# Lecture 2: Mappings of Probabilities to RKHS and Applications

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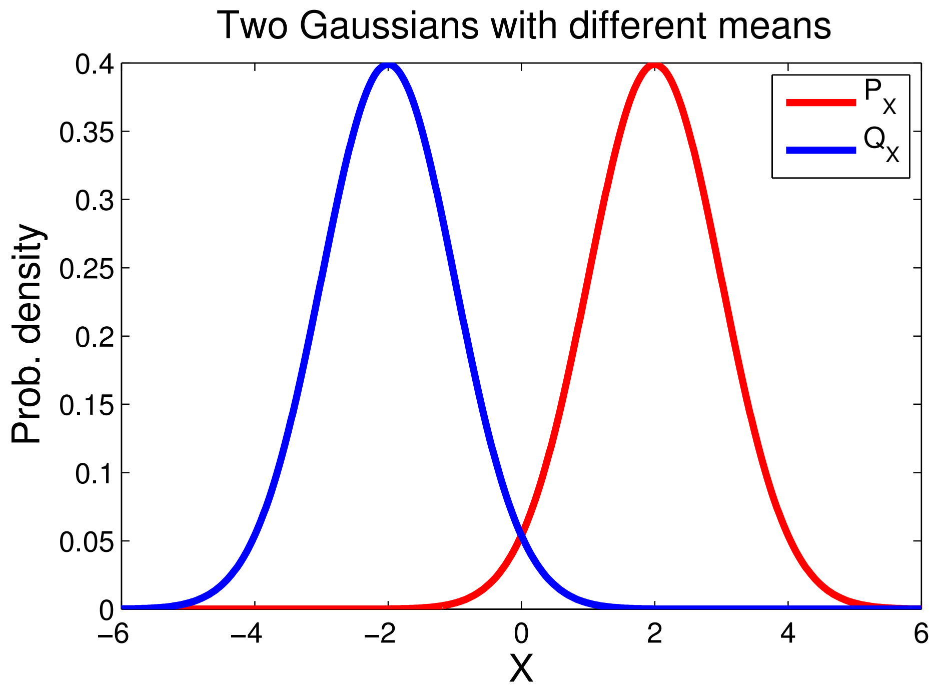
# Outline

- Kernel metric on the space of probability measures
  - Function revealing differences in distributions
  - Distance between means in space of features (RKHS)
  - Independence measure: features of joint minus product of marginals
- Characteristic kernels: feature space mappings of probabilities unique
- Two-sample, independence tests for (almost!) any data type
  - distributions on strings, images, graphs, groups (rotation matrices), semigroups,...

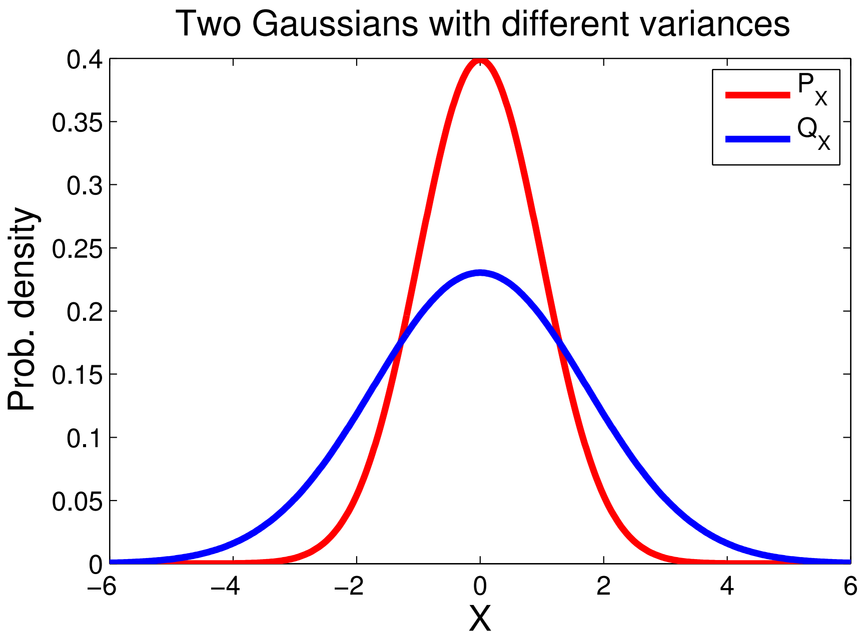
# Feature mean difference

- Simple example: 2 Gaussians with different means
- Answer: t-test



# Feature mean difference

- Two Gaussians with same means, different variance
- Idea: look at difference in means of features of the RVs
- In Gaussian case: second order features of form $\varphi(x) = x^2$



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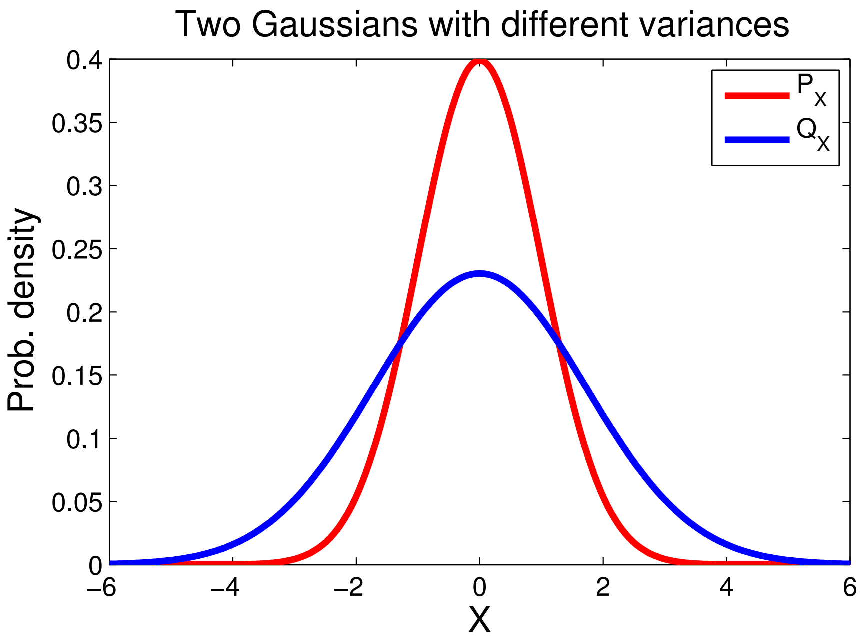
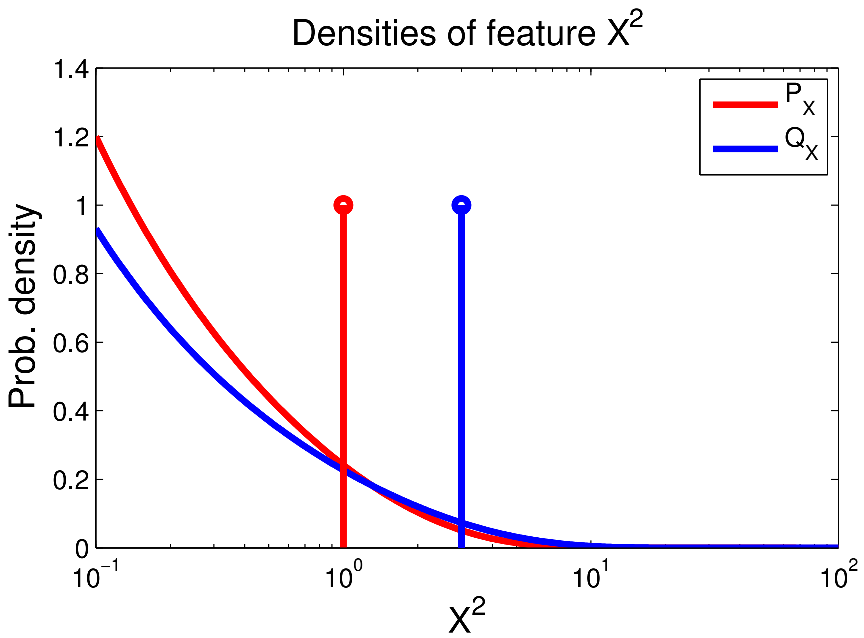
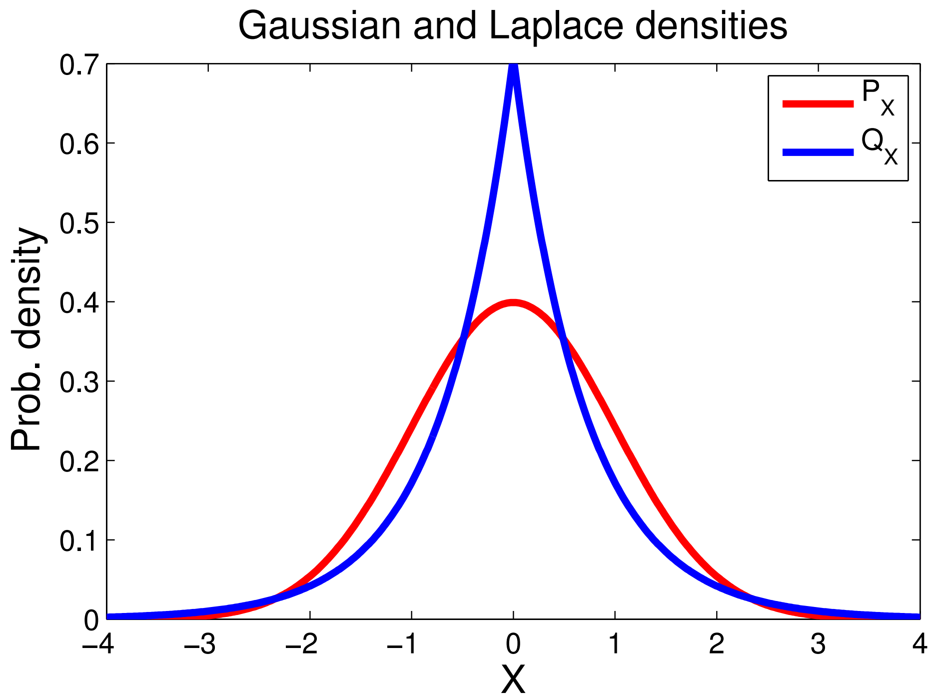


# Feature mean difference

- Gaussian and Laplace distributions
- Same mean *and* same variance
- Difference in means using higher order features...RKHS



# Probabilities in feature space: the mean trick

## The reproducing property (kernel trick)

- Given $x \in \mathcal{X}$ for some set $\mathcal{X}$, define feature map $\varphi(x) \in \mathcal{F}$,

$$\varphi(x) = [\ldots \varphi_i(x) \ldots] \in \ell_2$$

- For positive definite $k(x, x')$,

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

- The reproducing property: $\forall f \in \mathcal{F}$,

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

# Probabilities in feature space: the mean trick

The reproducing property (kernel trick)

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- The reproducing property: $\forall f \in \mathcal{F}$,

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

The mean trick

- Given $\mathsf{P}$ a Borel probability measure on $\mathcal{X}$, define feature map $\mu_{\mathsf{P}} \in \mathcal{F}$

$$\mu_{\mathsf{P}} = [\ldots \mathbf{E}_{\mathsf{P}} [\varphi_i(\mathsf{x})] \ldots]$$

- For positive definite $k(x, x')$,

$$\mathbf{E}_{\mathsf{P},\mathsf{Q}} k(\mathsf{x}, \mathsf{y}) = \langle \mu_{\mathsf{P}}, \mu_{\mathsf{Q}} \rangle_{\mathcal{F}}$$

for $\mathsf{x} \sim \mathsf{P}$ and $\mathsf{y} \sim \mathsf{Q}$.

- The mean trick: (we call $\mu_{\mathsf{P}}$ a mean/distribution embedding)

$$\mathbf{E}_{\mathsf{P}}(f(\mathsf{x})) =: \langle \mu_{\mathsf{P}}, f(\cdot) \rangle_{\mathcal{F}}$$

# Does the feature space mean exist?

Does there exist an element $\mu_{\mathsf{P}} \in \mathcal{F}$ such that

$$\mathbf{E}_{\mathsf{P}} f(\mathsf{x}) = \mathbf{E}_{\mathsf{P}} \langle f(\cdot), \varphi(\mathsf{x}) \rangle_{\mathcal{F}} = \langle f(\cdot), \mathbf{E}_{\mathsf{P}} \varphi(\mathsf{x}) \rangle_{\mathcal{F}} = \langle f(\cdot), \mu_{\mathsf{P}}(\cdot) \rangle_{\mathcal{F}} \qquad \forall f \in \mathcal{F}$$

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Yes: You can exchange expectation and innner product (i.e. $\varphi(\mathsf{x})$ is Bochner integrable [Steinwart and Christmann, 2008]) under the condition

$$\mathbf{E}_{\mathsf{P}} \|\varphi(\mathsf{x})\|_{\mathcal{F}} = \mathbf{E}_{\mathsf{P}} \sqrt{k(\mathsf{x}, \mathsf{x})} < \infty$$

# The maximum mean discrepancy

The maximum mean discrepancy is the distance between feature means:

$$MMD^2(\mathsf{P},\mathsf{Q}) = \|\mu_{\mathsf{P}} - \mu_{\mathsf{Q}}\|^2_{\mathcal{F}} = \langle \mu_{\mathsf{P}}, \mu_{\mathsf{P}} \rangle_{\mathcal{F}} + \langle \mu_{\mathsf{Q}}, \mu_{\mathsf{Q}} \rangle_{\mathcal{F}} - 2 \langle \mu_{\mathsf{P}}, \mu_{\mathsf{Q}} \rangle_{\mathcal{F}}$$
$$= \underbrace{\mathbf{E}_{\mathsf{P}} k(\mathsf{x},\mathsf{x}')}_{\text{(a)}} + \underbrace{\mathbf{E}_{\mathsf{Q}} k(\mathsf{y},\mathsf{y}')}_{\text{(a)}} - 2\underbrace{\mathbf{E}_{\mathsf{P},\mathsf{Q}} k(\mathsf{x},\mathsf{y})}_{\text{(b)}}$$

(a)= within distrib. similarity, (b)= cross-distrib. similarity

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Proof:

$$\begin{aligned}
\|\mu_{\mathbf{P}} - \mu_{\mathbf{Q}}\|^2_{\mathcal{F}} &= \langle \mu_{\mathbf{P}} - \mu_{\mathbf{Q}}, \mu_{\mathbf{P}} - \mu_{\mathbf{Q}} \rangle_{\mathcal{F}} \\
&= \langle \mu_{\mathbf{P}}, \mu_{\mathbf{P}} \rangle + \langle \mu_{\mathbf{Q}}, \mu_{\mathbf{Q}} \rangle - 2 \langle \mu_{\mathbf{P}}, \mu_{\mathbf{Q}} \rangle
\end{aligned}$$

# The maximum mean discrepancy

The maximum mean discrepancy is the distance between feature means:

$$
\begin{aligned}
MMD^2(\mathsf{P},\mathsf{Q}) = \|\mu_{\mathsf{P}} - \mu_{\mathsf{Q}}\|_{\mathcal{F}}^2 &= \langle \mu_{\mathsf{P}}, \mu_{\mathsf{P}} \rangle_{\mathcal{F}} + \langle \mu_{\mathsf{Q}}, \mu_{\mathsf{Q}} \rangle_{\mathcal{F}} - 2\,\langle \mu_{\mathsf{P}}, \mu_{\mathsf{Q}} \rangle_{\mathcal{F}} \\
&= \underbrace{\mathbf{E}_{\mathsf{P}} k(\mathsf{x},\mathsf{x}')}_{\text{(a)}} + \underbrace{\mathbf{E}_{\mathsf{Q}} k(\mathsf{y},\mathsf{y}')}_{\text{(a)}} - 2\underbrace{\mathbf{E}_{\mathsf{P},\mathsf{Q}} k(\mathsf{x},\mathsf{y})}_{\text{(b)}}
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Proof:

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$$= \underbrace{\mathbf{E}_{\mathbf{P}} k(x, x')}_{\text{(a)}} + \underbrace{\mathbf{E}_{\mathbf{Q}} k(y, y')}_{\text{(a)}} - 2\underbrace{\mathbf{E}_{\mathbf{P},\mathbf{Q}} k(x, y)}_{\text{(b)}}$$

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&= \mathbf{E}_{\mathbf{P}}[\mu_{\mathbf{P}}(x)] + \ldots \\
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&= \mathbf{E}_{\mathsf{P}} k(\mathsf{x},\mathsf{x}') + \mathbf{E}_{\mathsf{Q}} k(\mathsf{y},\mathsf{y}') - 2\mathbf{E}_{\mathsf{P},\mathsf{Q}} k(\mathsf{x},\mathsf{y})
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\end{aligned}
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(a)= within distrib. similarity, (b)= cross-distrib. similarity

Unbiased empirical estimate of first term (quadratic time)

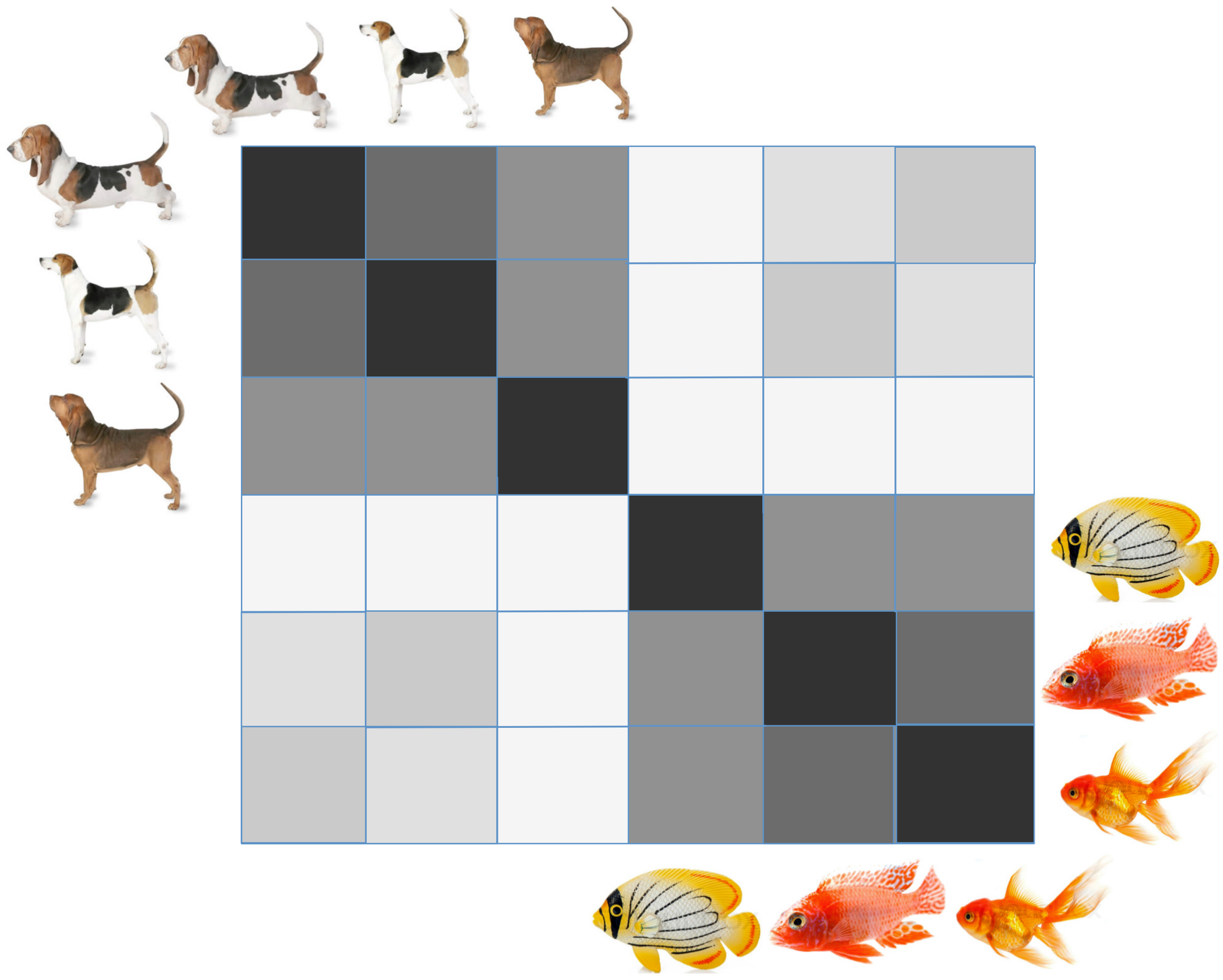
$$
\widehat{\mathbb{E}}_{\mathbf{P}} k(x,x') = \frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j\neq i}^{m} k(x_i, x_j)
$$

# The maximum mean discrepancy

$$\sim P$$

$$\sim Q$$

# The maximum mean discrepancy



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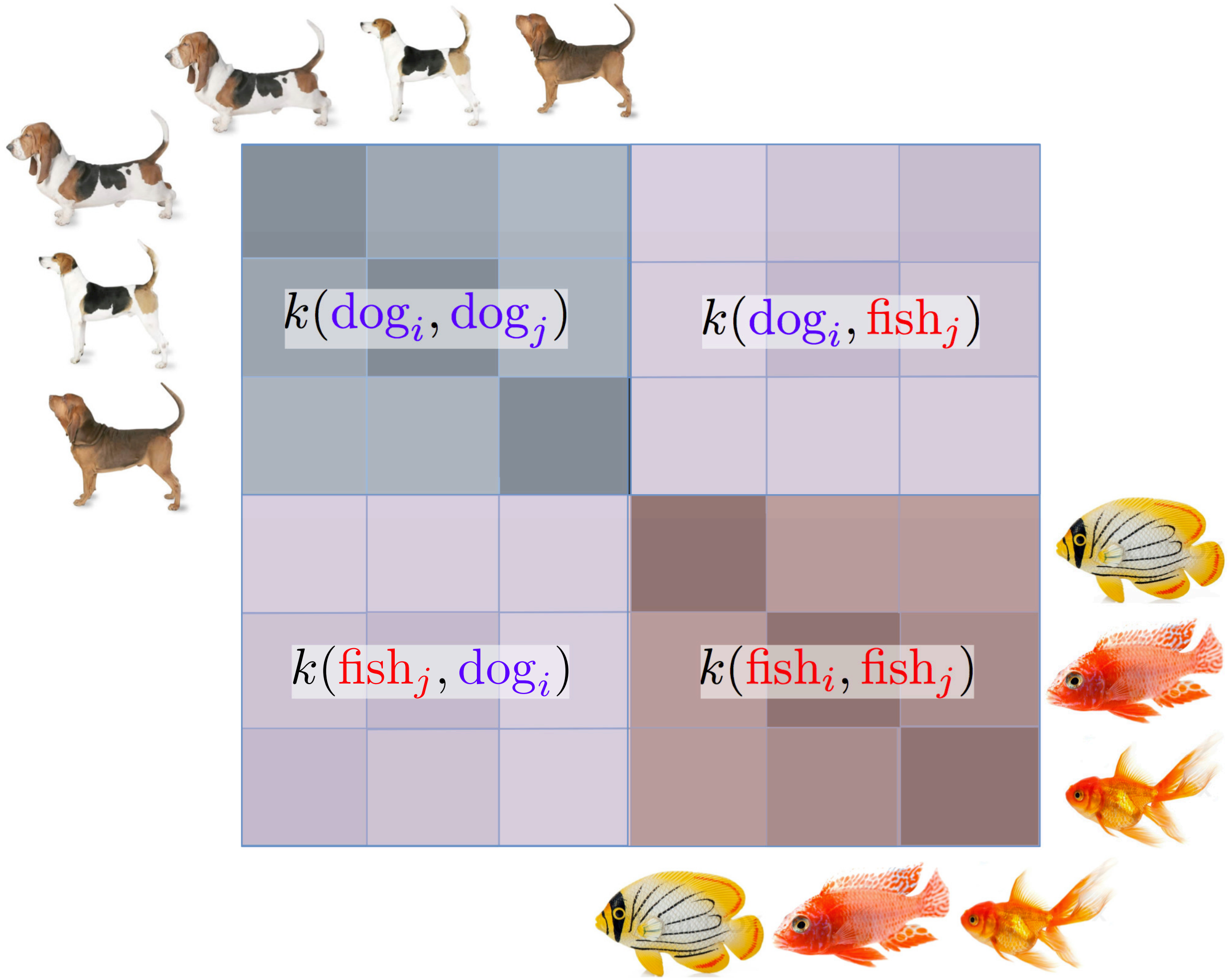


$$\widehat{MMD}^2 = \overline{K_{P,P}} + \overline{K_{Q,Q}} - 2\overline{K_{P,Q}}$$

(diagonal terms removed from $K_{P,P}$ and $K_{Q,Q}$)

# Function Showing Difference in Distributions

- Are **P** and **Q** different?

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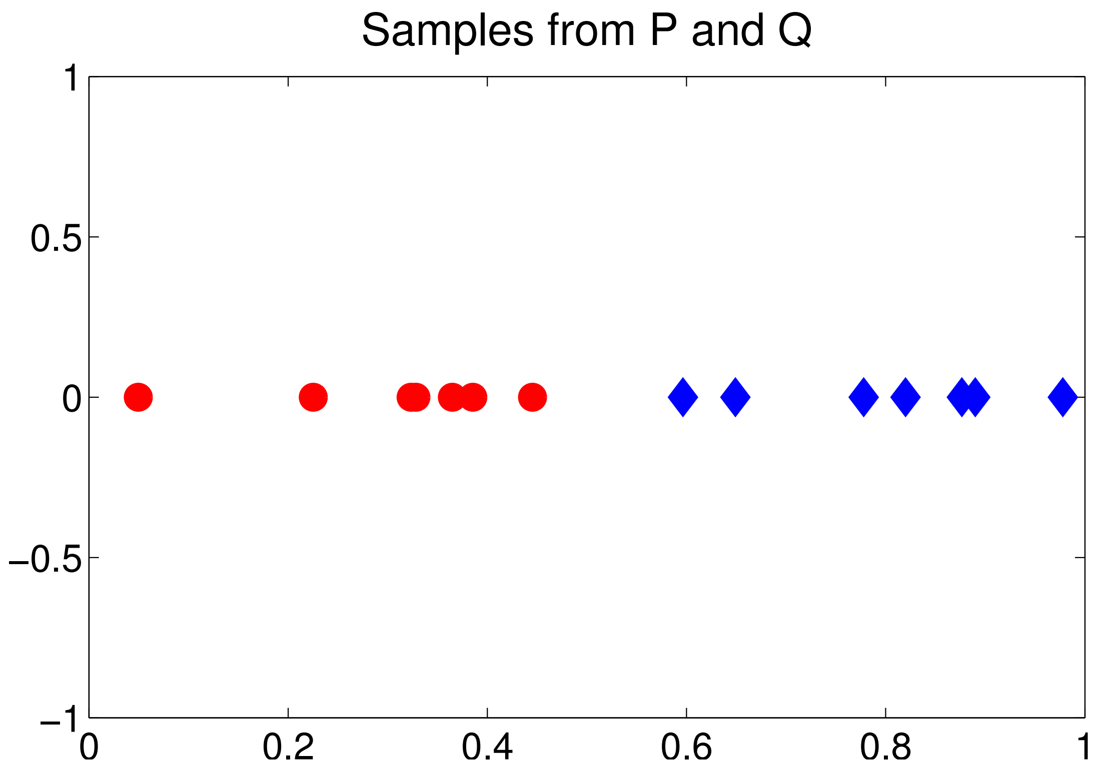

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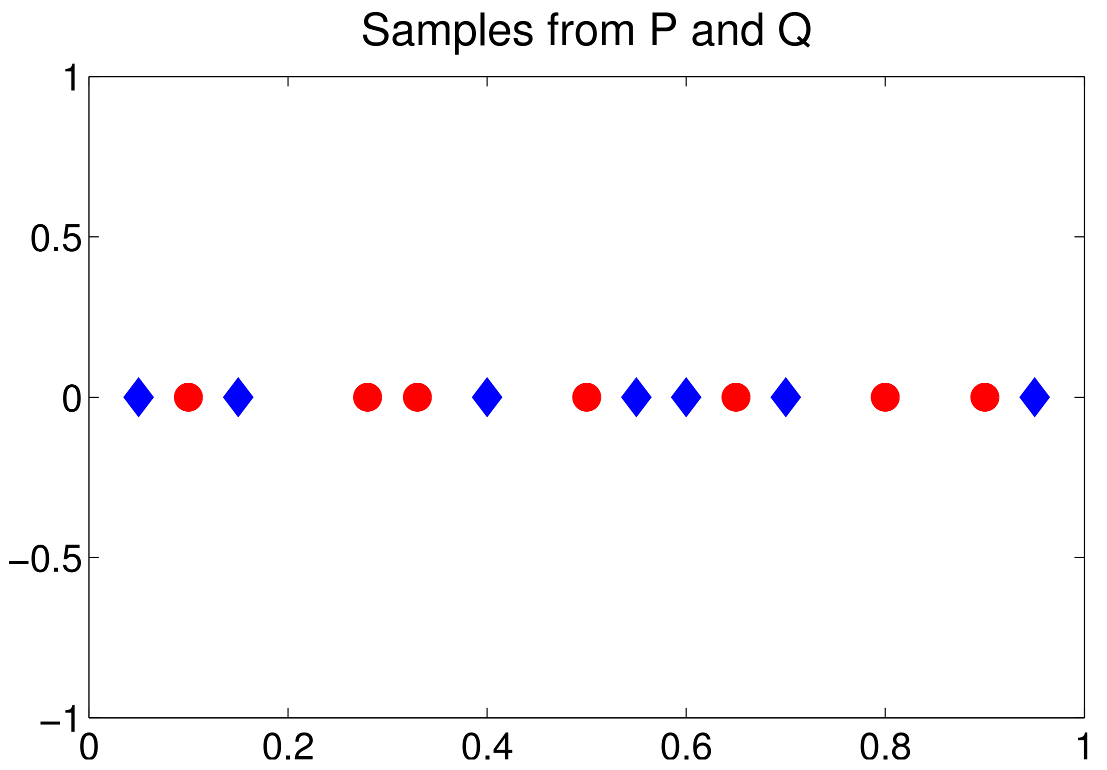
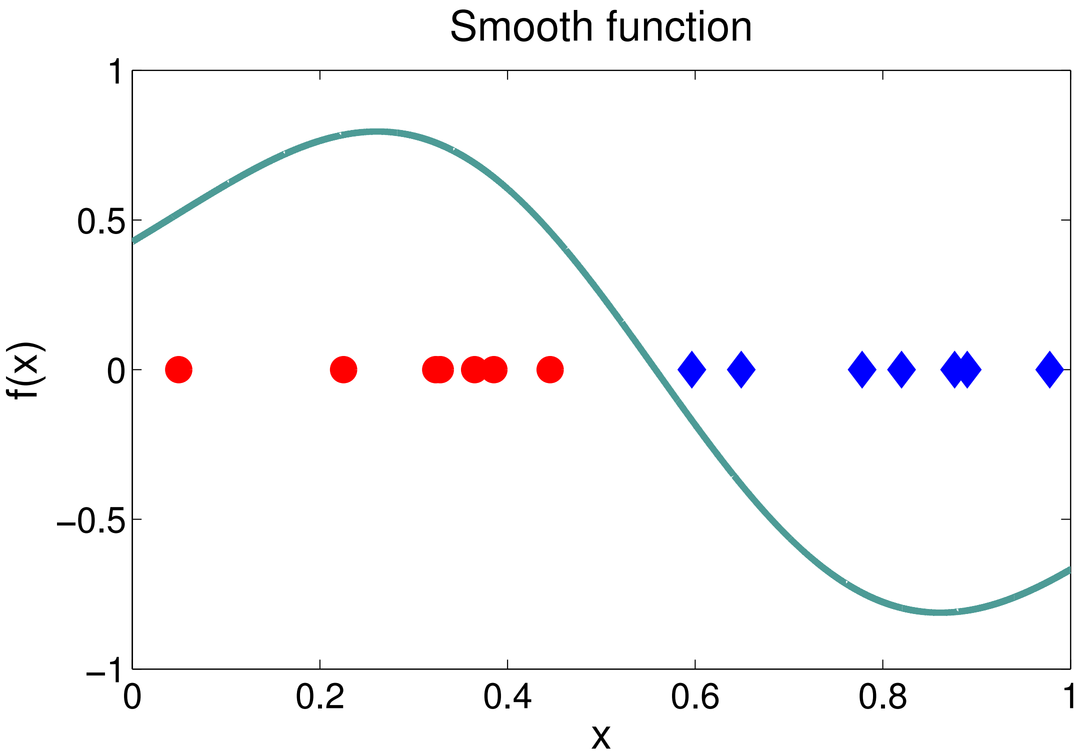


# Function Showing Difference in Distributions

- Maximum mean discrepancy: smooth function for **P** vs **Q**

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



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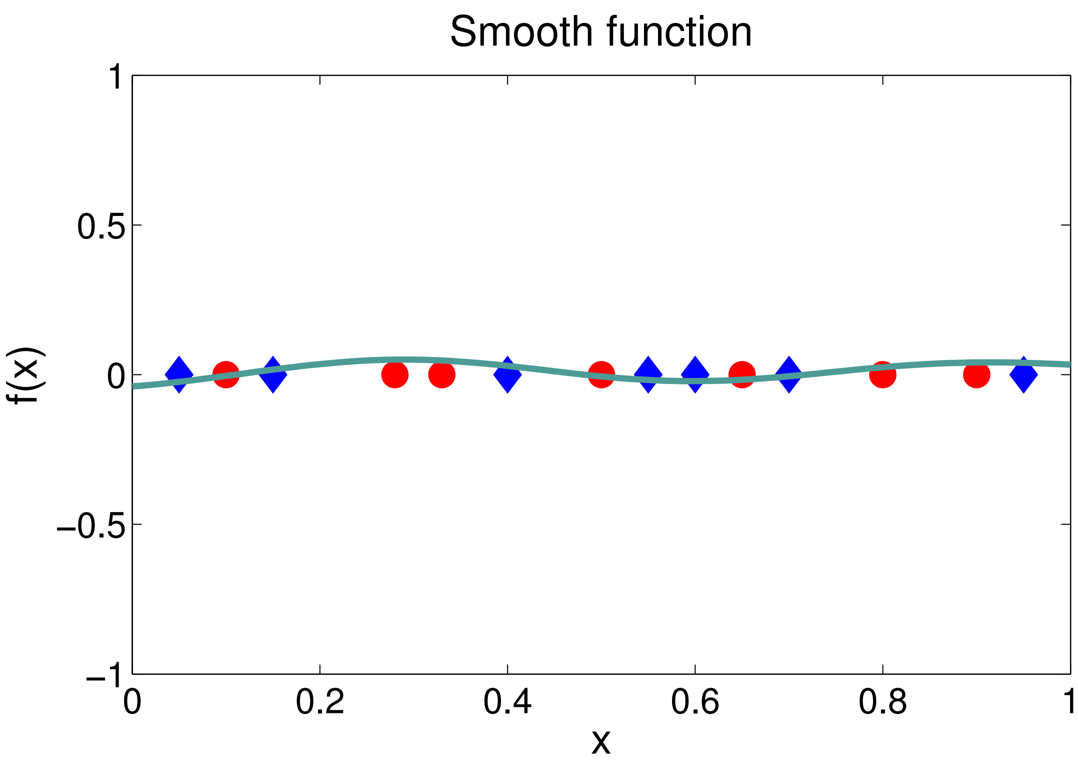

# Function Showing Difference in Distributions

- What if the function is not smooth?

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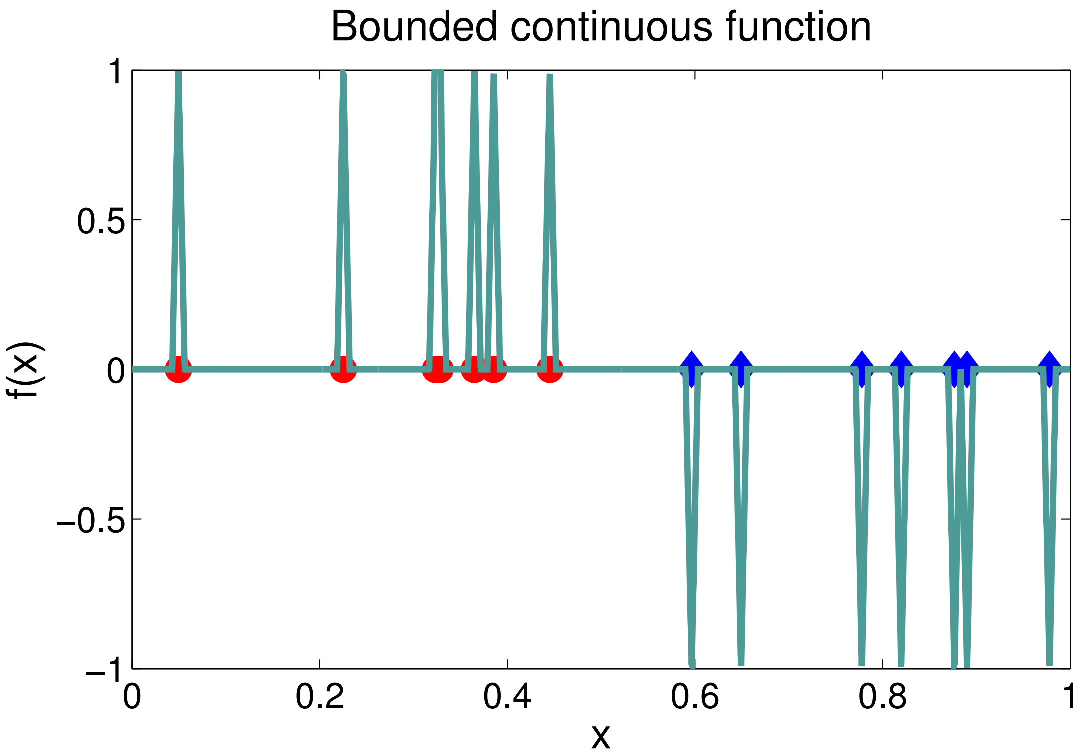

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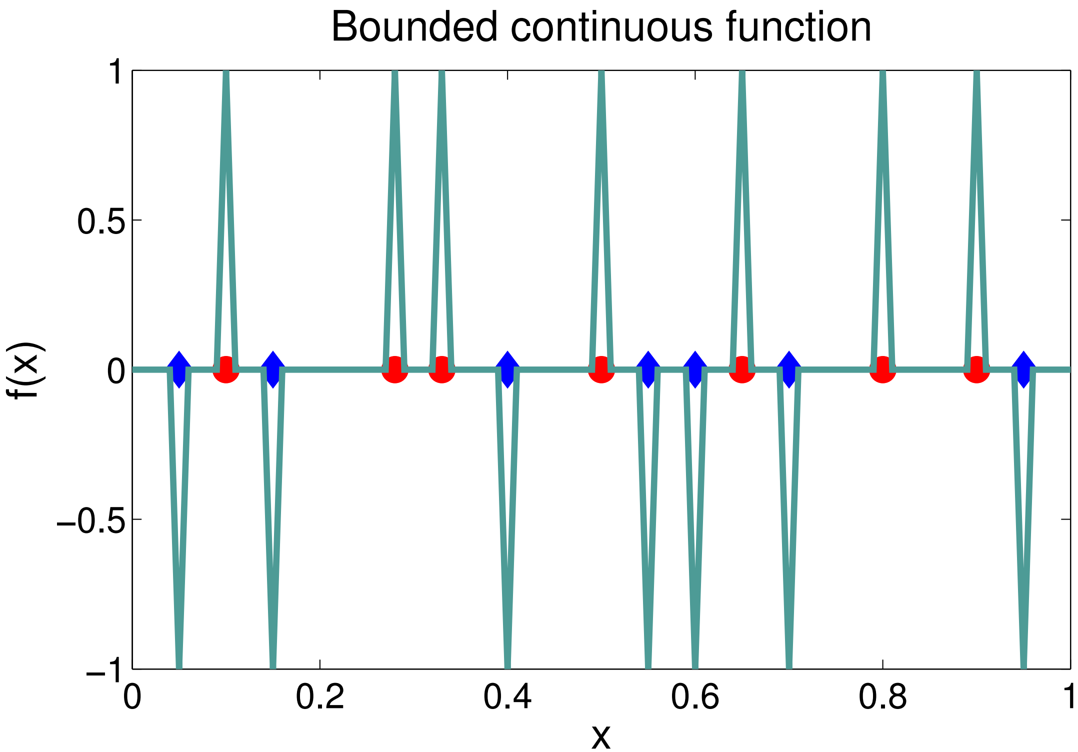

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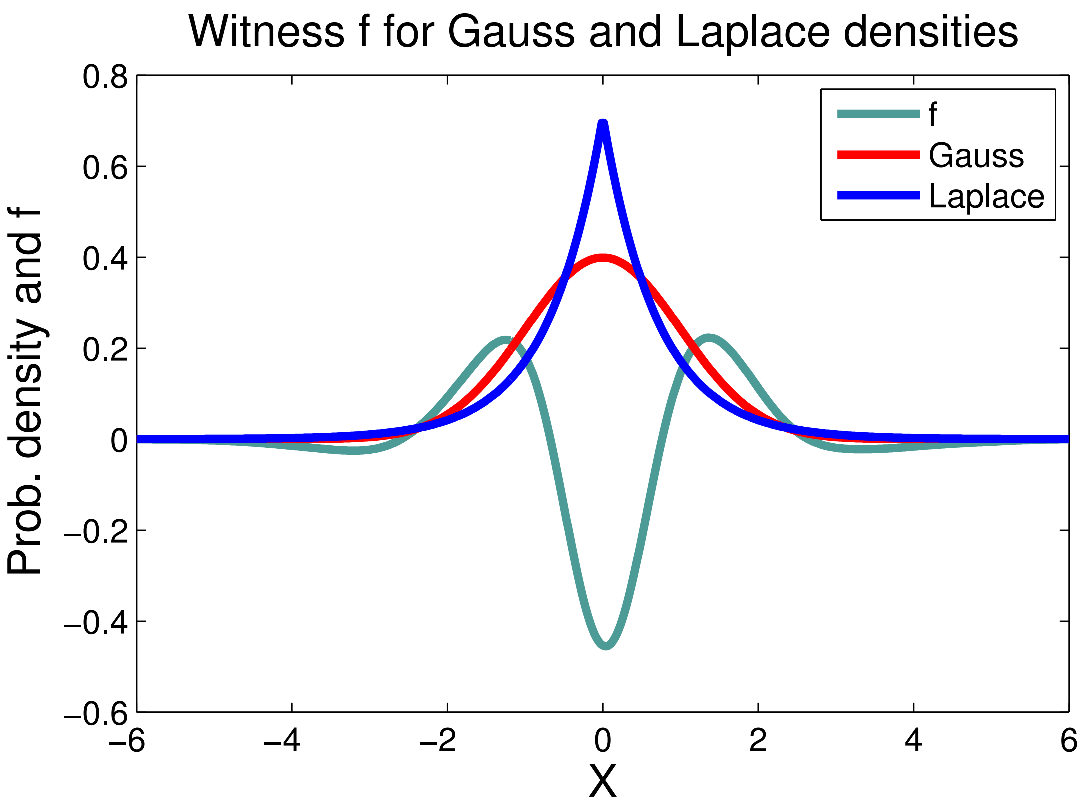
- Gauss **P** vs Laplace **Q**



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- Maximum mean discrepancy: smooth function for $\mathbf{P}$ vs $\mathbf{Q}$

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- Classical results: $\mathrm{MMD}(\mathbf{P},\mathbf{Q};F) = 0$ iff $\mathbf{P}=\mathbf{Q}$, when
  - $F =$bounded continuous [Dudley, 2002]
  - $F =$ bounded variation 1 (Kolmogorov metric) [Müller, 1997]
  - $F =$ bounded Lipschitz (Earth mover's distances) [Dudley, 2002]

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- $\mathrm{MMD}(\mathsf{P},\mathsf{Q};F) = 0$ iff $\mathsf{P}=\mathsf{Q}$ when $F=$the unit ball in a characteristic RKHS $\mathcal{F}$ (coming soon!) [ISMB06, NIPS06a, NIPS07b, NIPS08a, JMLR10]

# Function Showing Difference in Distributions

- Maximum mean discrepancy: smooth function for $\mathsf{P}$ vs $\mathsf{Q}$

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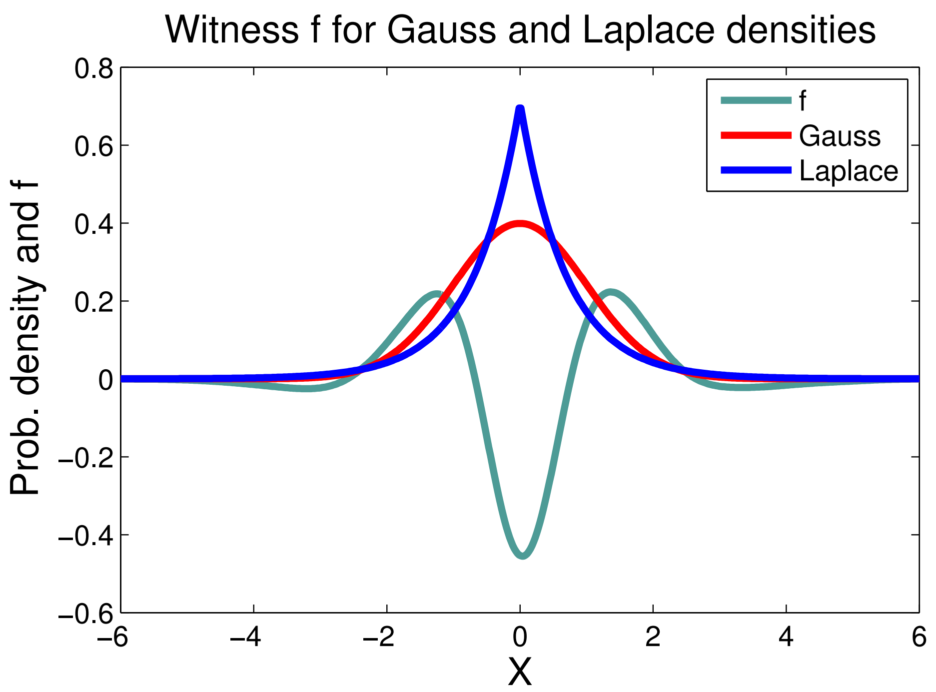
How do smooth functions relate to feature maps?

# Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

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

$$= \sup_{f\in F}\left[\mathbf{E}_{\mathbf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathbf{Q}} f(\mathsf{y})\right]$$



# Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

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

$$= \sup_{f \in F} \left[ \mathbf{E}_{\mathbf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathbf{Q}} f(\mathsf{y}) \right]$$

use

$$\mathbf{E}_{\mathbf{P}}(f(\mathsf{x})) \quad =: \quad \langle \mu_{\mathbf{P}}, f \rangle_{\mathcal{F}}$$

# Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

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

$$= \sup_{f \in F} \left[ \mathbf{E}_{\mathbf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathbf{Q}} f(\mathsf{y}) \right]$$

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use

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# Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

$$\begin{aligned}
&\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) \\
&= \sup_{f \in F} \left[ \mathbf{E}_{\mathbf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathbf{Q}} f(\mathsf{y}) \right] \\
&= \sup_{f \in F} \langle f, \mu_{\mathbf{P}} - \mu_{\mathbf{Q}} \rangle_{\mathcal{F}} \\
&= \|\mu_{\mathbf{P}} - \mu_{\mathbf{Q}}\|_{\mathcal{F}}
\end{aligned}$$

use

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

since $F := \{f \in \mathcal{F} : \|f\| \leq 1\}$

$\boxed{\text{Function view and feature view equivalent}}$

# MMD for independence: HSIC

- Dependence measure: the Hilbert Schmidt Independence Criterion [ALT05, NIPS07a, ALT07, ALT08, JMLR10]

  Related to [Feuerverger, 1993]and [Székely and Rizzo, 2009, Székely et al., 2007]

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# MMD for independence: HSIC

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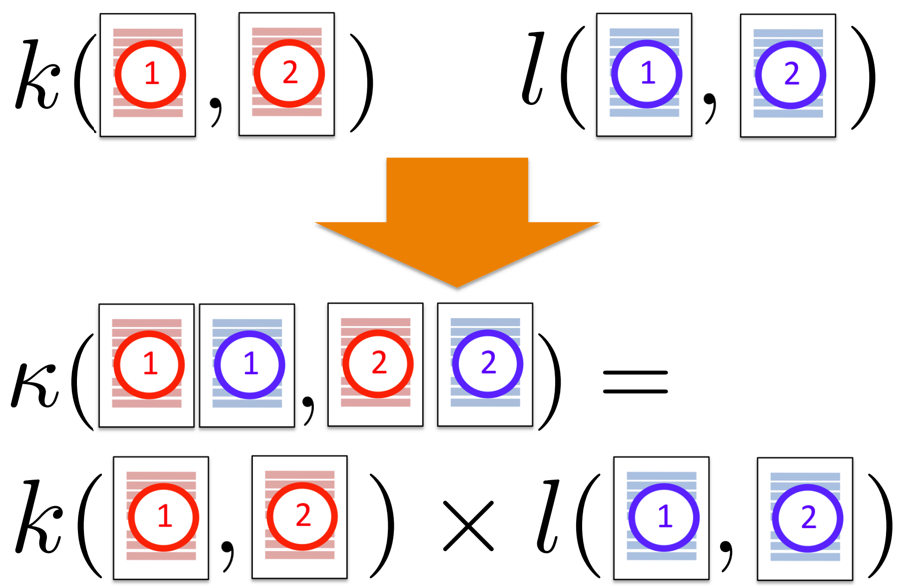

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$$HSIC(\mathbf{P}_{XY}, \mathbf{P}_X \mathbf{P}_Y) := \left\| \mu_{\mathbf{P}_{XY}} - \mu_{\mathbf{P}_X \mathbf{P}_Y} \right\|^2$$

HSIC using expectations of kernels:

Define RKHS $\mathcal{F}$ on $\mathcal{X}$ with kernel $k$, RKHS $\mathcal{G}$ on $\mathcal{Y}$ with kernel $l$. Then

$$\begin{aligned}
&\mathrm{HSIC}(\mathbf{P}_{XY}, \mathbf{P}_X \mathbf{P}_Y) \\
&= \mathbf{E}_{XY} \mathbf{E}_{X'Y'} k(\mathsf{x}, \mathsf{x}') l(\mathsf{y}, \mathsf{y}') + \mathbf{E}_X \mathbf{E}_{X'} k(\mathsf{x}, \mathsf{x}') \mathbf{E}_Y \mathbf{E}_{Y'} l(\mathsf{y}, \mathsf{y}') \\
&\quad - 2\mathbf{E}_{X'Y'} \left[ \mathbf{E}_X k(\mathsf{x}, \mathsf{x}') \mathbf{E}_Y l(\mathsf{y}, \mathsf{y}') \right].
\end{aligned}$$

# HSIC: empirical estimate and intuition

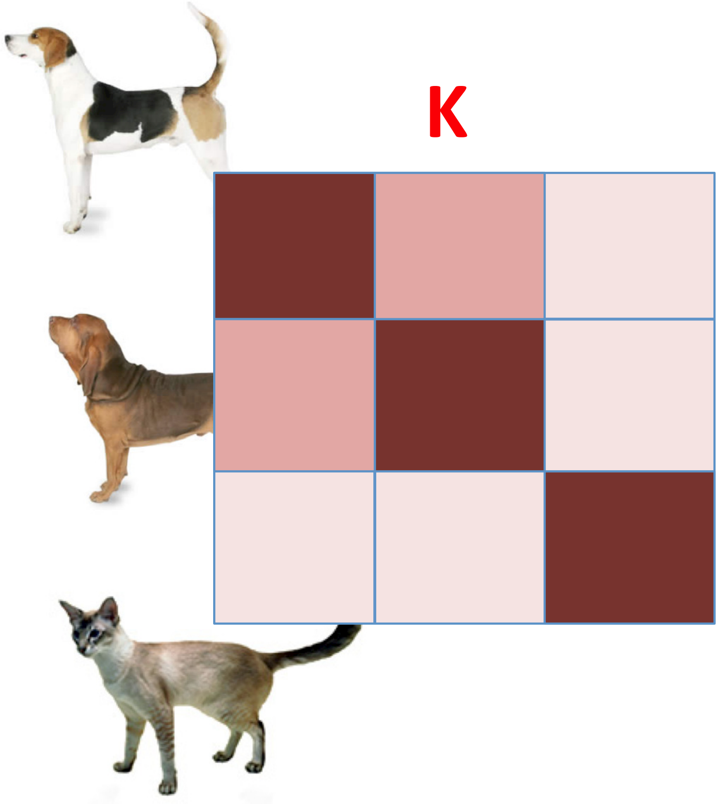
Their noses guide them through life, and they're never happier than when following an interesting scent. They need plenty of exercise, about an hour a day if possible.

A large animal who slings slobber, exudes a distinctive houndy odor, and wants nothing more than to follow his nose. They need a significant amount of exercise and mental stimulation.

Known for their curiosity, intelligence, and excellent communication skills, the Javanese breed is perfect if you want a responsive, interactive pet, one that will blow in your ear and follow you everywhere.

Text from dogtime.com and petfinder.com

# HSIC: empirical estimate and intuition

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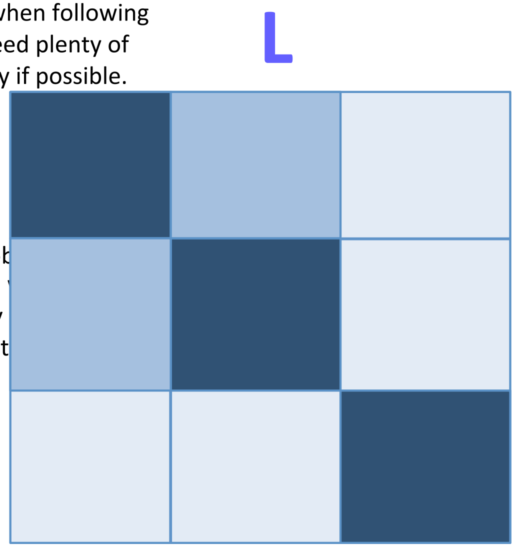


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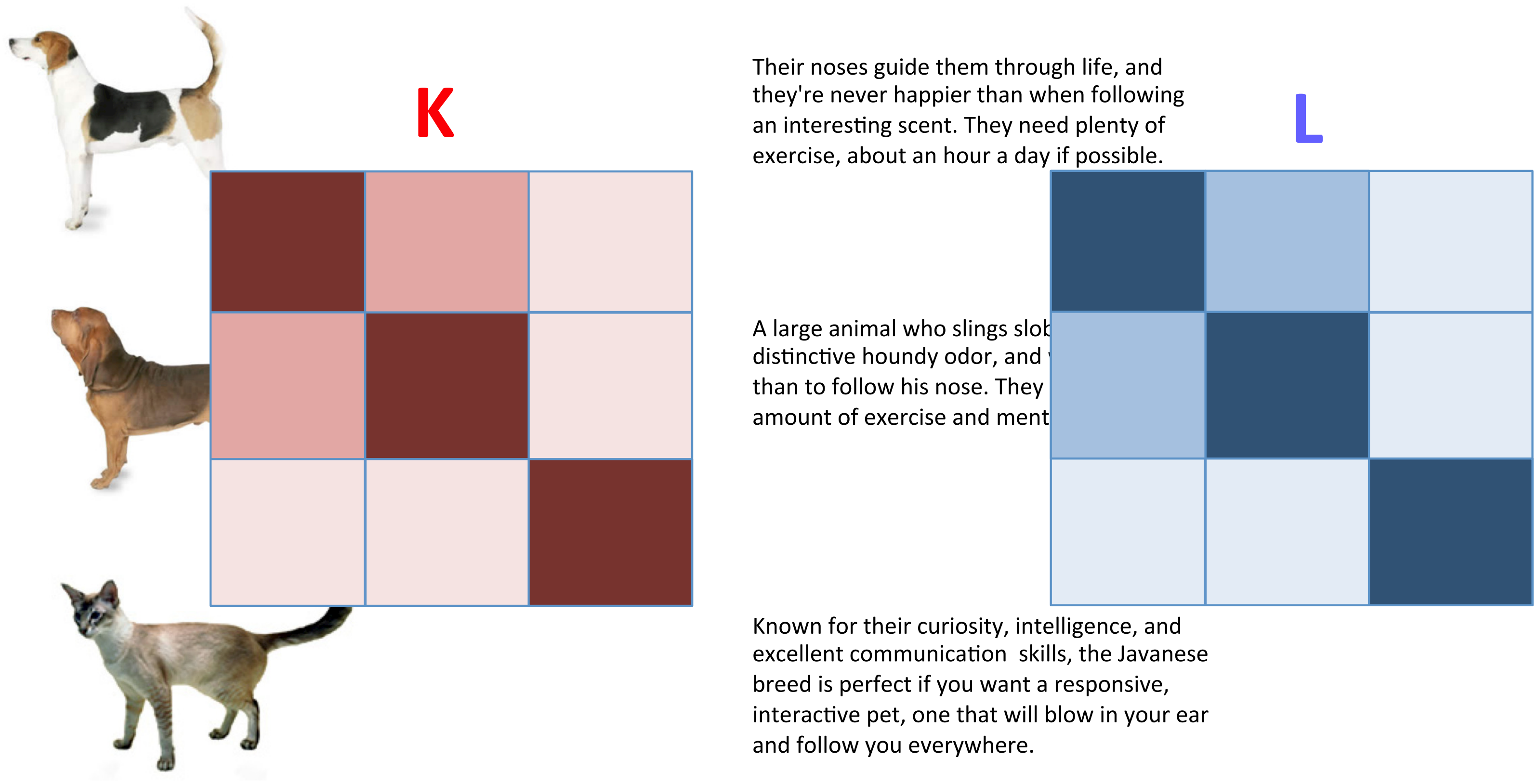



Text from dogtime.com and petfinder.com

Empirical $HSIC(\mathbf{P}_{XY}, \mathbf{P}_X\mathbf{P}_Y)$:

$$\frac{1}{n^2}\left(HKH \circ HLH\right)_{++}$$

# Characteristic kernels (Via Fourier, on the torus $\mathbb{T}$)

# Characteristic Kernels (via Fourier)

Reminder:

Characteristic: MMD a metric (MMD $= 0$ iff $\mathbf{P} = \mathbf{Q}$) [NIPS07b, JMLR10]

In the next slides:

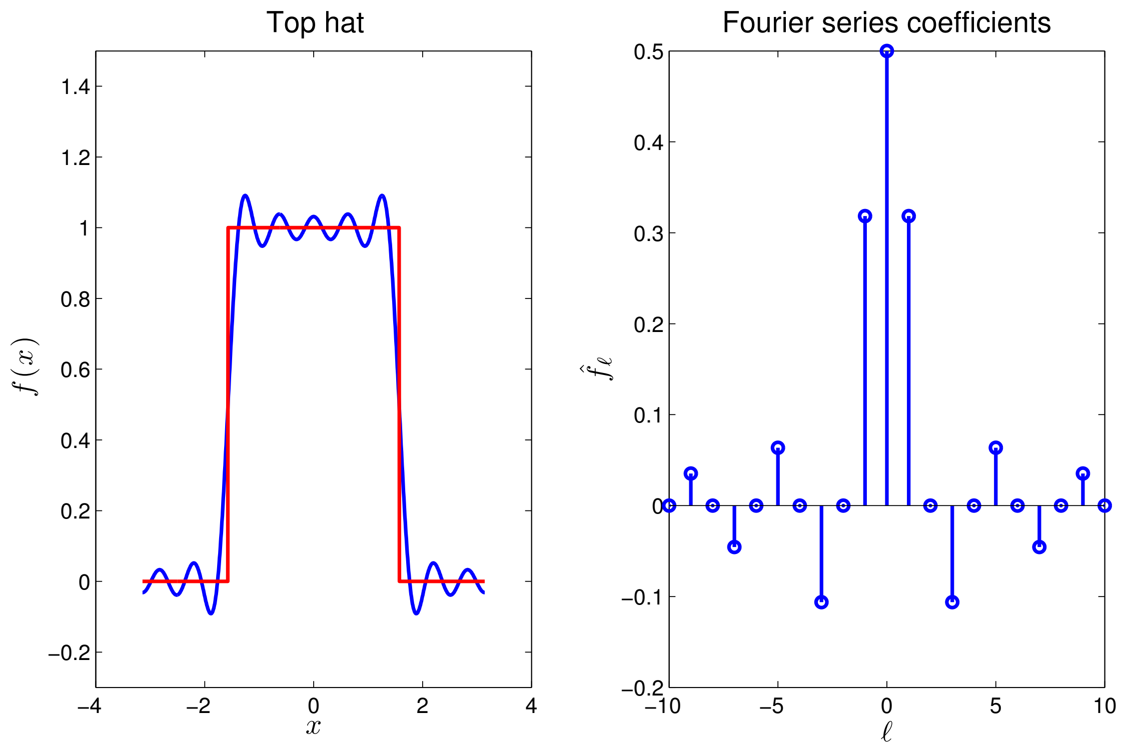
1. Characteristic property on $[-\pi, \pi]$ with periodic boundary
2. Characteristic property on $\mathbb{R}^d$

# Characteristic Kernels (via Fourier)

Reminder: Fourier series

- Function $[-\pi, \pi]$ with periodic boundary.

$$f(x) = \sum_{\ell=-\infty}^{\infty} \hat{f}_\ell \exp(\imath \ell x) = \sum_{l=-\infty}^{\infty} \hat{f}_\ell \left(\cos(\ell x) + \imath \sin(\ell x)\right).$$



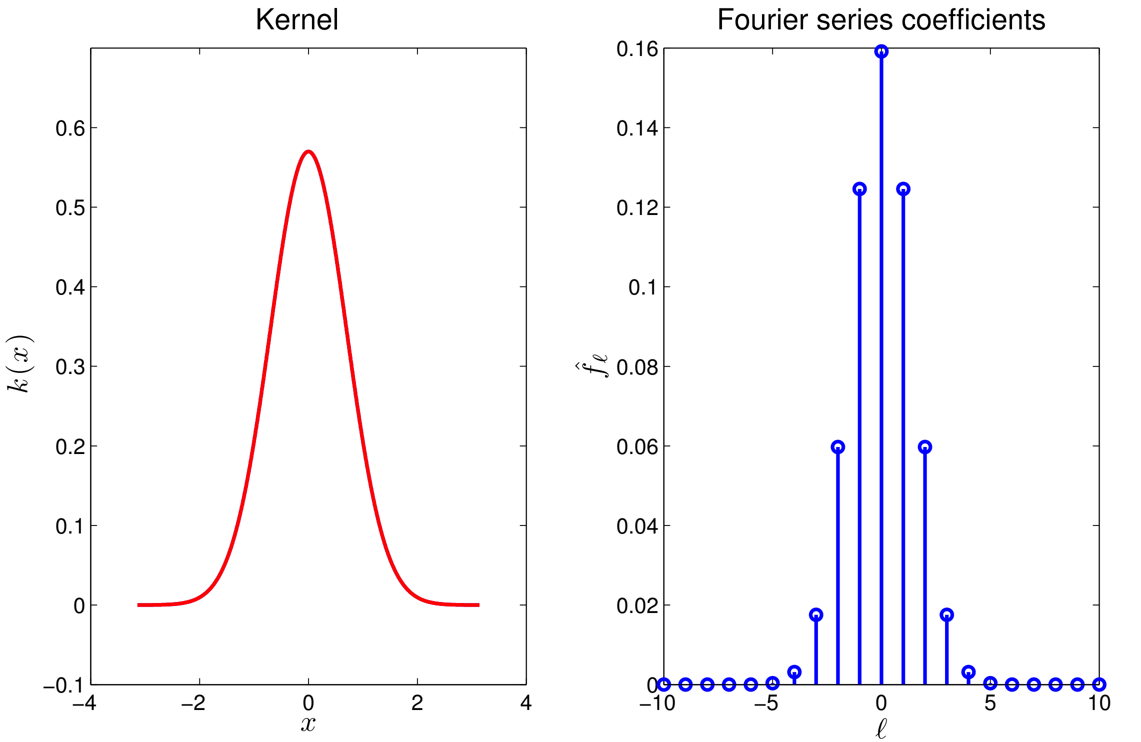
# Characteristic Kernels (via Fourier)

Reminder: Fourier series of kernel

$$k(x,y) = k(x-y) = k(z), \qquad k(z) = \sum_{\ell=-\infty}^{\infty} \hat{k}_\ell \exp(\imath \ell z),$$

E.g., $$k(x) = \frac{1}{2\pi}\vartheta\left(\frac{x}{2\pi}, \frac{\imath\sigma^2}{2\pi}\right), \qquad \hat{k}_\ell = \frac{1}{2\pi}\exp\left(\frac{-\sigma^2\ell^2}{2}\right).$$

$\vartheta$ is the Jacobi theta function, close to Gaussian when $\sigma^2$ sufficiently narrower than $[-\pi, \pi]$.



# Characteristic Kernels (via Fourier)

Maximum mean embedding via Fourier series:

- Fourier series for $\mathbf{P}$ is characteristic function $\bar{\phi}_{\mathbf{P}}$
- Fourier series for mean embedding is product of fourier series! (convolution theorem)

$$\mu_{\mathbf{P}}(x) = E_{\mathbf{P}} k(\mathsf{x} - x) = \int_{-\pi}^{\pi} k(x-t)\, d\mathbf{P}(t) \qquad \hat{\mu}_{\mathbf{P},\ell} = \hat{k}_\ell \times \bar{\phi}_{\mathbf{P},\ell}$$

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- MMD can be written in terms of Fourier series:

$$\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) := \left\| \sum_{\ell=-\infty}^{\infty} \left[ \left( \bar{\phi}_{\mathbf{P},\ell} - \bar{\phi}_{\mathbf{Q},\ell} \right) \hat{k}_\ell \right] \exp(\imath \ell x) \right\|_{\mathcal{F}}$$

# A simpler Fourier expression for MMD

- From previous slide,

$$\text{MMD}(\mathbf{P}, \mathbf{Q}; F) := \left\| \sum_{\ell=-\infty}^{\infty} \left[ \left( \bar{\phi}_{\mathbf{P},\ell} - \bar{\phi}_{\mathbf{Q},\ell} \right) \hat{k}_\ell \right] \exp(\imath \ell x) \right\|_{\mathcal{F}}$$

- The squared norm of a function $f$ in $\mathcal{F}$ is:

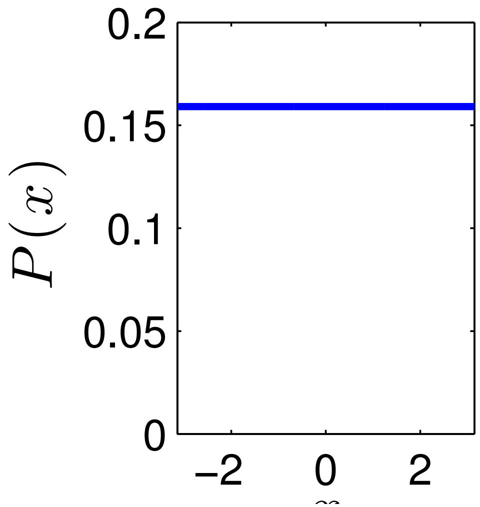
$$\|f\|_{\mathcal{F}}^2 = \langle f, f \rangle_{\mathcal{F}} = \sum_{l=-\infty}^{\infty} \frac{|\hat{f}_\ell|^2}{\hat{k}_\ell}.$$

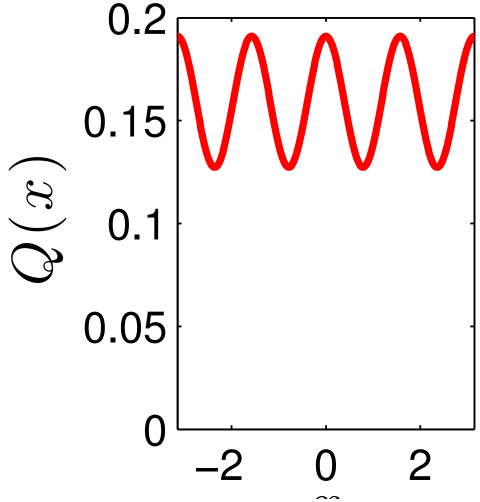
- Simple, interpretable expression for squared MMD:

$$\text{MMD}^2(\mathbf{P}, \mathbf{Q}; F) = \sum_{l=-\infty}^{\infty} \frac{[|\phi_{\mathbf{P},\ell} - \phi_{\mathbf{Q},\ell}|^2 \hat{k}_\ell]^2}{\hat{k}_\ell} = \sum_{l=-\infty}^{\infty} |\phi_{\mathbf{P},\ell} - \phi_{\mathbf{Q},\ell}|^2 \hat{k}_\ell$$

# Example

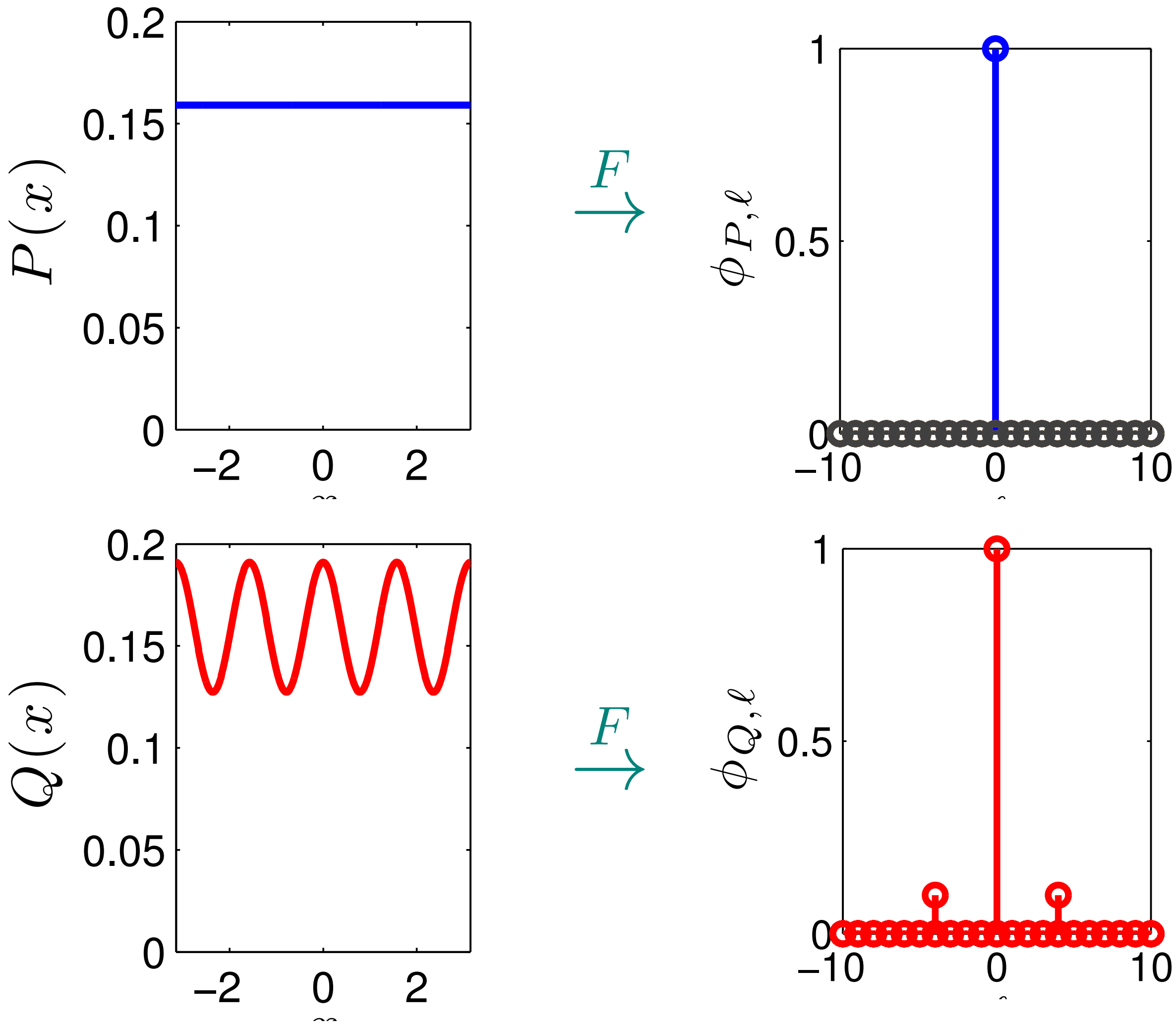
- Example: **P** differs from **Q** at one frequency



# Characteristic Kernels (2)

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



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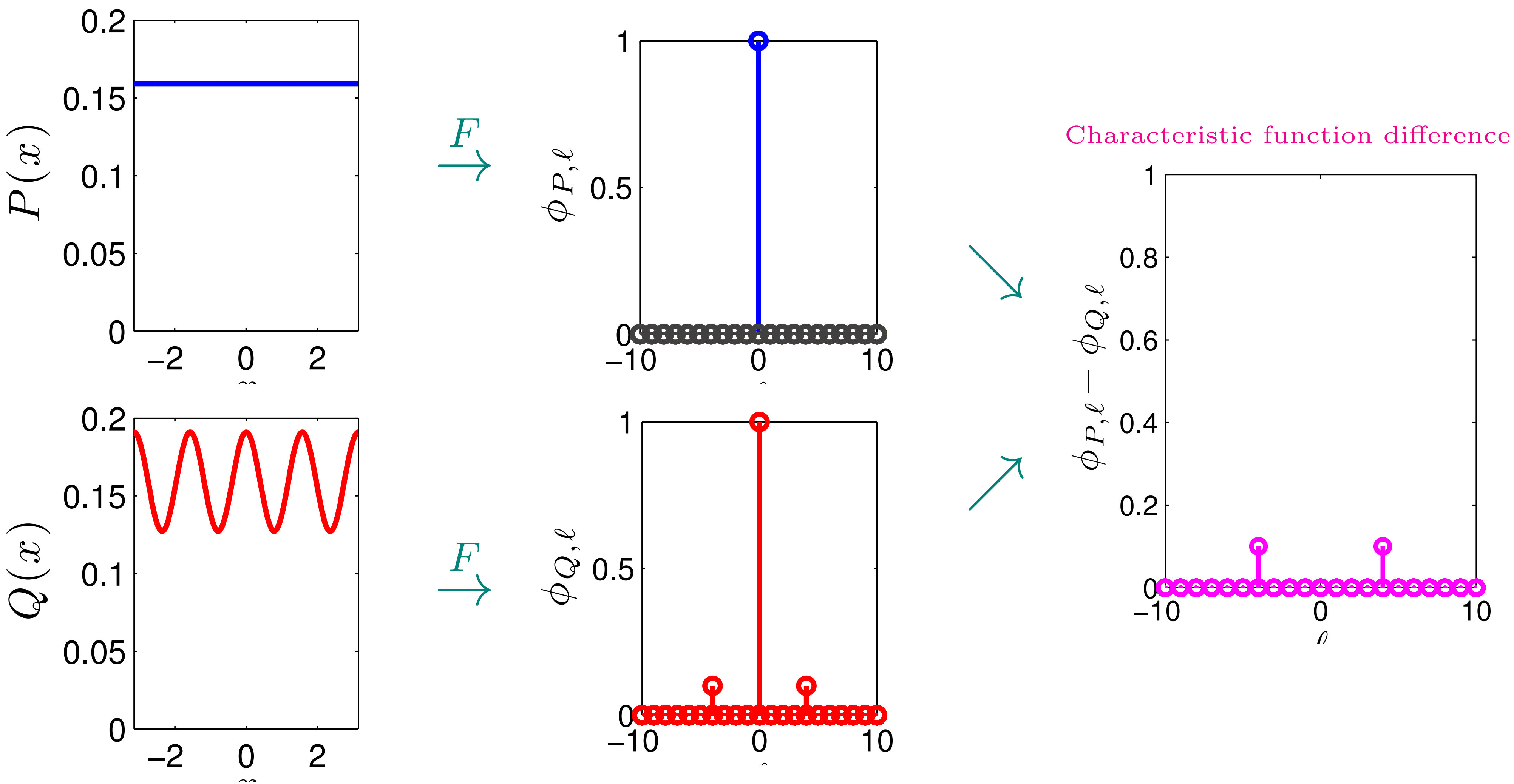
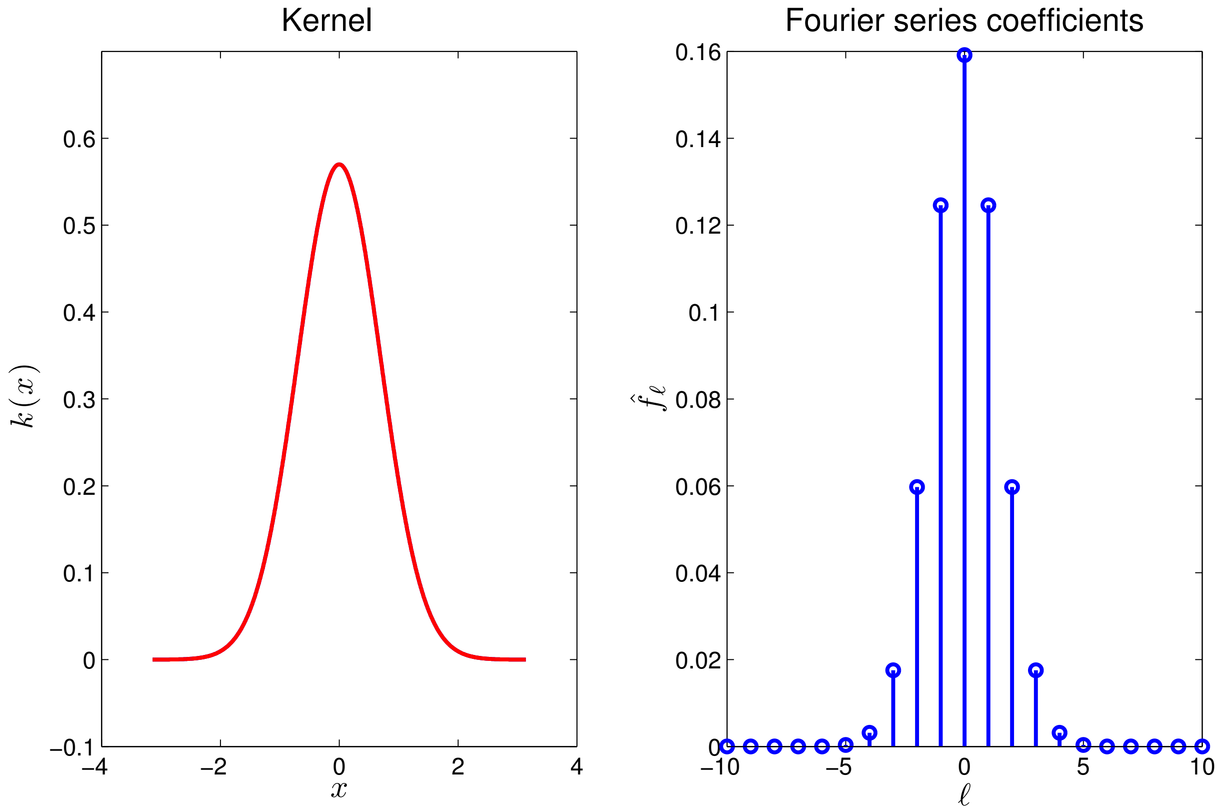


# Example

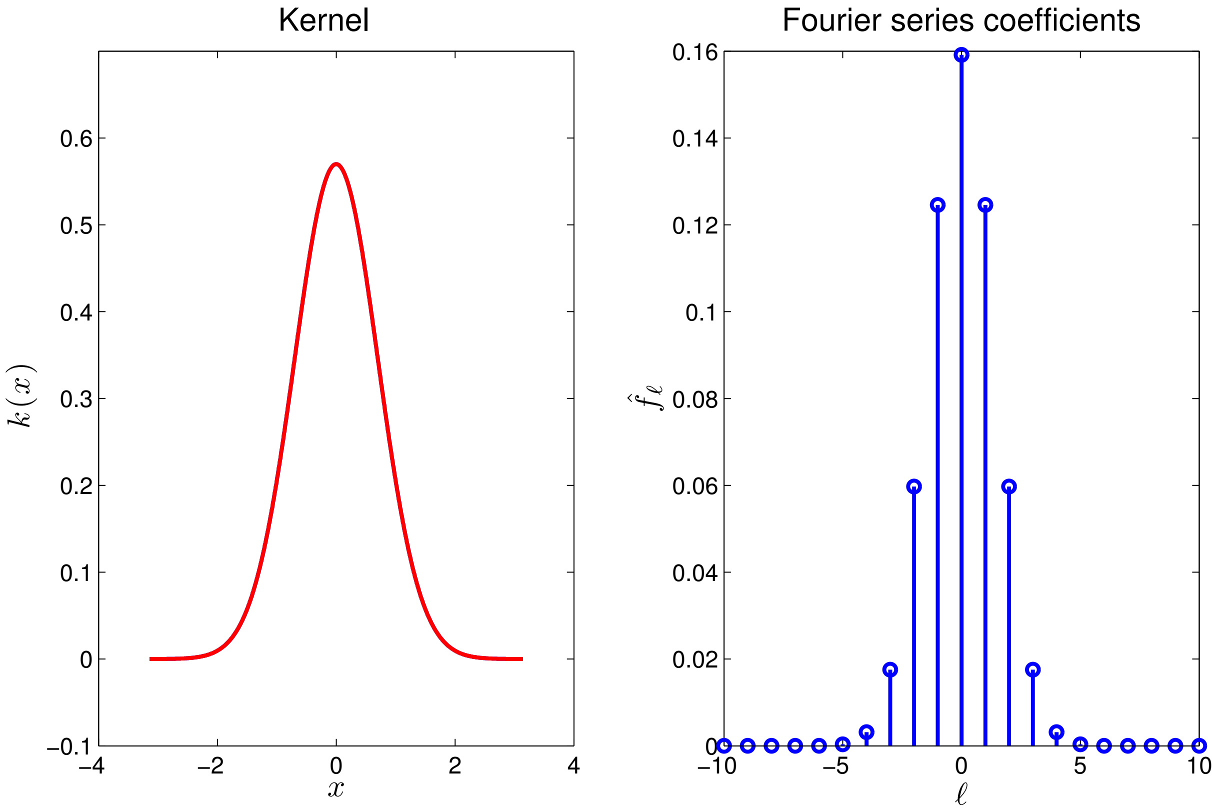
Is the Gaussian-spectrum kernel characteristic?




$$\mathrm{MMD}^2(\mathbf{P}, \mathbf{Q}; F) := \sum_{l=-\infty}^{\infty} |\phi_{\mathbf{P},\ell} - \phi_{\mathbf{Q},\ell}|^2 \hat{k}_\ell$$

# Example

Is the Gaussian-spectrum kernel characteristic? YES

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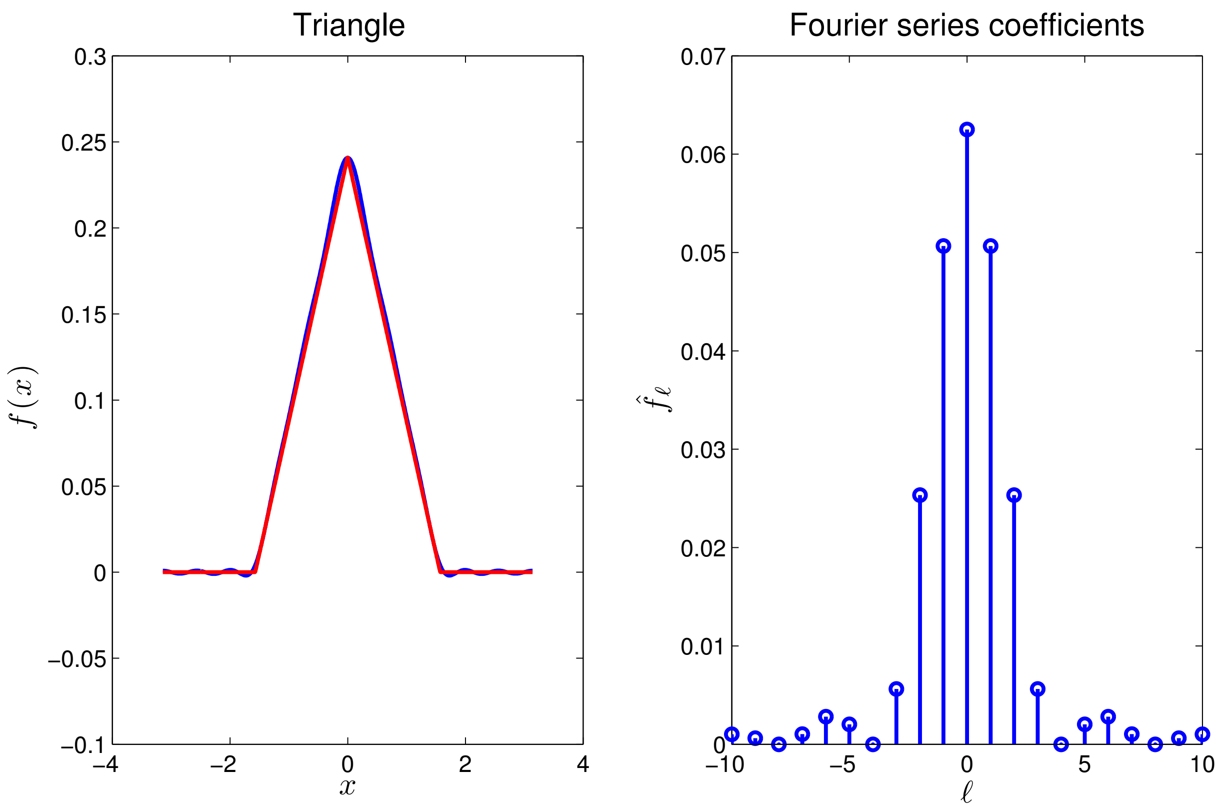
Is the triangle kernel characteristic?

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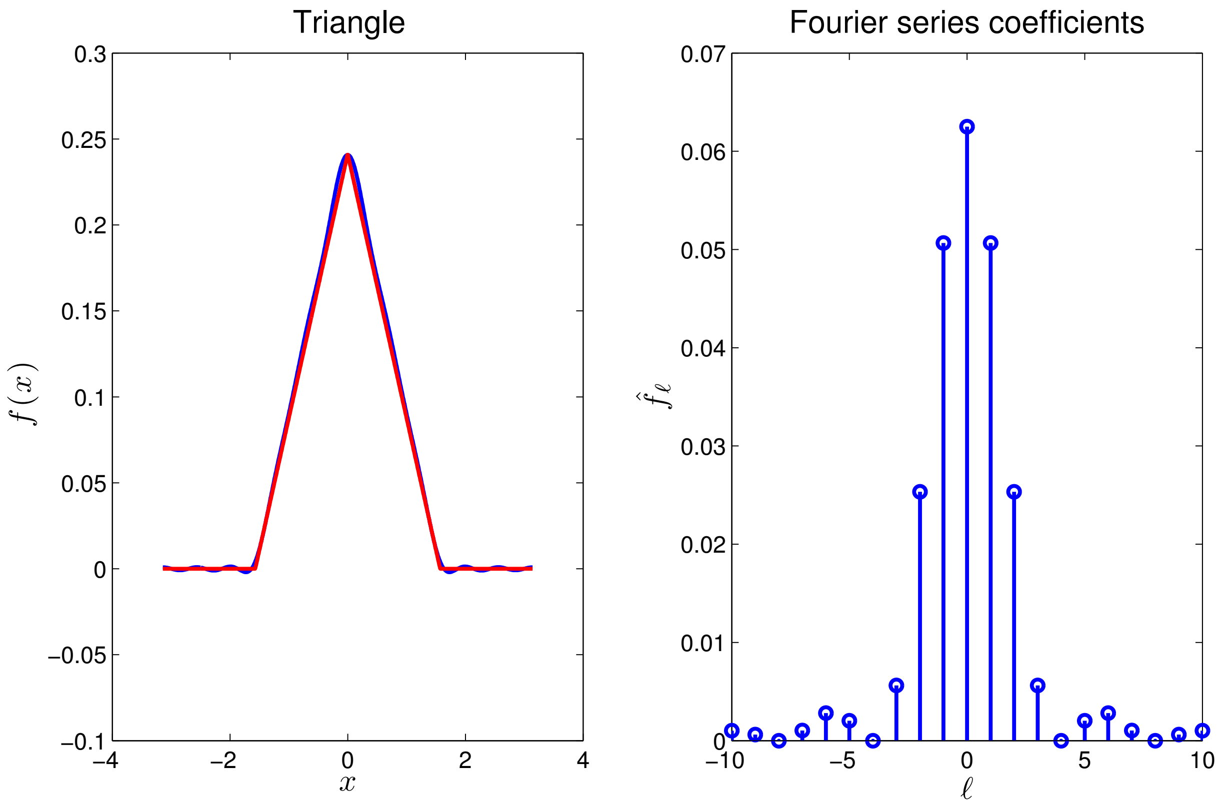
# Example

Is the triangle kernel characteristic? NO

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# Characteristic kernels (Via Fourier, on $\mathbb{R}^d$)

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- Can we prove characteristic on $\mathbb{R}^d$?

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$$\phi_{\mathbf{P}}(\omega) = \int_{\mathbb{R}^d} e^{ix^\top \omega} d\mathbf{P}(x)$$

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$$k(z) = \int_{\mathbb{R}^d} e^{-iz^\top \omega} d\Lambda(\omega)$$

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# Characteristic Kernels (via Fourier)

Fourier representation of MMD:

$$\mathrm{MMD}^2(\mathbf{P}, \mathbf{Q}; F) = \int |\phi_{\mathbf{P}}(\omega) - \phi_{\mathbf{Q}}(\omega)|^2 \, d\Lambda(\omega)$$

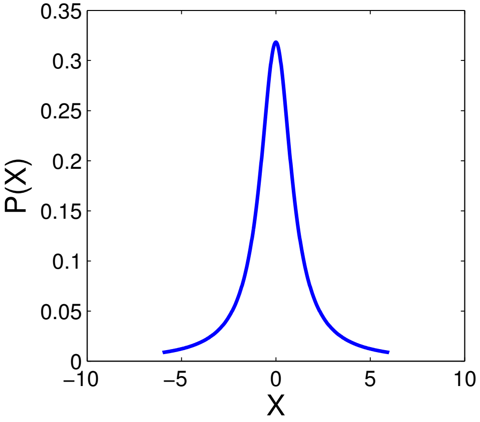
$\phi_{\mathbf{P}}$ characteristic function of $\mathbf{P}$

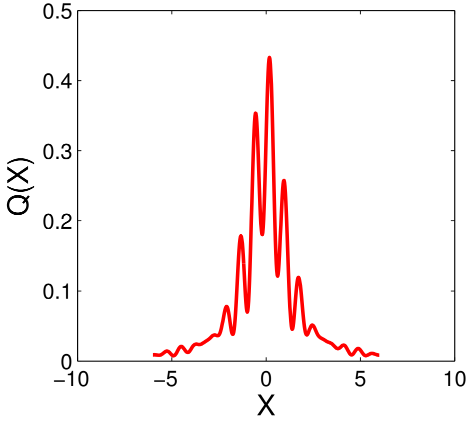
Proof: Using Bochner's theorem (a)... and Fubini's theorem (b)

$$\begin{aligned}
\mathrm{MMD}^2(\mathbf{P}, \mathbf{Q}) &:= \mathbb{E}_{\mathbf{P}} k(\mathsf{x} - \mathsf{x}') + \mathbb{E}_{\mathbf{Q}} k(\mathsf{y} - \mathsf{y}') - 2\mathbb{E}_{\mathbf{P},\mathbf{Q}} k(\mathsf{x}, \mathsf{y}) \\
&= \int \int \left[ k(s - t) \, d(\mathbf{P} - \mathbf{Q})(s) \right] d(\mathbf{P} - \mathbf{Q})(t) \\
&\stackrel{(a)}{=} \int \int \int_{\mathbb{R}^d} e^{-i(s-t)^T \omega} \, d\Lambda(\omega) \, d(\mathbf{P} - \mathbf{Q})(s) \, d(\mathbf{P} - \mathbf{Q})(t) \\
&\stackrel{(b)}{=} \int \int_{\mathbb{R}^d} e^{-ix^T \omega} \, d(\mathbf{P} - \mathbf{Q})(s) \int_{\mathbb{R}^d} e^{iy^T \omega} \, d(\mathbf{P} - \mathbf{Q})(t) \, d\Lambda(\omega) \\
&= \int_{\mathbb{R}^d} |\phi_{\mathbf{P}}(\omega) - \phi_{\mathbf{Q}}(\omega)|^2 \, d\Lambda(\omega)
\end{aligned}$$

# Example

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



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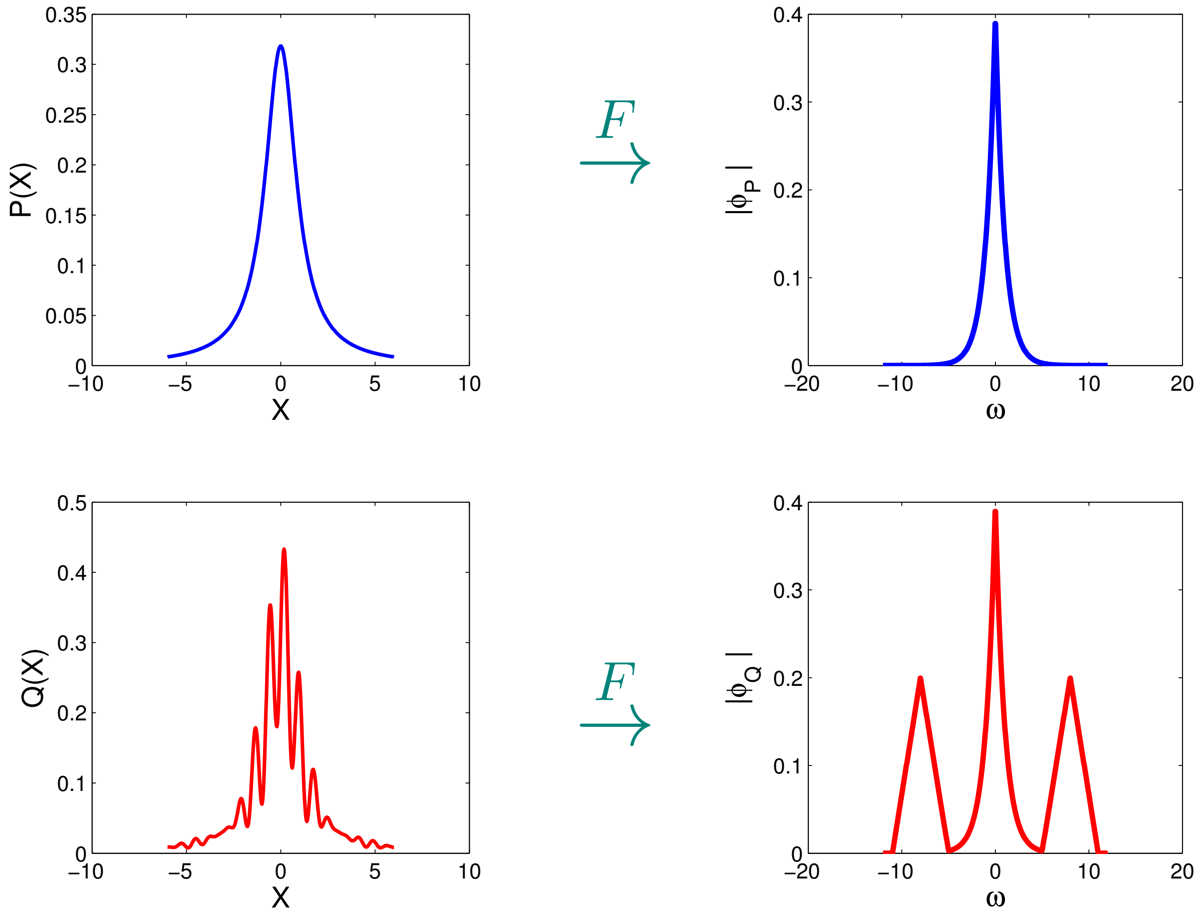

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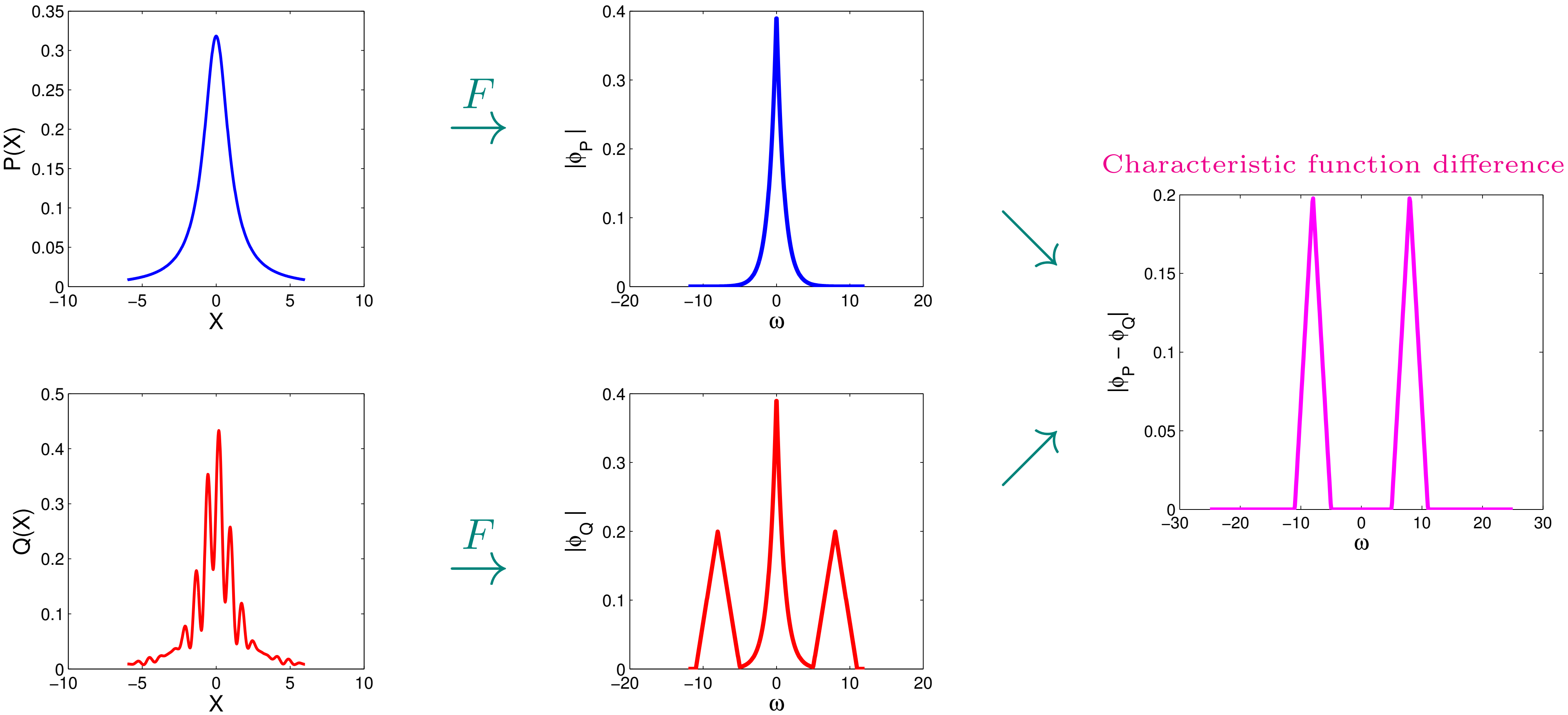
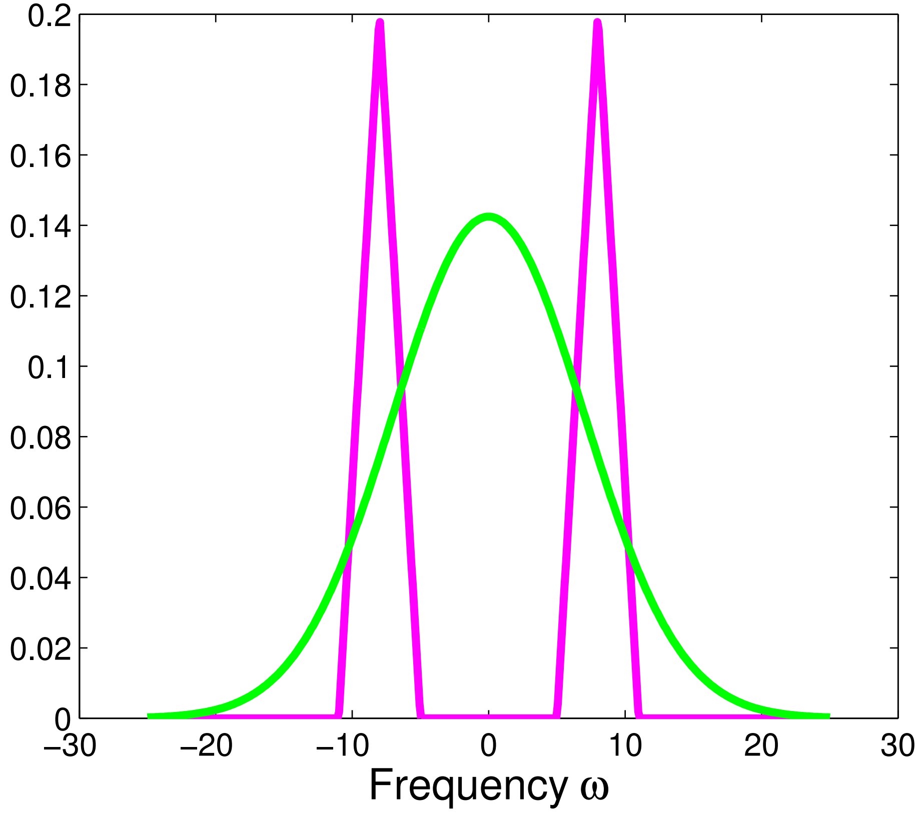


# Example

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

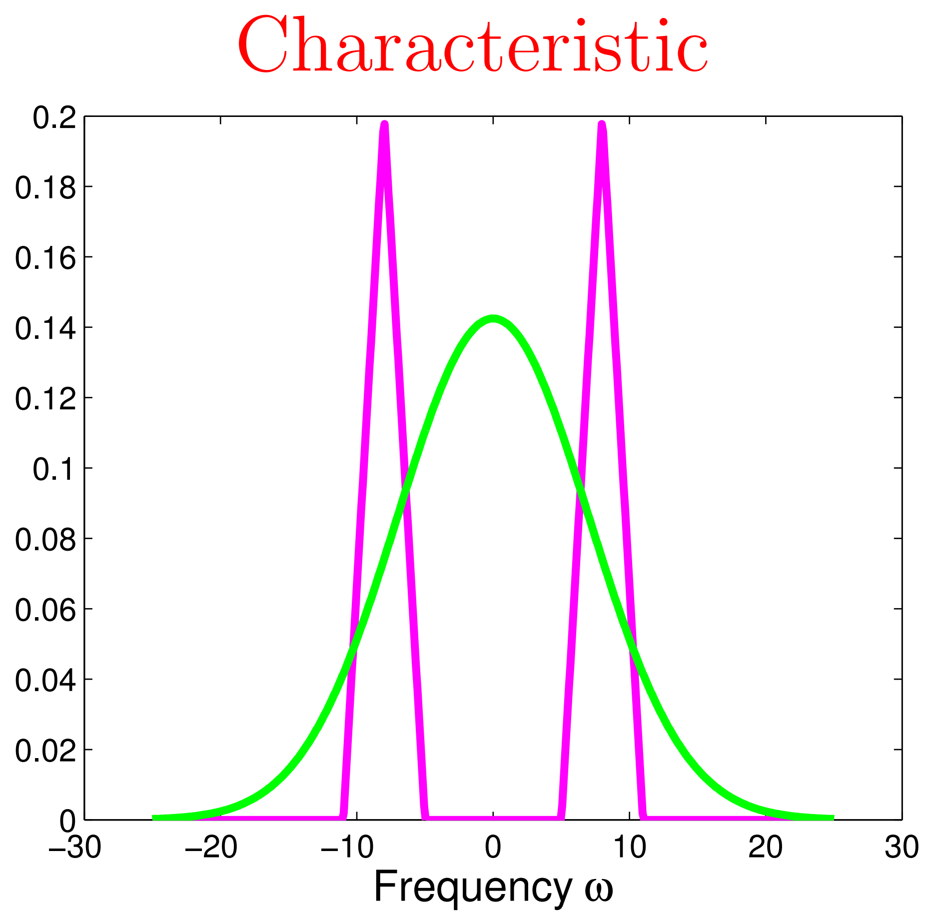
**Exponentiated quadratic** kernel

Difference $|\phi_P - \phi_Q|$



# Example

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

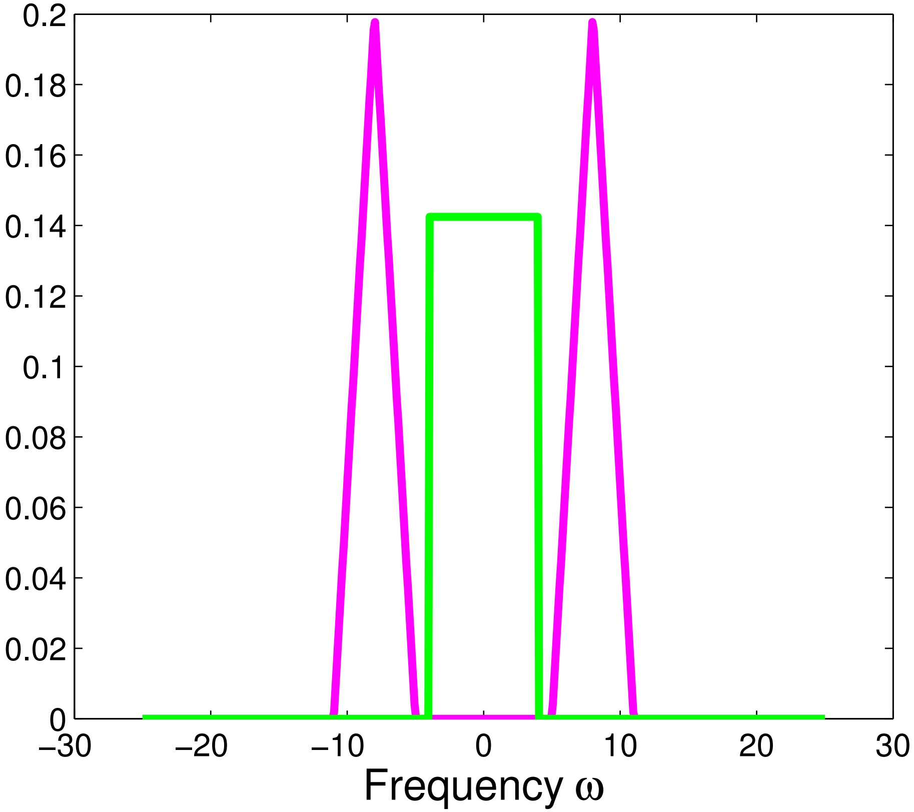


# Example

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

**Sinc** kernel

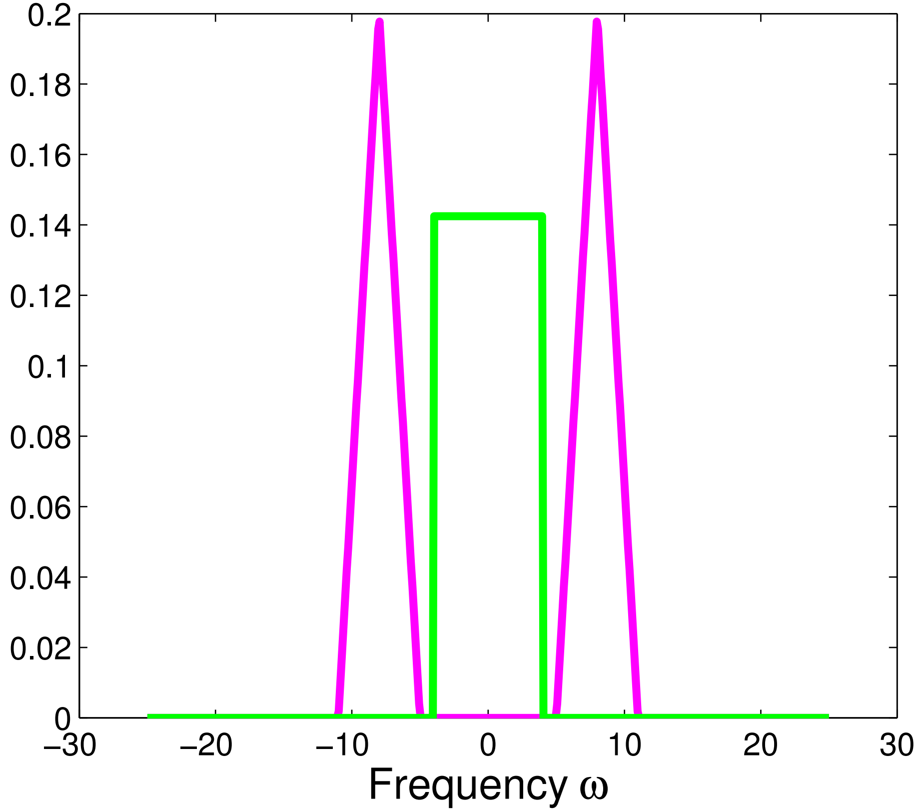
Difference $|\phi_P - \phi_Q|$



# Example

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

NOT characteristic

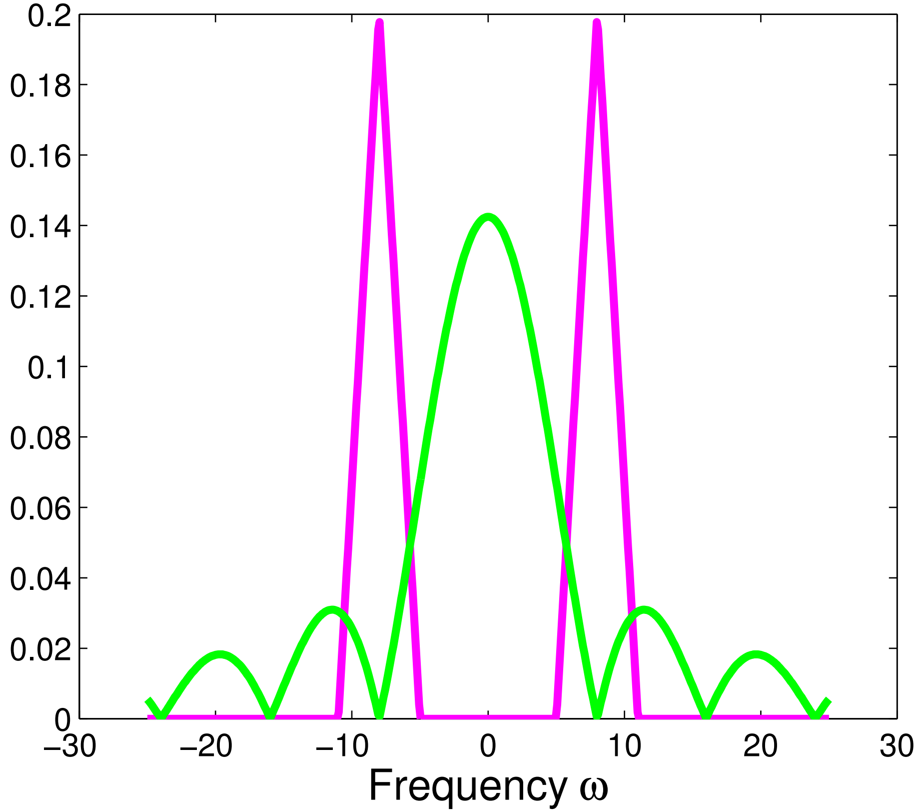


# Example

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

**Triangle** (B-spline) kernel

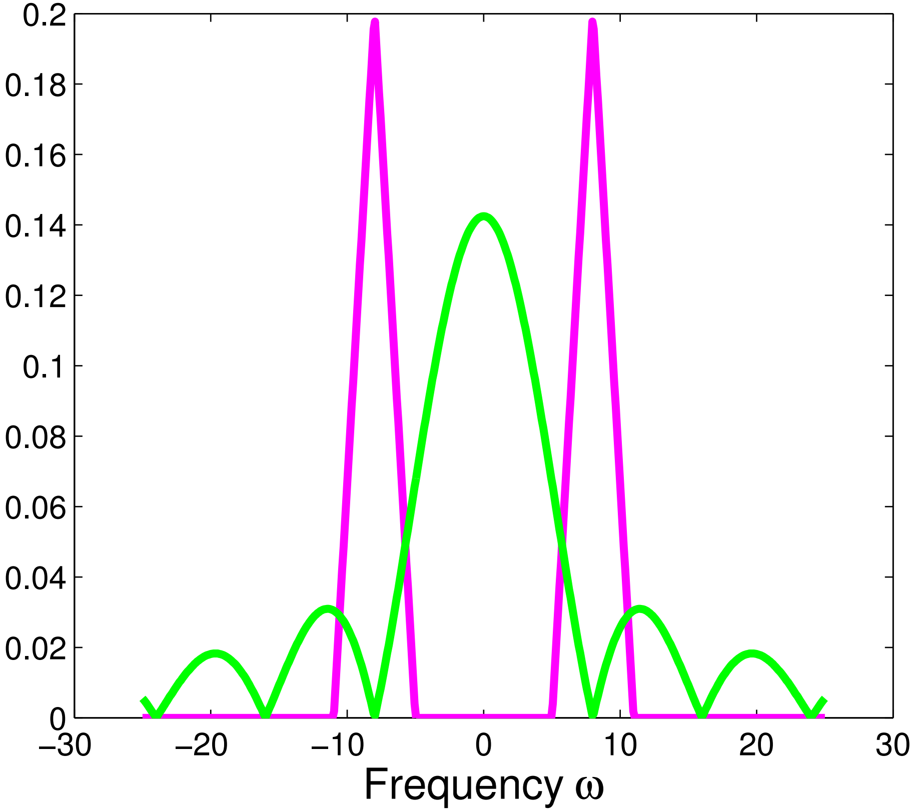
Difference $|\phi_P - \phi_Q|$



# Example

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

???



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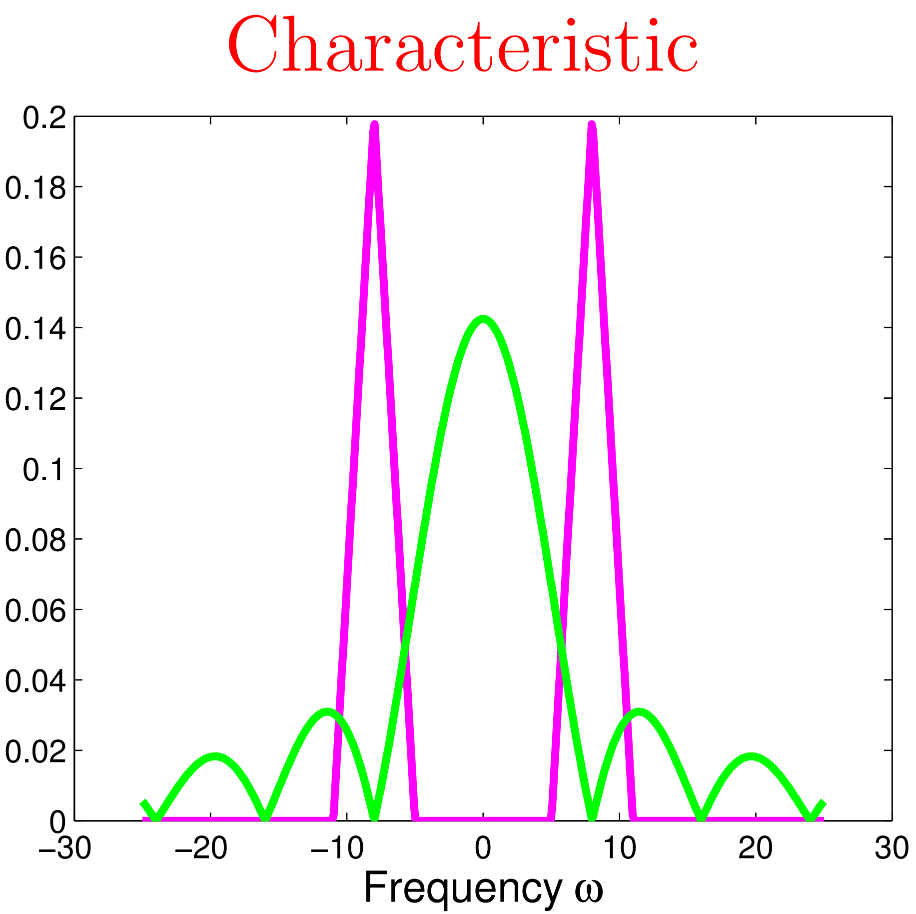


# Summary: Characteristic Kernels

Characteristic kernel: (MMD $= 0$ iff $\mathbf{P} = \mathbf{Q}$) [NIPS07b, COLT08]

Main theorem: A translation invariant $k$ characteristic for prob. measures on $\mathbb{R}^d$ if and only if $\mathrm{supp}(\Lambda) = \mathbb{R}^d$ (i.e. support zero on at most a countable set) [COLT08, JMLR10]

Corollary: continuous, compactly supported $k$ characteristic (since Fourier spectrum $\Lambda(\omega)$ cannot be zero on an interval). 1-D proof sketch from [Mallat, 1999, Theorem 2.6] proof on $\mathbb{R}^d$ via distribution theory in [Sriperumbudur et al., 2010, Corollary 10 p. 1535]

# $k$ characteristic iff $\mathrm{supp}(\Lambda) = \mathbb{R}^d$

Proof: $\mathrm{supp}\,\{\Lambda\} = \mathbb{R}^d \implies$ k characteristic:

Recall Fourier definition of MMD:

$$\mathrm{MMD}^2(\mathbf{P}, \mathbf{Q}) = \int_{\mathbb{R}^d} |\phi_{\mathbf{P}}(\omega) - \phi_{\mathbf{Q}}(\omega)|^2 \, d\Lambda(\omega).$$

Characteristic functions $\phi_{\mathbf{P}}(\omega)$ and $\phi_{\mathbf{Q}}(\omega)$ uniformly continuous, hence their difference cannot be non-zero only on a countable set.

Map $\phi_{\mathbf{P}}$ uniformly continuous: $\forall \epsilon > 0, \quad \exists \delta > 0$ such that $\forall (\omega_1, \omega_2) \in \Omega$ for which $d(\omega_1, \omega_2) < \delta$, we have $d(\phi_{\mathbf{P}}(\omega_1), \phi_{\mathbf{P}}(\omega_2)) < \epsilon$. **Uniform:** $\delta$ depends only on $\epsilon$, not on $\omega_1, \omega_2$.

# $k$ characteristic iff $\mathrm{supp}(\Lambda) = \mathbb{R}^d$

Proof: $k$ characteristic $\implies \mathrm{supp}\{\Lambda\} = \mathbb{R}^d$ :

**Proof by contrapositive.**

Given $\mathrm{supp}\{\Lambda\} \subsetneq \mathbb{R}^d$, hence $\exists$ open interval $U$ such that $\Lambda(\omega)$ zero on $U$.

Construct densities $p(x)$, $q(x)$ such that $\phi_{\mathbf{P}}, \phi_{\mathbf{Q}}$ differ only inside $U$

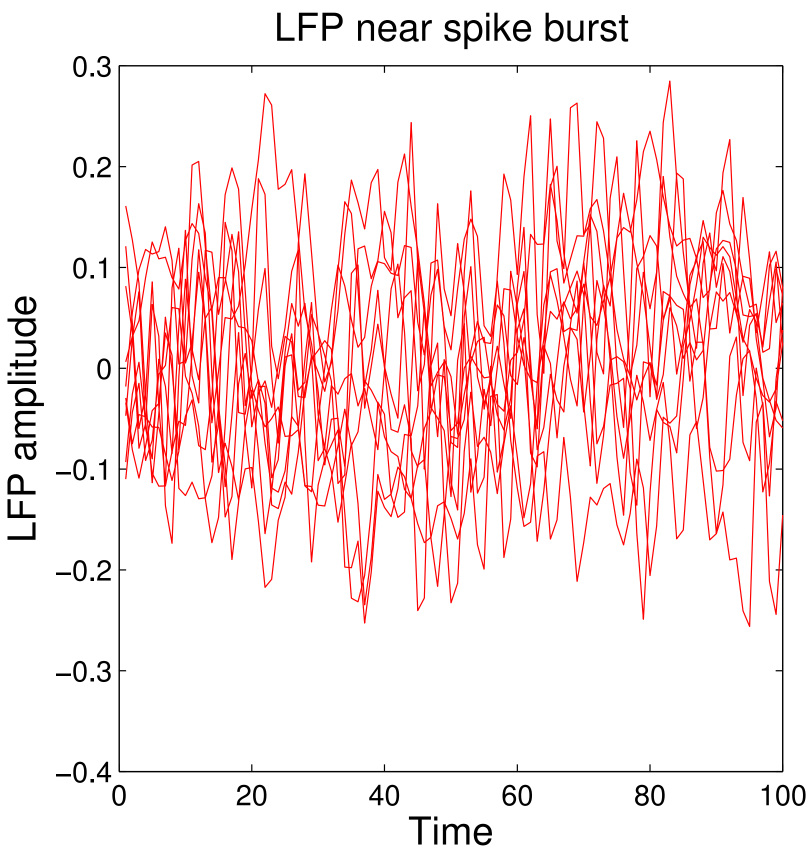
# Further extensions

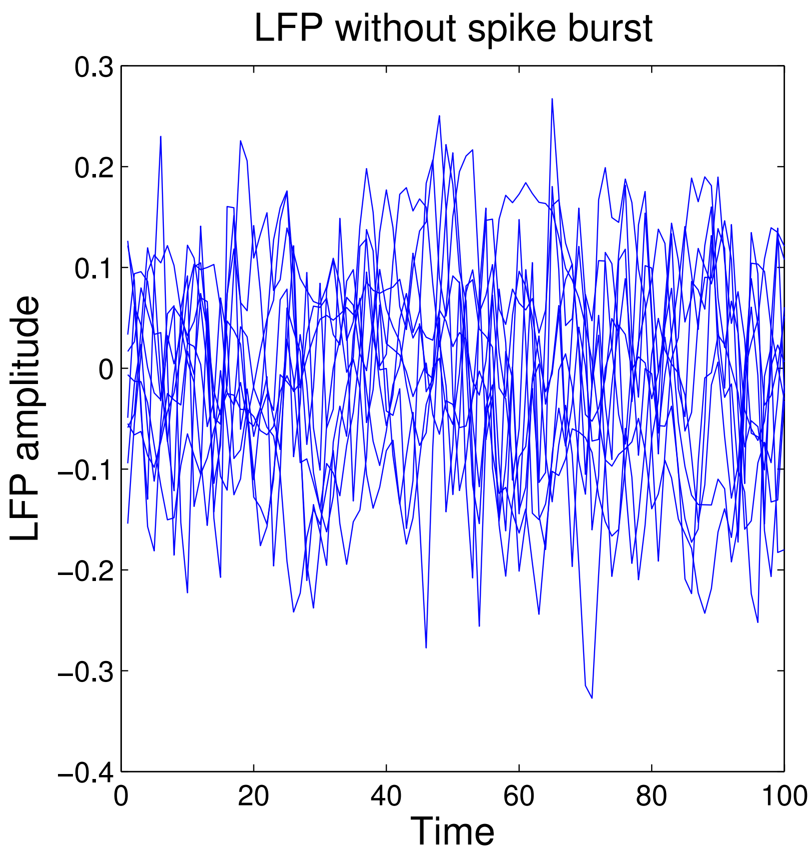
- Similar reasoning wherever extensions of Bochner's theorem exist: [Fukumizu et al., 2009]
  - Locally compact Abelian groups (periodic domains, as we saw)
  - Compact, non-Abelian groups (orthogonal matrices)
  - The semigroup $\mathbb{R}_n^+$ (histograms)
- Related kernel statistics: Fisher statistic [Harchaoui et al., 2008](zero iff $\mathbf{P} = \mathbf{Q}$ for characteristic kernels), other distances [Zhou and Chellappa, 2006](not yet shown to establish whether $\mathbf{P} = \mathbf{Q}$), energy distances

# Statistical hypothesis testing

# Motivating question: differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?



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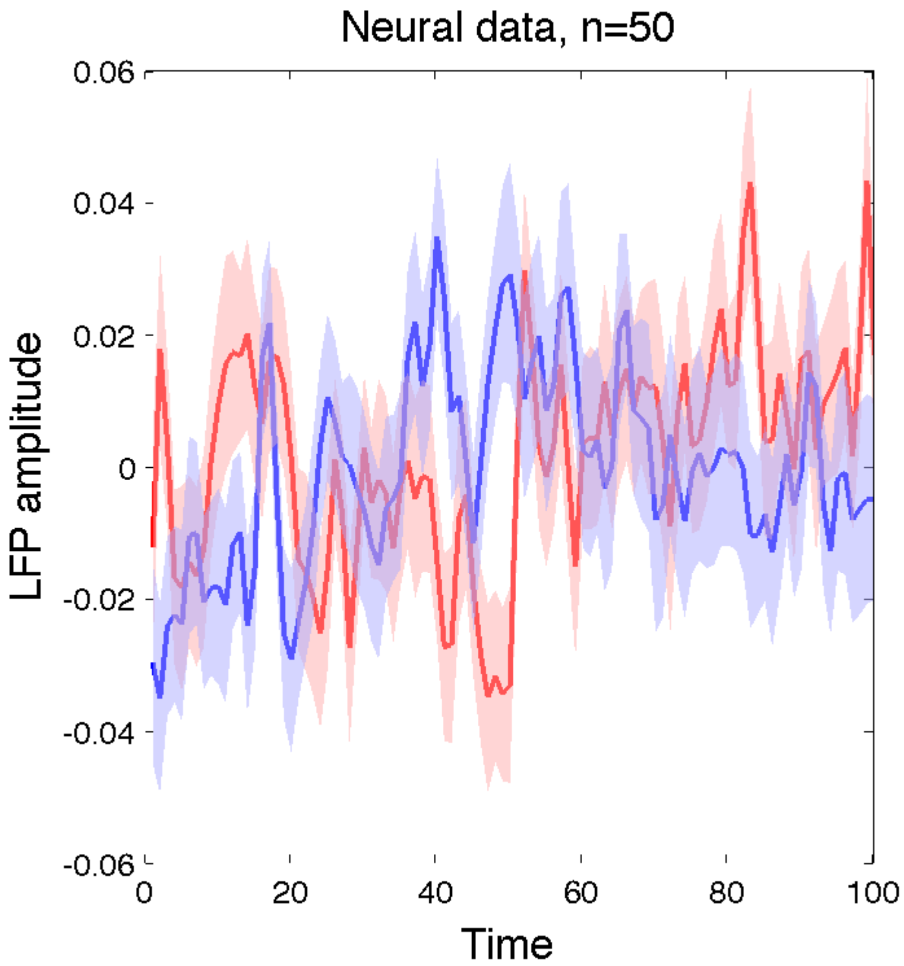

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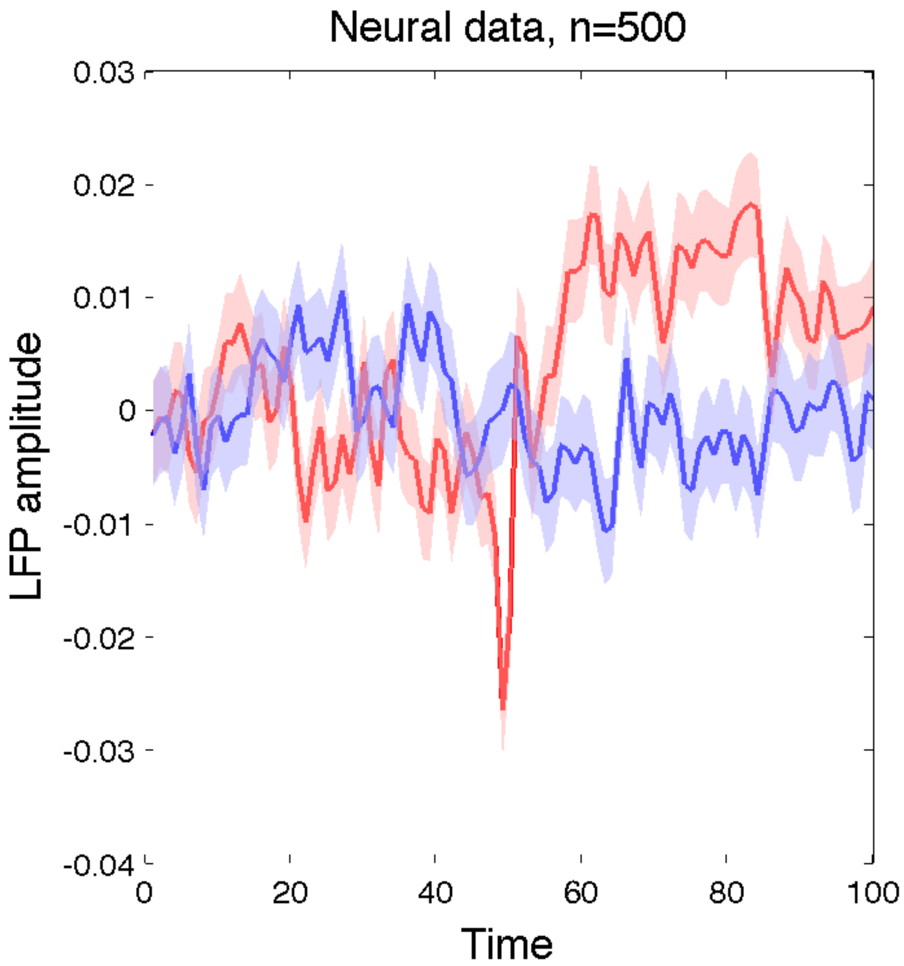

# Statistical test using MMD (1)

- Two hypotheses:
  - $H_0$: null hypothesis ($\mathbf{P} = \mathbf{Q}$)
  - $H_1$: alternative hypothesis ($\mathbf{P} \neq \mathbf{Q}$)

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- Two hypotheses:
  - $H_0$: null hypothesis ($\mathbf{P} = \mathbf{Q}$)
  - $H_1$: alternative hypothesis ($\mathbf{P} \neq \mathbf{Q}$)
- Observe samples $\boldsymbol{x} := \{x_1, \ldots, x_n\}$ from $\mathbf{P}$ and $\boldsymbol{y}$ from $\mathbf{Q}$
- If empirical $\mathrm{MMD}(\boldsymbol{x}, \boldsymbol{y}; F)$ is
  - "far from zero": reject $H_0$
  - "close to zero": accept $H_0$

# Statistical test using MMD (2)

- "far from zero" vs "close to zero" - threshold?
- One answer: asymptotic distribution of $\widehat{\mathrm{MMD}}^2$

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- An unbiased empirical estimate (quadratic cost):

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$$\widehat{\mathrm{MMD}}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} \underbrace{k(x_i, x_j) - k(x_i, y_j) - k(y_i, x_j) + k(y_i, y_j)}_{h((x_i, y_i), (x_j, y_j))}$$

- When $\mathbf{P} \neq \mathbf{Q}$, asymptotically normal

$$(\sqrt{n}) \left( \widehat{\mathrm{MMD}}^2 - \mathrm{MMD}^2 \right) \sim \mathcal{N}(0, \sigma_u^2)$$

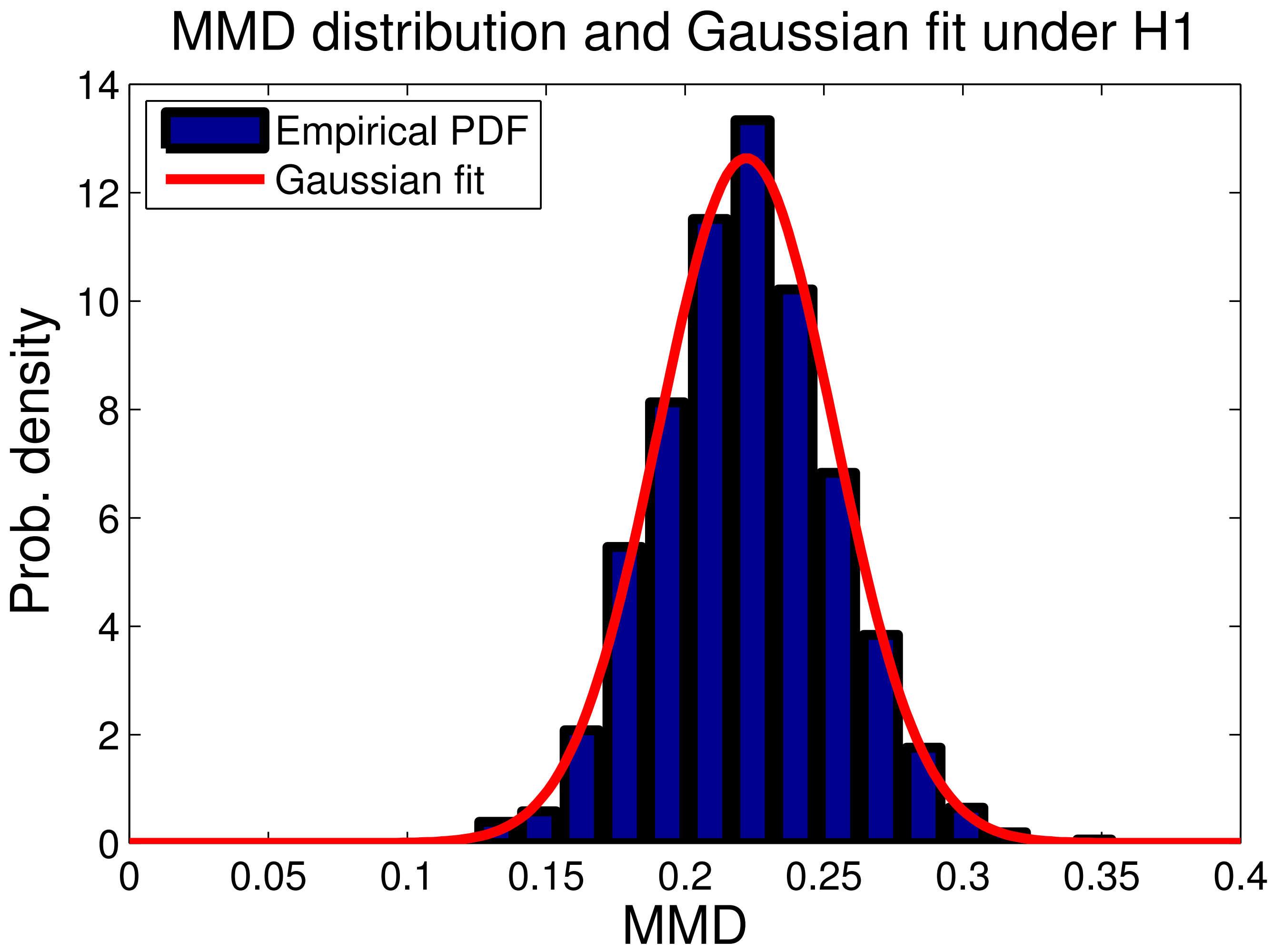
[Hoeffding, 1948, Serfling, 1980]

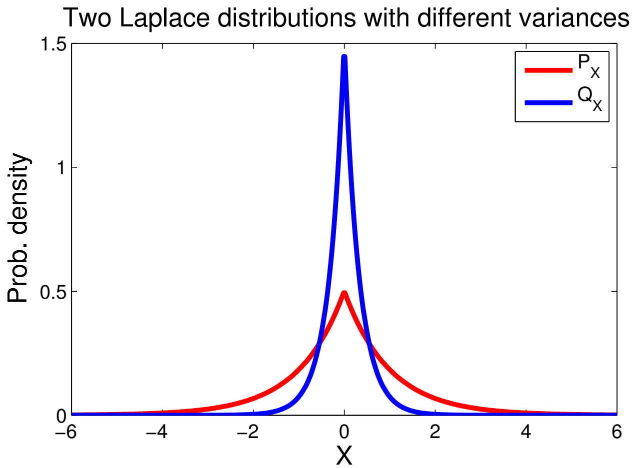
- Expression for the variance: $z_i := (x_i, y_i)$

$$\sigma_u^2 = 4 \left( \mathbb{E}_{\mathsf{z}} \left[ (\mathbb{E}_{\mathsf{z}'} h(\mathsf{z}, \mathsf{z}'))^2 \right] - \left[ \mathbb{E}_{\mathsf{z}, \mathsf{z}'} (h(\mathsf{z}, \mathsf{z}')) \right]^2 \right)$$

# Statistical test using MMD (3)

- Example: laplace distributions with different variance



# Statistical test using MMD (4)

- When $\mathbf{P} = \mathbf{Q}$, U-statistic degenerate: $\mathbb{E}_{\mathsf{z}'}[h(\mathsf{z}, \mathsf{z}')] = 0$ [Anderson et al., 1994]
- Distribution is

$$n\mathrm{MMD}(\boldsymbol{x}, \boldsymbol{y}; F) \sim \sum_{l=1}^{\infty} \lambda_l \left[ z_l^2 - 2 \right]$$

- where
  - $z_l \sim \mathcal{N}(0, 2)$ i.i.d
  - $\int_{\mathcal{X}} \underbrace{\tilde{k}(x, x')}_{\text{centred}} \psi_i(x) d\mathbf{P}(x) = \lambda_i \psi_i(x')$

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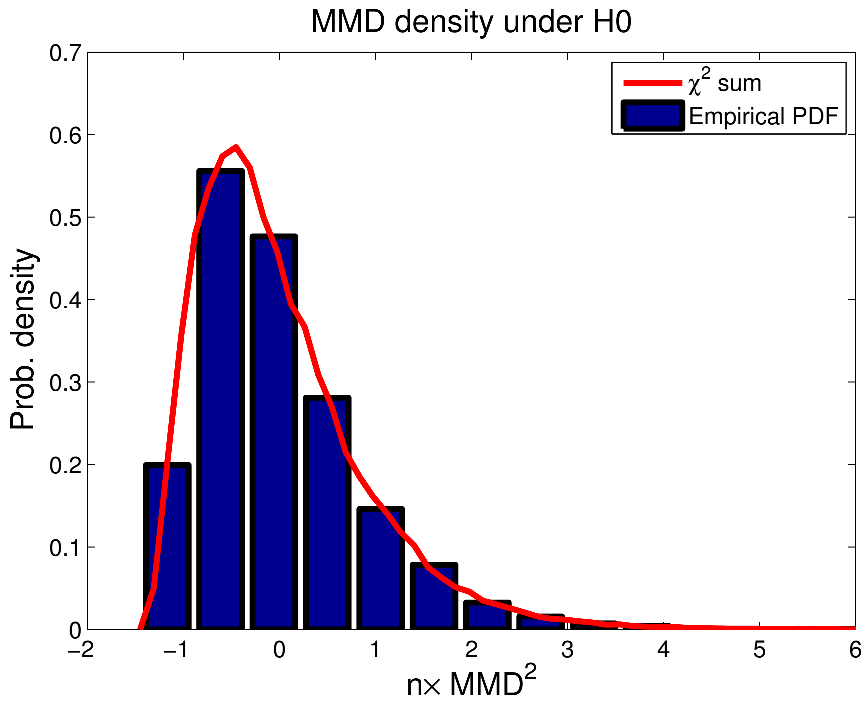
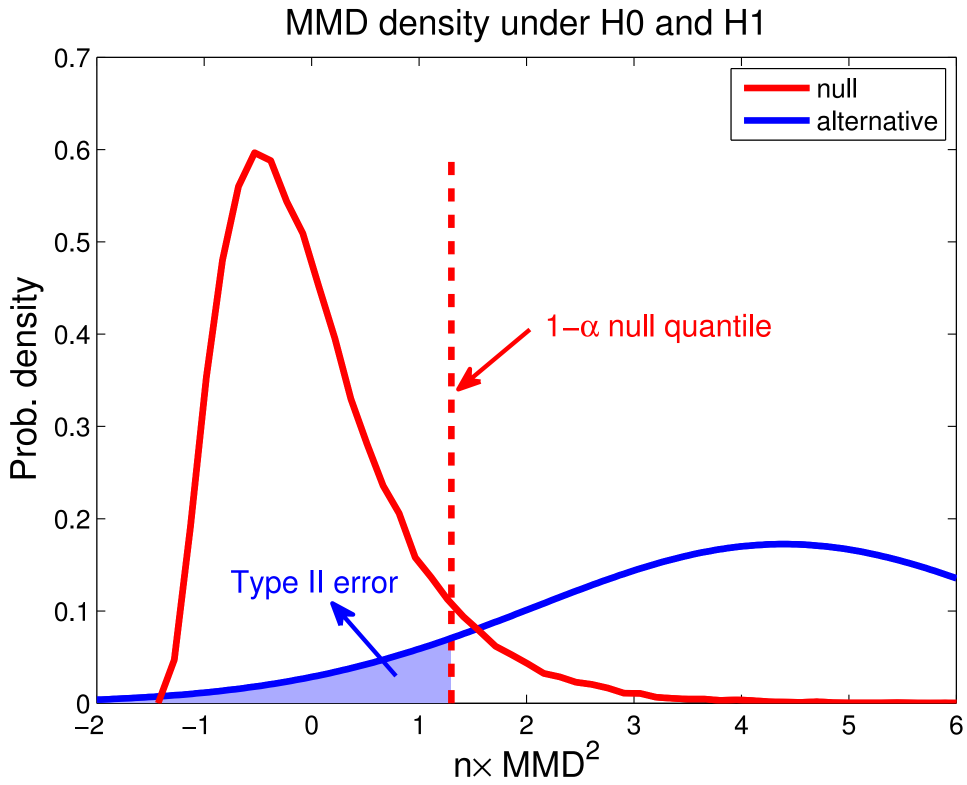


# Statistical test using MMD (5)

- Given $\mathbf{P} = \mathbf{Q}$, want threshold $T$ such that $\mathbf{P}(\mathrm{MMD} > T) \leq 0.05$

$$\widehat{MMD}^2 = \overline{K_{P,P}} + \overline{K_{Q,Q}} - 2\overline{K_{P,Q}}$$



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- Given $\mathbf{P} = \mathbf{Q}$, want threshold $T$ such that $\mathbf{P}(\text{MMD} > T) \leq 0.05$
- Permutation for empirical CDF [Arcones and Giné, 1992, Alba Fernández et al., 2008]
- Pearson curves by matching first four moments [Johnson et al., 1994]
- Large deviation bounds [Hoeffding, 1963, McDiarmid, 1989]
- Consistent test using kernel eigenspectrum [NIPS09b]

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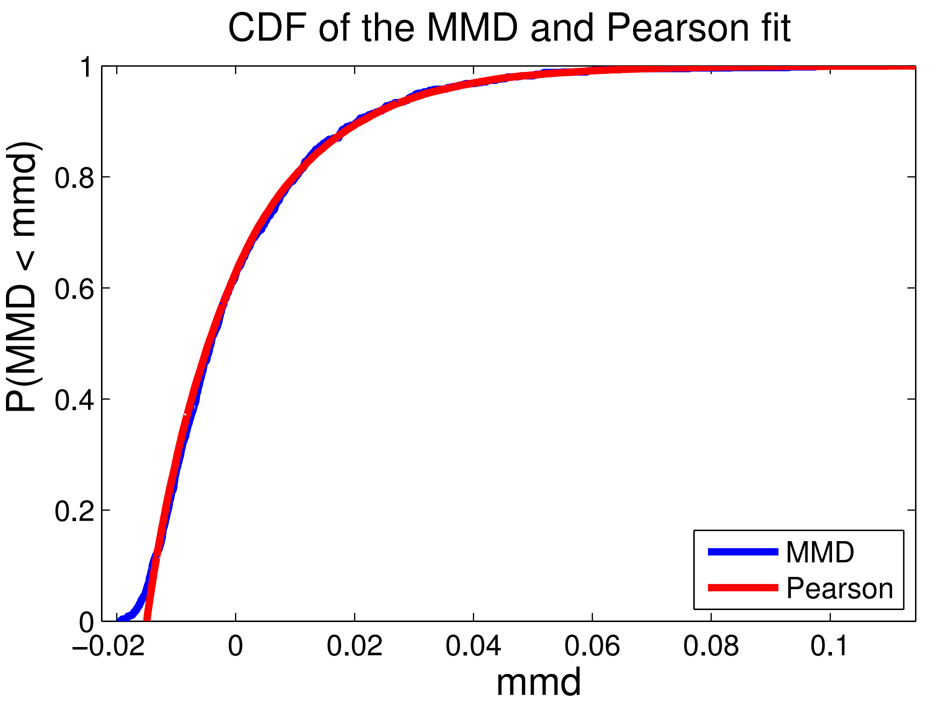

# Approximate null distribution of $\widehat{MMD}$ via permutation

Empirical MMD:

$$w = (\underbrace{1, 1, 1, \ldots 1}_{n}, \underbrace{-1 \ldots, -1, -1, -1}_{n})^\top$$

$$\frac{1}{n^2} \sum \left( \begin{bmatrix} K_{P,P} & K_{P,Q} \\ K_{Q,P} & K_{Q,Q} \end{bmatrix} \odot \left[ w w^\top \right] \right) \approx \widehat{\mathrm{MMD}}^2$$

# Approximate null distribution of $\widehat{MMD}$ via permutation

Permuted case: [Alba Fernández et al., 2008]

$$w = (\underbrace{1, -1, 1, \ldots 1}_{n}, \underbrace{-1 \ldots, 1, -1, -1}_{n})^\top$$

(equal number of $+1$ and $-1$)

$$\frac{1}{n^2} \sum \left( \begin{bmatrix} K_{P,P} & K_{P,Q} \\ K_{Q,P} & K_{Q,Q} \end{bmatrix} \odot \left[ ww^\top \right] \right) = [?]$$

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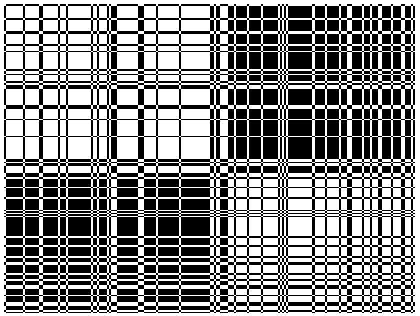
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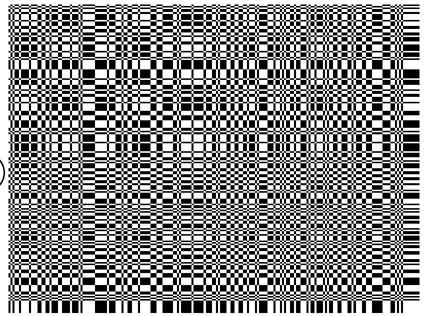
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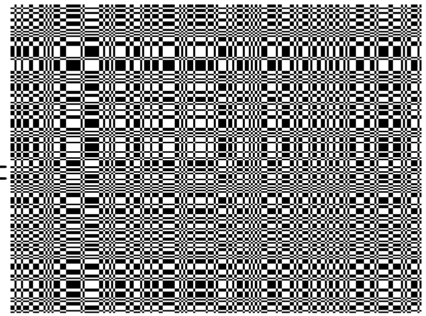
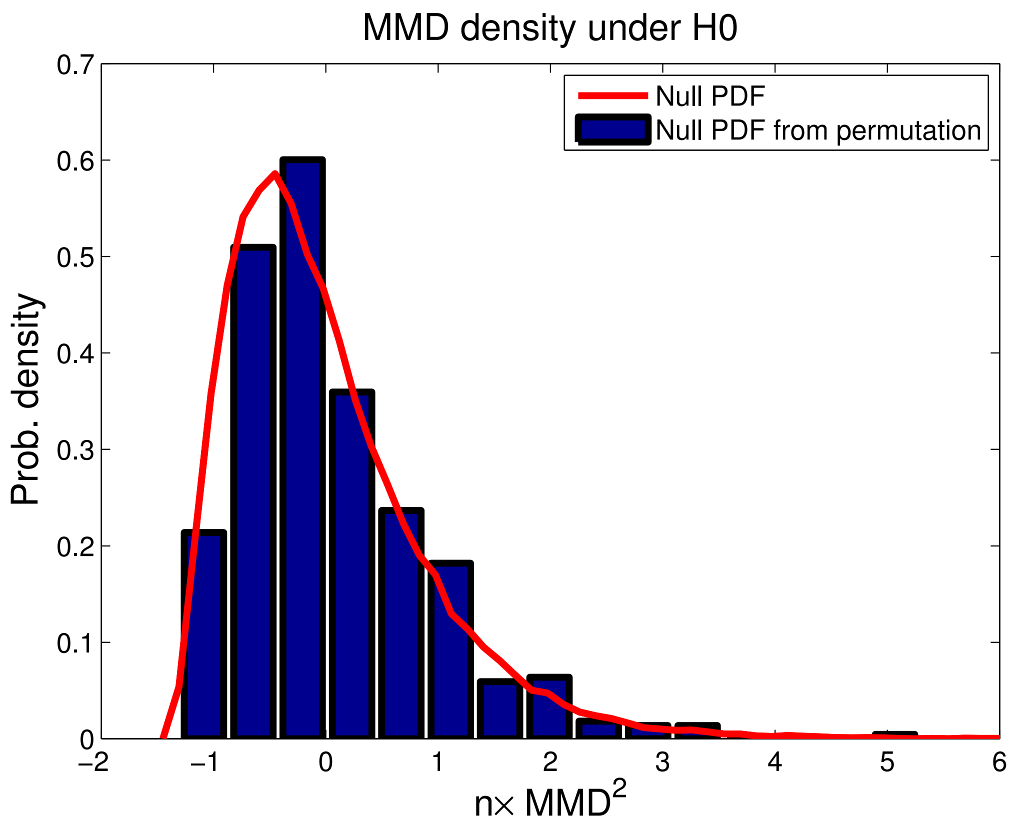


Figure thanks to Kacper Chwialkowski.

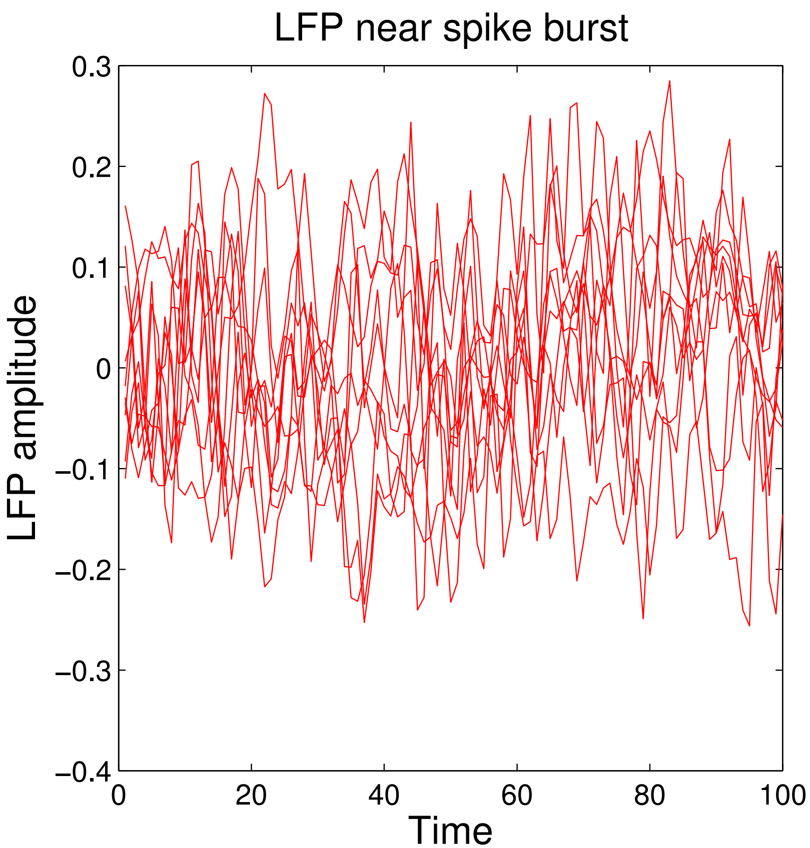
# Approximate null distribution of $\widehat{MMD}^2$ via permutation

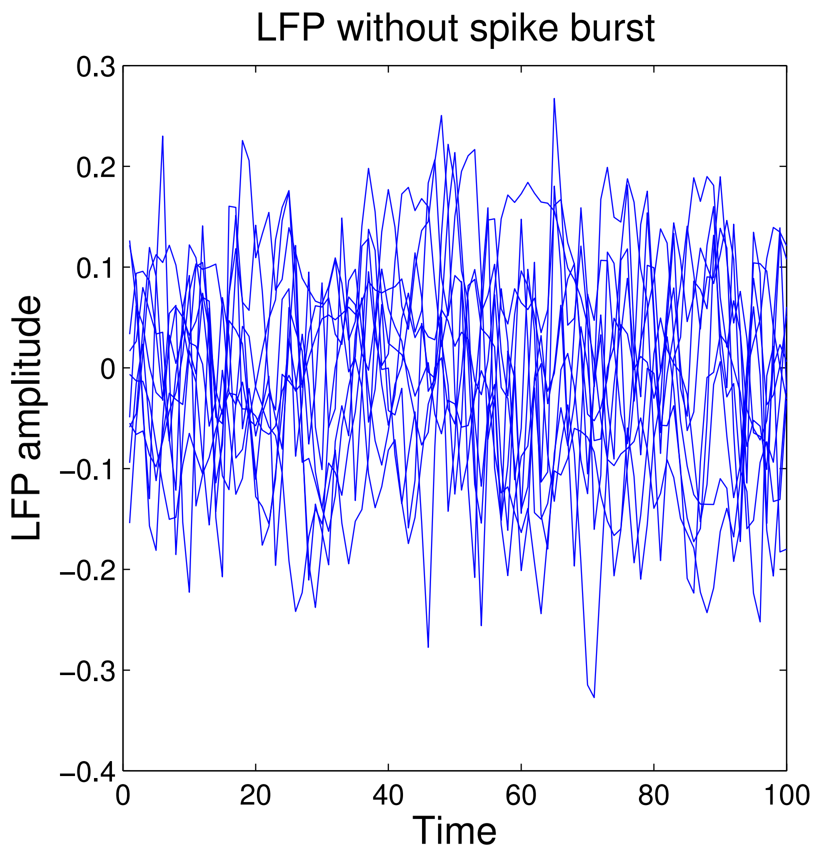
$$\widehat{MMD}_p^2 \approx \frac{1}{n^2} \sum \left( \begin{bmatrix} K_{P,P} & K_{P,Q} \\ K_{Q,P} & K_{Q,Q} \end{bmatrix} \odot \left[ w w^\top \right] \right)$$



# Detecting differences in brain signals

Do local field potential (LFP) signals change when measured near a spike burst?



# Neuro data: consistent test w/o permutation

- Maximum mean discrepancy (MMD): distance between **P** and **Q**

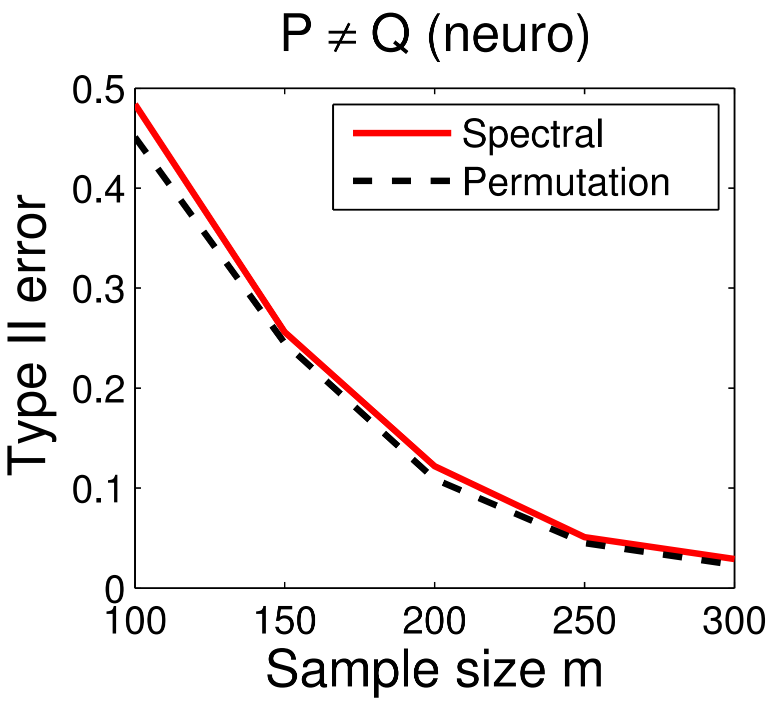
$$\mathrm{MMD}(\mathbf{P}, \mathbf{Q}; F) := \|\mu_{\mathbf{P}} - \mu_{\mathbf{Q}}\|^2_{\mathcal{F}}$$

- Is $\widehat{\mathrm{MMD}}$ significantly $> 0$?

- $\mathbf{P} = \mathbf{Q}$, null distrib. of $\widehat{\mathrm{MMD}}$:

$$n\widehat{\mathrm{MMD}} \underset{D}{\rightarrow} \sum_{l=1}^{\infty} \lambda_l (z_l^2 - 2),$$

  – $\lambda_l$ is $l$th eigenvalue of kernel $\tilde{k}(x_i, x_j)$




Use Gram matrix spectrum for $\hat{\lambda}_l$: consistent test without permutation

# Hypothesis testing with HSIC

# Distribution of HSIC at independence

- (Biased) empirical HSIC a v-statistic

$$HSIC_b = \frac{1}{n^2}\mathrm{trace}(KHLH)$$

  - Statistical testing: How do we find when this is larger enough that the null hypothesis $\mathbf{P} = \mathbf{P}_x \mathbf{P}_y$ is unlikely?
  - Formally: given $\mathbf{P} = \mathbf{P}_x \mathbf{P}_y$, what is the threshold $T$ such that $\mathbf{P}(\mathrm{HSIC} > T) < \alpha$ for small $\alpha$?

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- Associated U-statistic degenerate when $\mathbf{P} = \mathbf{P}_{\mathsf{x}}\mathbf{P}_{\mathsf{y}}$ [Serfling, 1980]:

$$n\mathrm{HSIC}_b \xrightarrow{D} \sum_{l=1}^{\infty} \lambda_l z_l^2, \qquad z_l \sim \mathcal{N}(0,1)\mathrm{i.i.d.}$$

$$\lambda_l \psi_l(z_j) = \int h_{ijqr}\psi_l(z_i)dF_{i,q,r}, \quad h_{ijqr} = \frac{1}{4!}\sum_{(t,u,v,w)}^{(i,j,q,r)} k_{tu}l_{tu} + k_{tu}l_{vw} - 2k_{tu}l_{tv}$$

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- First two moments [NIPS07b]

$$\mathbf{E}(\mathrm{HSIC}_b) = \frac{1}{n}\mathrm{Tr}C_{xx}\mathrm{Tr}C_{yy}$$

$$\mathrm{var}(\mathrm{HSIC}_b) = \frac{2(n-4)(n-5)}{(n)_4}\|C_{xx}\|_{\mathrm{HS}}^2\|C_{yy}\|_{\mathrm{HS}}^2 + \mathrm{O}(n^{-3}).$$

# Statistical testing with HSIC

- Given $\mathbf{P} = \mathbf{P}_x\mathbf{P}_y$, what is the threshold $T$ such that $\mathbf{P}(\text{HSIC} > T) < \alpha$ for small $\alpha$?
- Null distribution via permutation [Feuerverger, 1993]
  - Compute HSIC for $\{x_i, y_{\pi(i)}\}_{i=1}^n$ for random permutation $\pi$ of indices $\{1, \ldots, n\}$. This gives HSIC for independent variables.
  - Repeat for many different permutations, get empirical CDF
  - Threshold $T$ is $1 - \alpha$ quantile of empirical CDF

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  - Repeat for many different permutations, get empirical CDF
  - Threshold $T$ is $1 - \alpha$ quantile of empirical CDF
- Approximate null distribution via moment matching [Kankainen, 1995]:

$$n\text{HSIC}_b(Z) \sim \frac{x^{\alpha-1}e^{-x/\beta}}{\beta^\alpha \Gamma(\alpha)}$$

where

$$\alpha = \frac{(\mathbf{E}(\text{HSIC}_b))^2}{\text{var}(\text{HSIC}_b)}, \quad \beta = \frac{\text{var}(\text{HSIC}_b)}{n\mathbf{E}(\text{HSIC}_b)}.$$

# Experiment: dependence testing for translation

## Are the French text extracts translations of English?

$X_1$: Honourable senators, I have a question for the Leader of the Government in the Senate with regard to the support funding to farmers that has been announced. Most farmers have not received any money yet.

$X_2$: No doubt there is great pressure on provincial and municipal governments in relation to the issue of child care, but the reality is that there have been no cuts to child care funding from the federal government to the provinces. In fact, we have increased federal investments for early childhood development.

...

$$\overset{?}{\Longleftrightarrow}$$

$Y_1$: Honorables sénateurs, ma question s'adresse au leader du gouvernement au Sénat et concerne l'aide financiére qu'on a annoncée pour les agriculteurs. La plupart des agriculteurs n'ont encore rien reu de cet argent.

$Y_2$: Il est évident que les ordres de gouvernements provinciaux et municipaux subissent de fortes pressions en ce qui concerne les services de garde, mais le gouvernement n'a pas réduit le financement qu'il verse aux provinces pour les services de garde. Au contraire, nous avons augmenté le financement fédéral pour le développement des jeunes enfants.

...

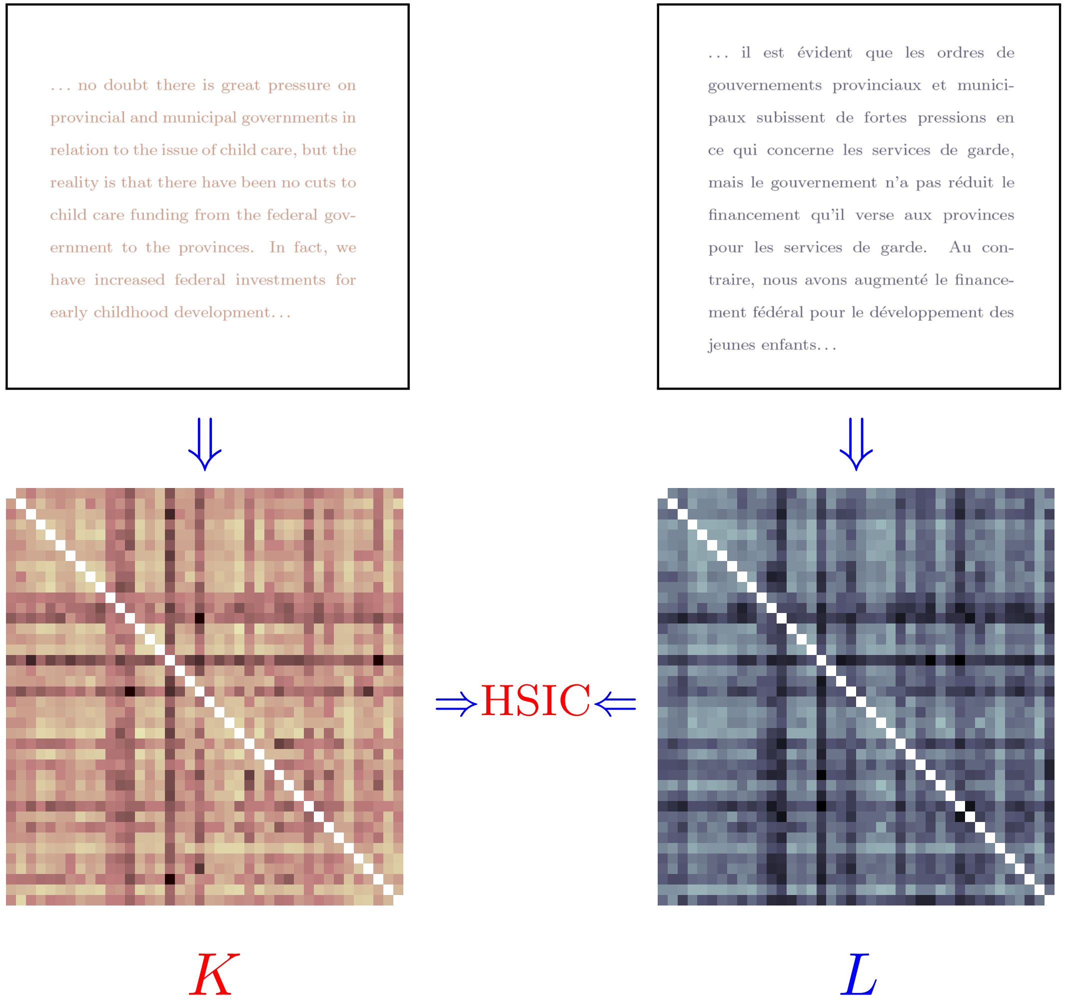
# Experiment: dependence testing for translation

- (Biased) empirical HSIC:

$$HSIC_b = \frac{1}{n^2} \text{trace}(KHLH)$$

- Translation example: [NIPS07b]
  Canadian Hansard
  (agriculture)

- 5-line extracts,
  $k$-spectrum kernel, $k = 10$,
  repetitions=300,
  sample size 10




- $k$-spectrum kernel: average Type II error 0 ($\alpha = 0.05$)

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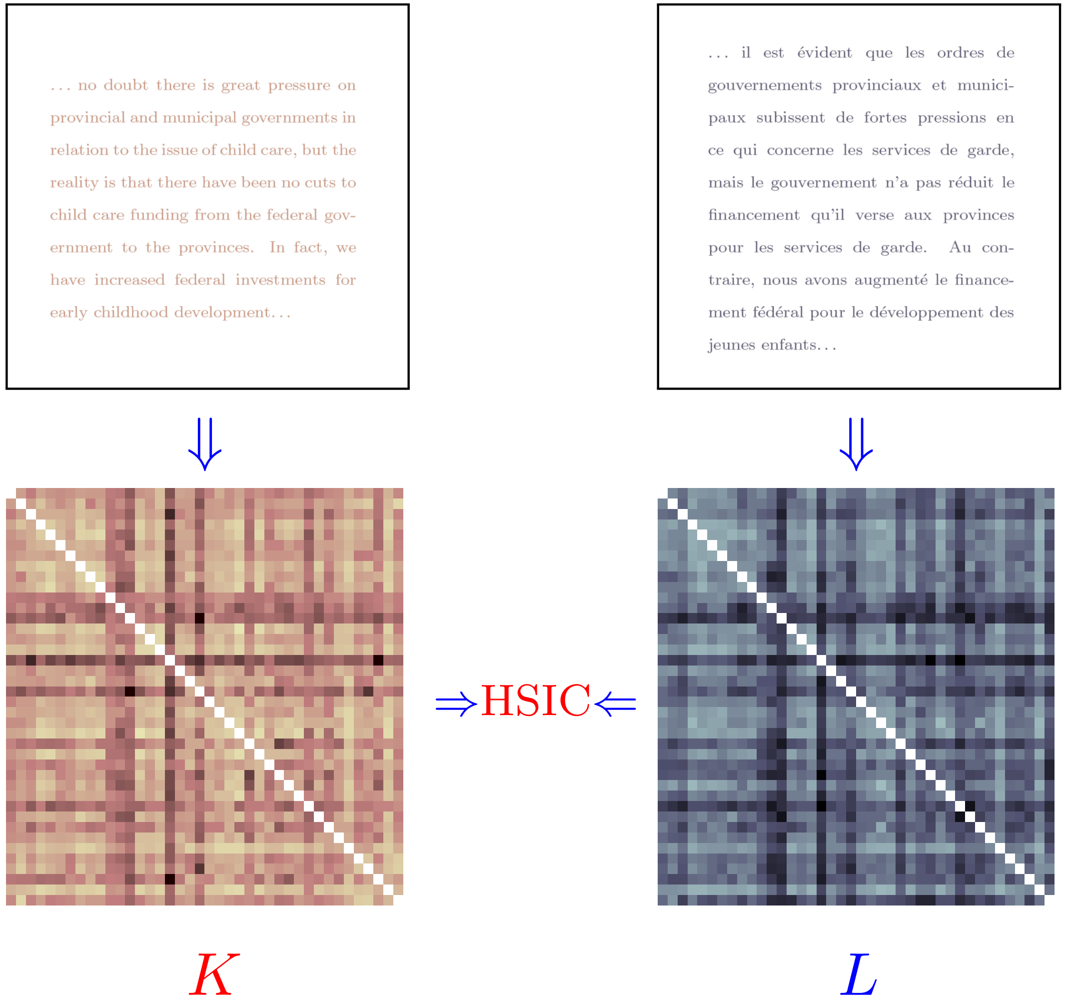


- $k$-spectrum kernel: average Type II error 0 ($\alpha = 0.05$)
- Bag of words kernel: average Type II error 0.18

# Summary

- MMD a distance between distributions [ISMB06, NIPS06a, JMLR10, JMLR12a]
  - high dimensionality
  - non-euclidean data (strings, graphs)
  - Nonparametric hypothesis tests
- Measure and test independence [ALT05, NIPS07a, NIPS07b, ALT08, JMLR10, JMLR12a]
- Characteristic RKHS: MMD a metric [NIPS07b, COLT08, NIPS08a]
  - Easy to check: does spectrum cover $\mathbb{R}^d$

# Co-authors

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  - Steffen Grunewalder
  - Guy Lever
  - Sam Patterson
  - Massimiliano Pontil
  - Dino Sejdinovic
- **External:**
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  - Wicher Bergsma, LSE
  - Kenji Fukumizu, ISM
  - Zaid Harchaoui, INRIA
  - Bernhard Schoelkopf, MPI
  - Alex Smola, CMU/Google
  - Le Song, Georgia Tech
  - Bharath Sriperumbudur, Cambridge

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- Sriperumbudur, B., Gretton, A., Fukumizu, K., Schoelkopf, B., Lanckriet, G. (2010). Hilbert space embeddings and metrics on probability measures. JMLR.
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- Gretton, A., Fukumizu, K., Teo, C., Song, L., Schoelkopf, B., Smola, A. (2008). A kernel statistical test of independence. NIPS
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## Energy distance, relation to kernel distances


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## Three way interaction


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- Fukumizu, K., Song, L., Gretton, A. (2013). Kernel Bayes rule: Bayesian inference with positive definite kernels, JMLR

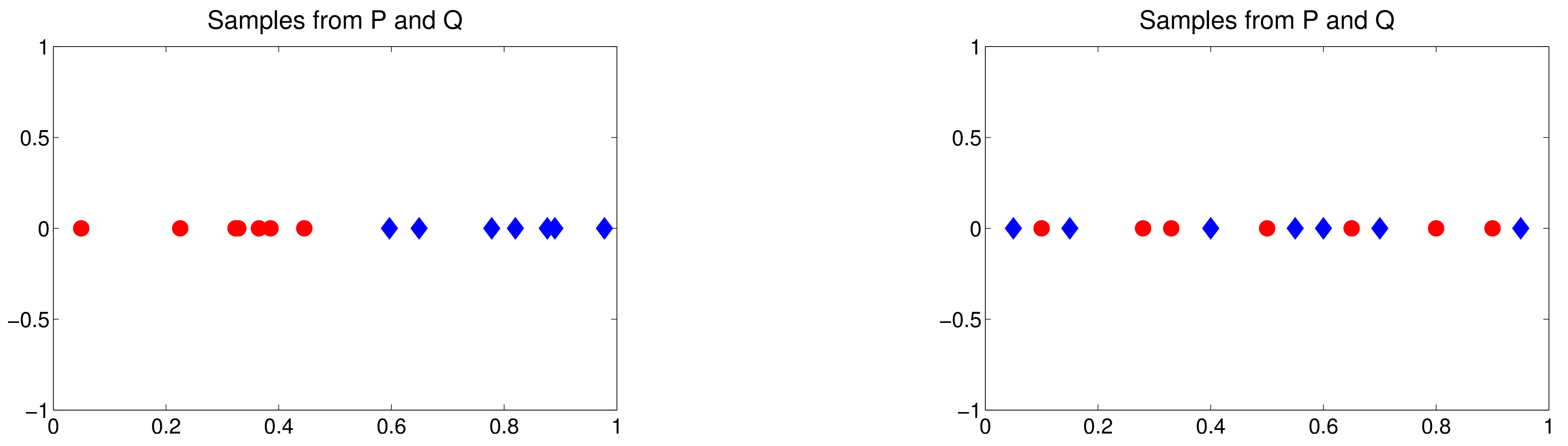
# Local departures from the null

What is a hard testing problem?

# Local departures from the null

## What is a hard testing problem?

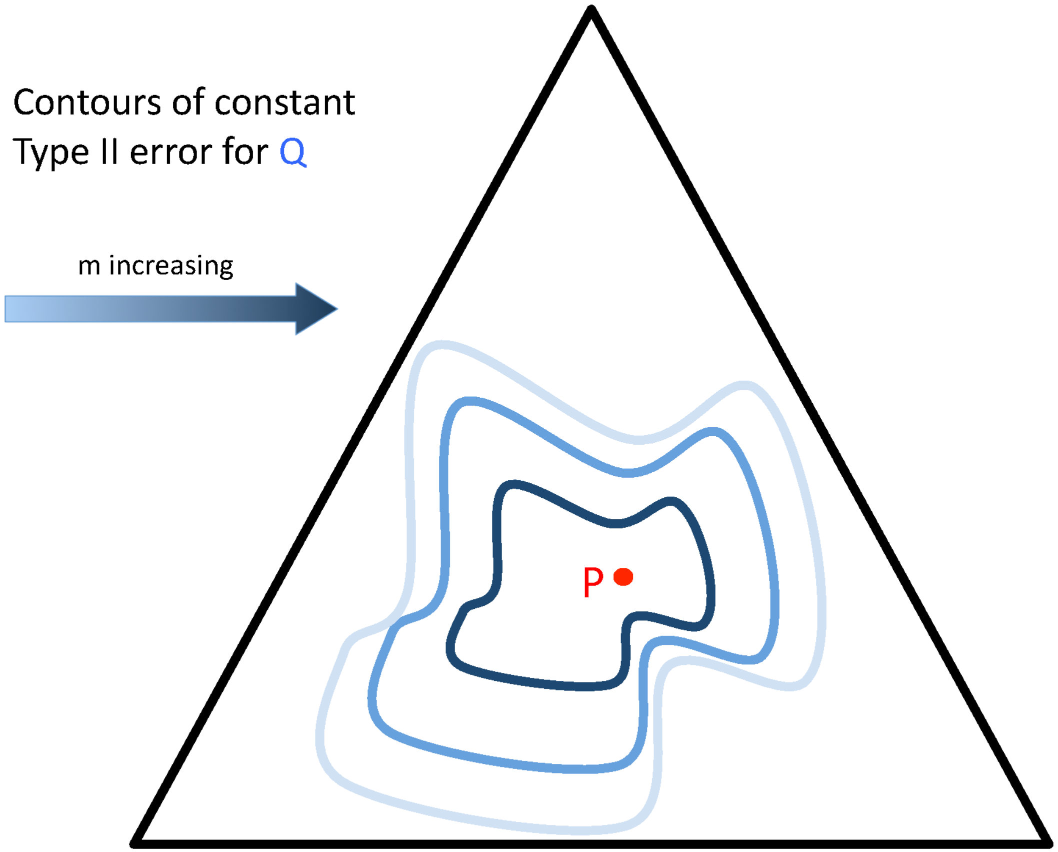
- First version: for fixed $m$, "closer" **P** and **Q** have higher Type II error



# Local departures from the null

## What is a hard testing problem?

- As $m$ increases, distinguish "closer" **P** and **Q** with fixed Type II error



# Local departures from the null

What is a hard testing problem?

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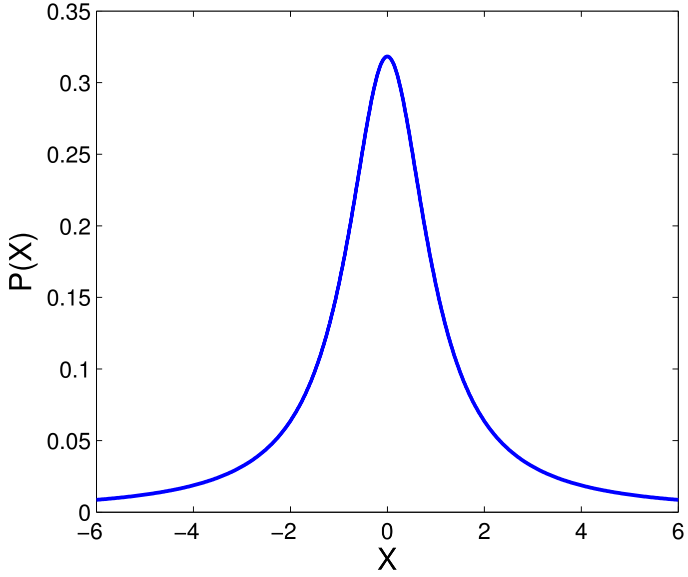
- Example: $f_{\mathbf{P}}$ and $f_{\mathbf{Q}}$ probability densities, $f_{\mathbf{Q}} = f_{\mathbf{P}} + \delta g$, where $\delta \in \mathbb{R}$, $g$ some *fixed* function such that $f_{\mathbf{Q}}$ is a valid density
  - If $\delta \sim m^{-1/2}$, Type II error approaches a constant

# More general local departures from null

- Example: $f_{\mathbf{P}}$ and $f_{\mathbf{Q}}$ probability densities, $f_{\mathbf{Q}} = f_{\mathbf{P}} + \delta g$, where $\delta \in \mathbb{R}$, $g$ some *fixed* function such that $f_{\mathbf{Q}}$ is a valid density

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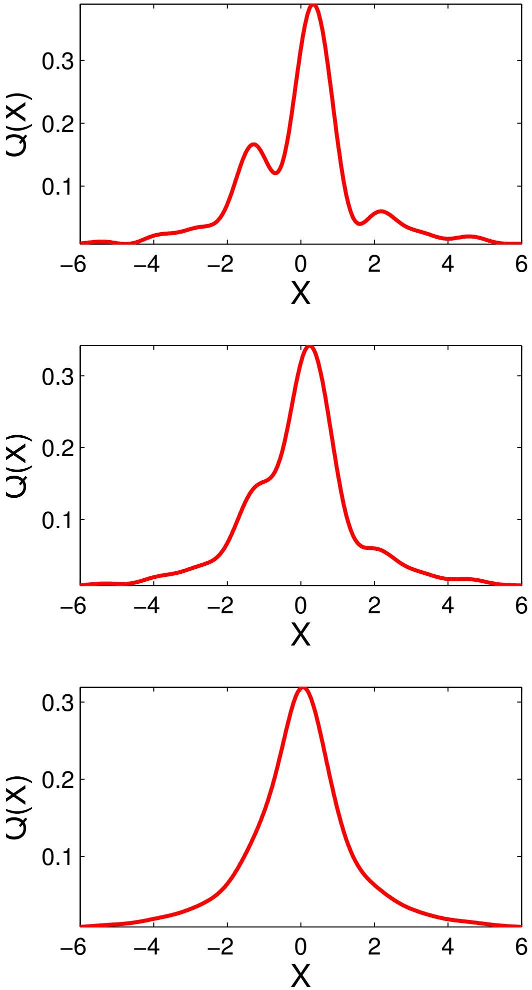

# Local departures from the null

What is a hard testing problem?

- As we see more samples $m$, distinguish "closer" $\mathbf{P}$ and $\mathbf{Q}$ with same Type II error
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- ...but **other choices also possible** – how to characterize them all?

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  - If $\delta \sim m^{-1/2}$, Type II error approaches a constant
- ...but **other choices also possible** – how to characterize them all?

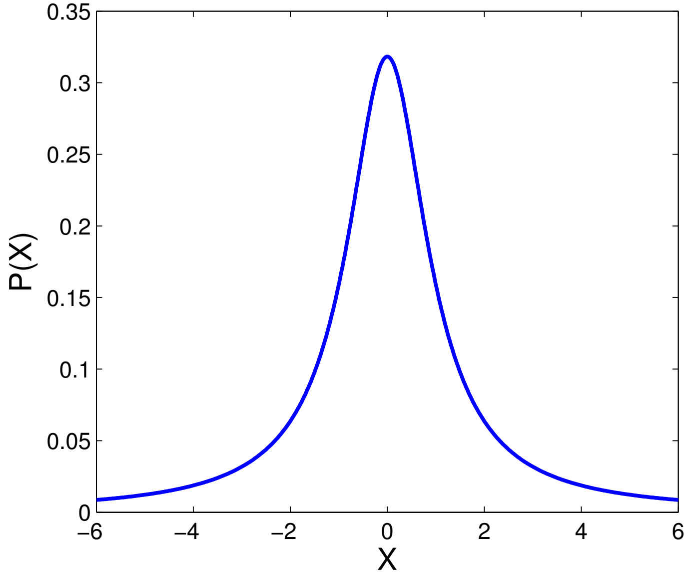
**General characterization of local departures from $\mathcal{H}_0$:**

- Write $\mu_{\mathbf{Q}} = \mu_{\mathbf{P}} + g_m$, where $g_m \in \mathcal{F}$ chosen such that $\mu_{\mathbf{P}} + g_m$ a valid distribution embedding
- Minimum distinguishable distance [JMLR12]

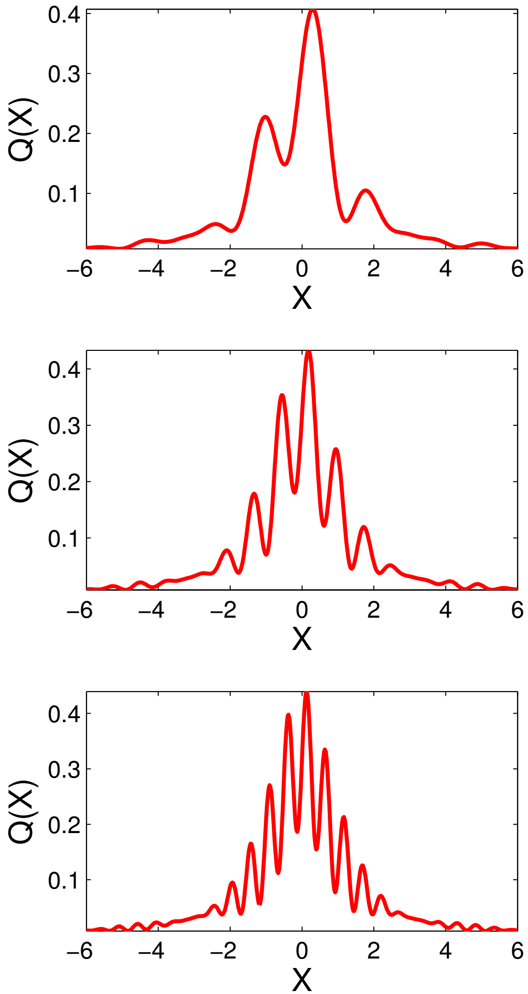
$$\|g_m\|_{\mathcal{F}} = cm^{-1/2}$$

# More general local departures from null

- More advanced example of a local departure from the null
- Recall: $\mu_{\mathbf{Q}} = \mu_{\mathbf{P}} + g_m$, and $\|g_m\|_{\mathcal{F}} = cm^{-1/2}$




VS



# Kernels vs kernels

- How does MMD relate to Parzen density estimate? [Anderson et al., 1994]

$$\hat{f}_{\mathbf{P}}(x) = \frac{1}{m}\sum_{i=1}^{m}\kappa\left(x_i - x\right), \text{ where } \kappa \text{ satisfies } \int_{\mathcal{X}}\kappa\left(x\right)dx = 1 \text{ and } \kappa\left(x\right) \geq 0.$$

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- $L_2$ distance between Parzen density estimates:

$$D_2(\hat{f}_{\mathbf{P}}, \hat{f}_{\mathbf{Q}})^2 = \int \left[\frac{1}{m}\sum_{i=1}^{m}\kappa(x_i - z) - \frac{1}{m}\sum_{i=1}^{m}\kappa(y_i - z)\right]^2 dz$$

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where $k(x - y) = \int \kappa(x - z)\kappa(y - z)dz$

# Kernels vs kernels

- How does MMD relate to Parzen density estimate? [Anderson et al., 1994]

$$\hat{f}_{\mathbf{P}}(x) = \frac{1}{m}\sum_{i=1}^{m}\kappa\left(x_i - x\right), \text{ where } \kappa \text{ satisfies } \int_{\mathcal{X}}\kappa\left(x\right)dx = 1 \text{ and } \kappa\left(x\right) \geq 0.$$

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- $f_{\mathbf{Q}} = f_{\mathbf{P}} + \delta g$, minimum distance to discriminate $f_{\mathbf{P}}$ from $f_{\mathbf{Q}}$ is $\delta = (m)^{-1/2}h_m^{-d/2}$, where $h_m$ is width of $\kappa$.

# Characteristic Kernels (via universality)

Characteristic: MMD a metric (MMD $= 0$ iff $\mathbf{P} = \mathbf{Q}$) [NIPS07b, COLT08]

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If $\mathcal{F}$ universal, then MMD $\{\mathbf{P}, \mathbf{Q}; F\} = 0$ iff $\mathbf{P} = \mathbf{Q}$

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Proof:

First, it is clear that $\mathbf{P} = \mathbf{Q}$ implies $\mathrm{MMD}\left\{\mathbf{P}, \mathbf{Q}; F\right\}$ is zero.

Converse: by the universality of $\mathcal{F}$, for any given $\epsilon > 0$ and $f \in C(\mathcal{X})$ $\exists g \in \mathcal{F}$

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We next make the expansion

$$|\mathbf{E}_{\mathsf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathsf{Q}} f(\mathsf{y})| \le |\mathbf{E}_{\mathsf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathsf{P}} g(\mathsf{x})| + |\mathbf{E}_{\mathsf{P}} g(\mathsf{x}) - \mathbf{E}_{\mathsf{Q}} g(\mathsf{y})| + |\mathbf{E}_{\mathsf{Q}} g(\mathsf{y}) - \mathbf{E}_{\mathsf{Q}} f(\mathsf{y})|.$$

The first and third terms satisfy

$$|\mathbf{E}_{\mathsf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathsf{P}} g(\mathsf{x})| \le \mathbf{E}_{\mathsf{P}} |f(\mathsf{x}) - g(\mathsf{x})| \le \epsilon.$$

# Characteristic Kernels (via universality)

Proof (continued):

Next, write

$$\mathbf{E}_{\mathsf{P}} g(\mathsf{x}) - \mathbf{E}_{\mathsf{Q}} g(\mathsf{y}) = \langle g(\cdot), \mu_{\mathsf{P}} - \mu_{\mathsf{Q}} \rangle_{\mathcal{F}} = 0,$$

since $\mathrm{MMD}\{\mathsf{P}, \mathsf{Q}; F\} = 0$ implies $\mu_{\mathsf{P}} = \mu_{\mathsf{Q}}$. Hence

$$|\mathbf{E}_{\mathsf{P}} f(\mathsf{x}) - \mathbf{E}_{\mathsf{Q}} f(\mathsf{y})| \leq 2\epsilon$$

for all $f \in C(\mathcal{X})$ and $\epsilon > 0$, which implies $\mathsf{P} = \mathsf{Q}$.

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