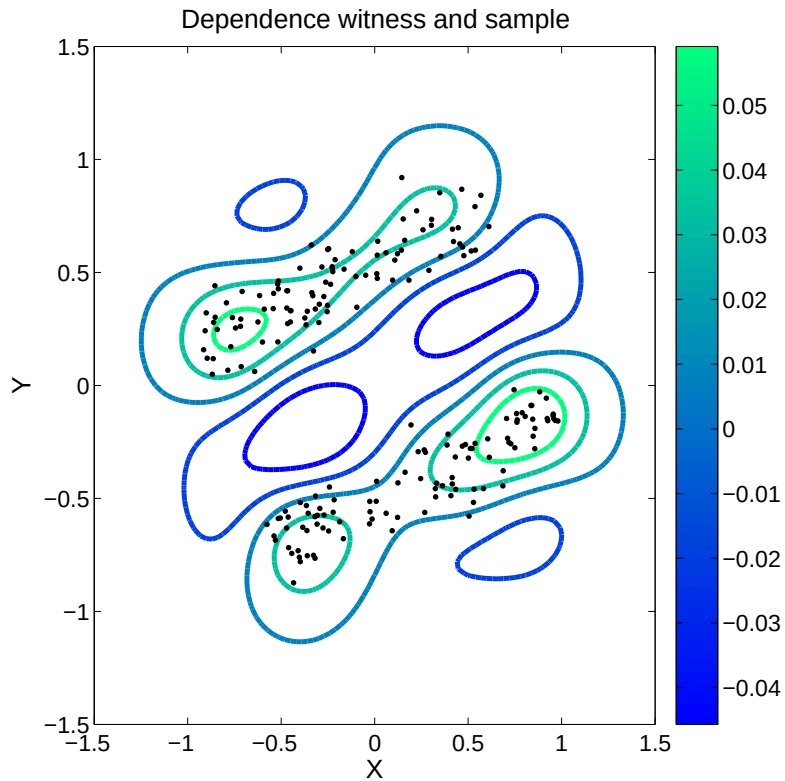
- The squared distance between these two mean elements is

$$\begin{aligned} \mathrm{MMD}^2(\mathbf{P}, \mathbf{P}_{\mathsf{x}} \mathbf{P}_{\mathsf{y}}; F \times G) &= \|\mu_{xy} - \mu_{x \perp\!\!\!\perp y}\|^2_{\mathcal{F} \times \mathcal{G}} \\ &=: \mathrm{HSIC}(\mathbf{P}, F, G) \end{aligned}$$

MMD for Independence (3)

- Witness function:

$$\sup_{\|f\|\leq 1} \langle f, \mu_{xy} - \mu_{x\perp\!\!\!\perp y} \rangle_{\mathcal{F}\times\mathcal{G}} = \|\mu_{xy} - \mu_{x\perp\!\!\!\perp y}\|_{\mathcal{F}\times\mathcal{G}}$$



Covariance in RKHS (1)

- Idea: avoid density estimation when testing $\mathbf{P} = \mathbf{P}_x \mathbf{P}_y$ [Rényi, 1959]

$$\mathrm{COCO}(\mathbf{P}; F, G) := \sup_{f \in F, g \in G} \left(\mathbf{E}_{\mathsf{x},\mathsf{y}}[f(\mathsf{x})g(\mathsf{y})] - \mathbf{E}_{\mathsf{x}}[f(\mathsf{x})]\mathbf{E}_{\mathsf{y}}[g(\mathsf{y})] \right)$$

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More formally:

- Covariance operator: $\Sigma_{xy} : \mathcal{G} \to \mathcal{F}$ such that

$$\langle f, \Sigma_{xy} g \rangle_{\mathcal{F}} = \mathbf{E}_{\mathsf{x},\mathsf{y}}[f(\mathsf{x})g(\mathsf{y})] - \mathbf{E}_{\mathsf{x}}[f(\mathsf{x})]\mathbf{E}_{\mathsf{y}}[g(\mathsf{y})]$$

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- COCO is the spectral norm of Σ_{xy} [Gretton et al., 2005b,c]:

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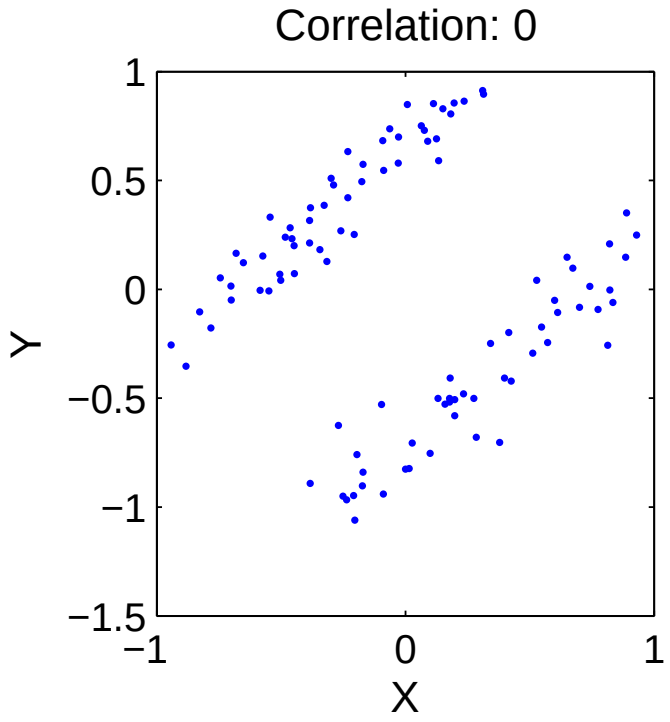
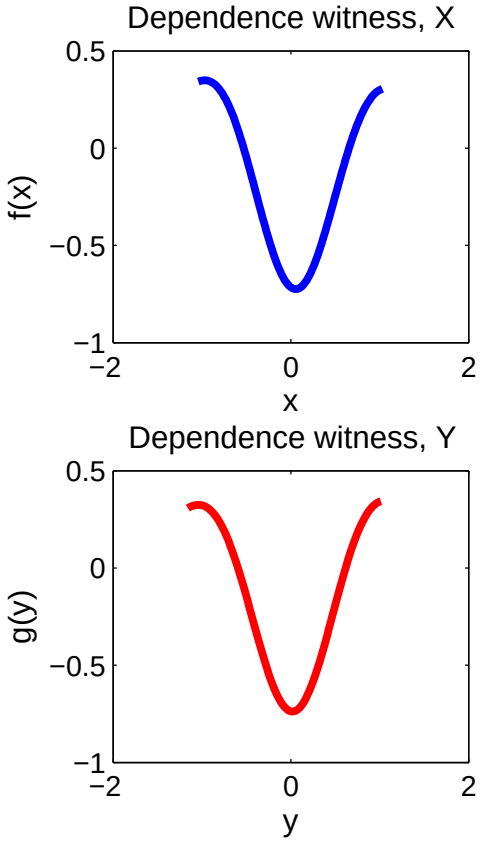
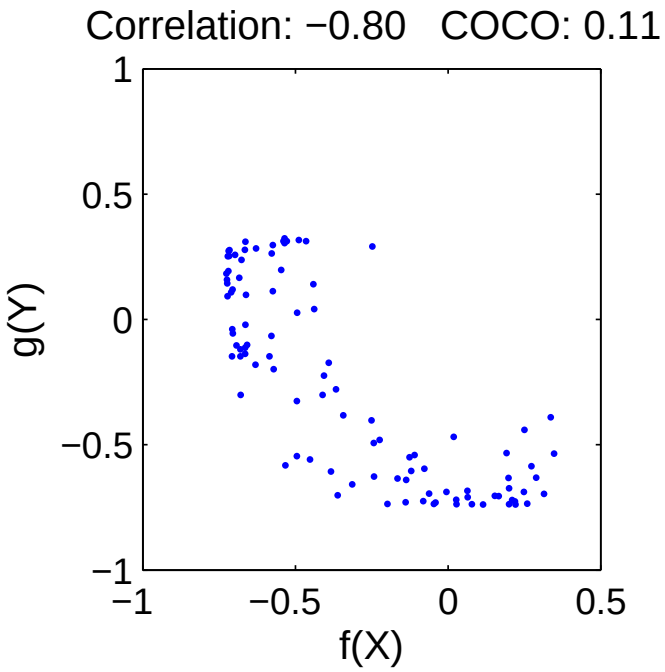
Covariance in RKHS (2)

- Example: variables with zero correlation
- Can we do better?







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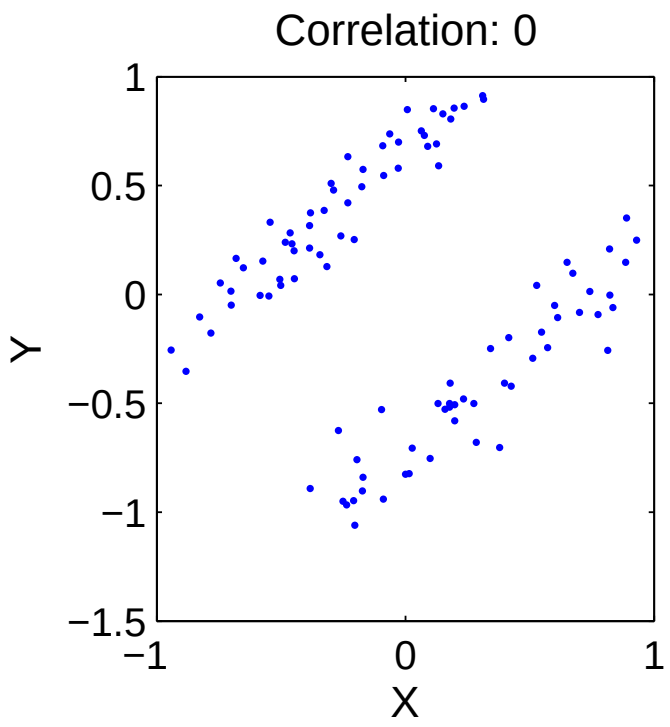

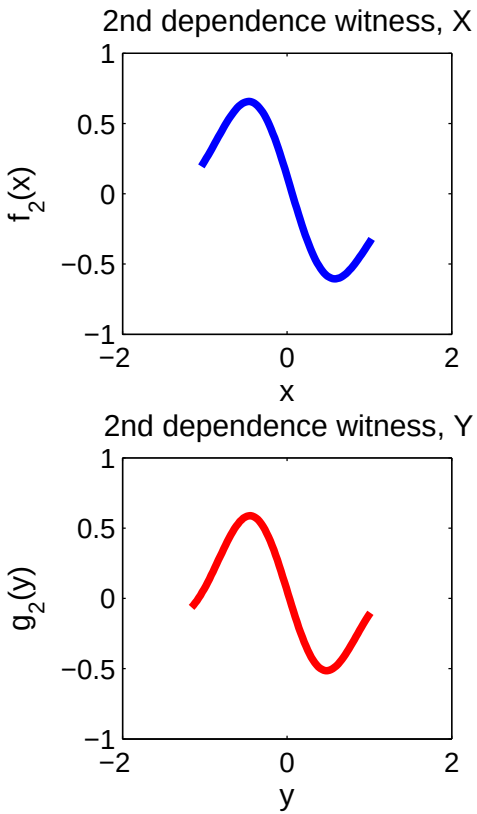

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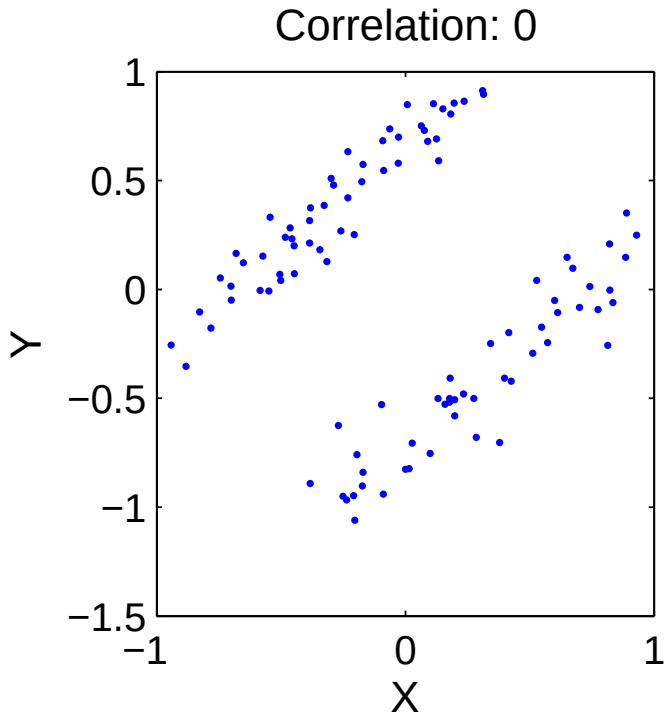

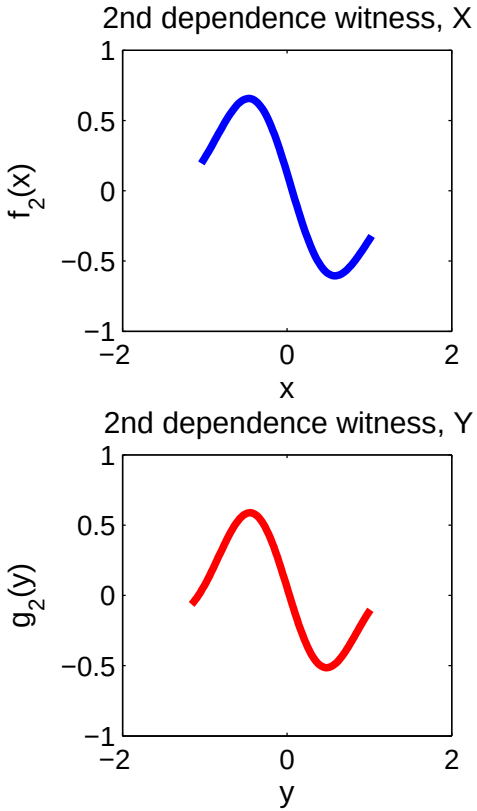

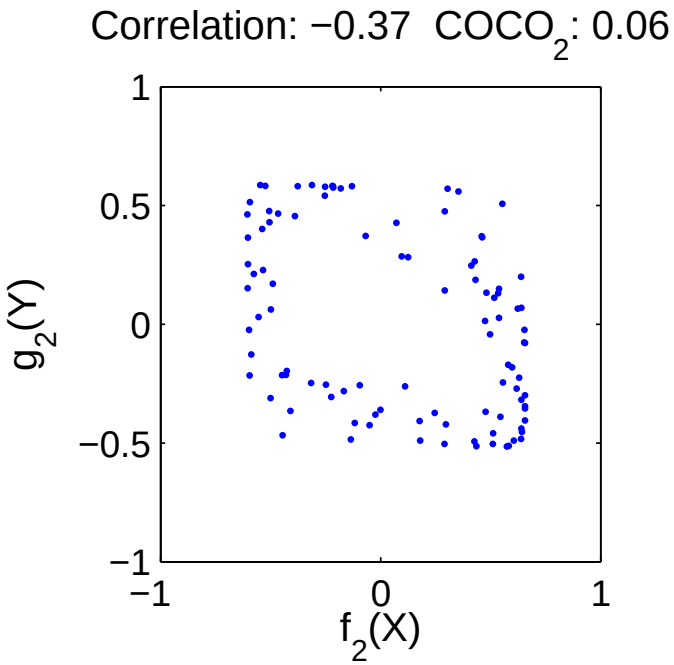

Hilbert-Schmidt Independence Criterion

- Given $\gamma_i := \mathrm{COCO}_i(\boldsymbol{z}; F, G), \quad \boldsymbol{z} := \{(x_1, y_1), \ldots, (x_m, y_m)\}$
- Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005a]

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- (Biased) empirical HSIC a v-statistic

$$HSIC(\boldsymbol{z}; F, G) := \frac{1}{m^2}\mathrm{trace}(\mathbf{KHLH}) \qquad H = I - \frac{1}{m}\mathbf{1}\mathbf{1}^\top$$

End of Part 1

- Embeddings of distributions into RKHSs
- Injective for characteristic kernels
  - Easy to check for translation invariant kernels: support of spectrum is $\mathbb{R}^d$.
- HSIC: distance between embedding of $\mathbf{P}$ and of $\mathbf{P}_{\mathsf{x}}\mathbf{P}_{\mathsf{y}}$
- Next part:

$$HSIC(\boldsymbol{z}; F, G) := \frac{1}{m^2}\mathrm{trace}(\mathbf{KHLH})$$

Questions?

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