Representing and comparing probabilities with kernels: Part 2

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Comparing two samples

- **Given:** Samples from unknown distributions P and Q.
- **Goal:** do P and Q differ?

$\sim P$

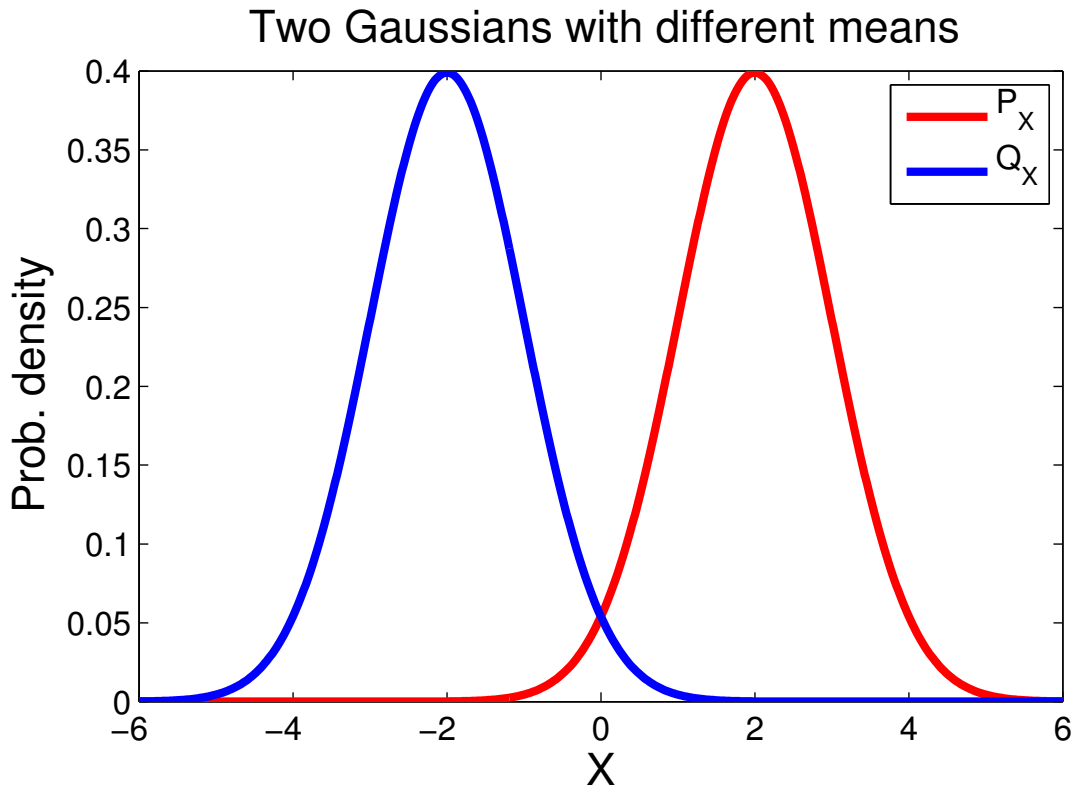
$\sim Q$

Outline

- Maximum Mean Discrepancy (MMD)...
  - ...as a difference in feature means
  - ...as an integral probability metric (not just a technicality!)
- A statistical test based on the MMD
- Next slides: training generative adversarial networks with MMD
  - Gradient regularisation and data adaptivity

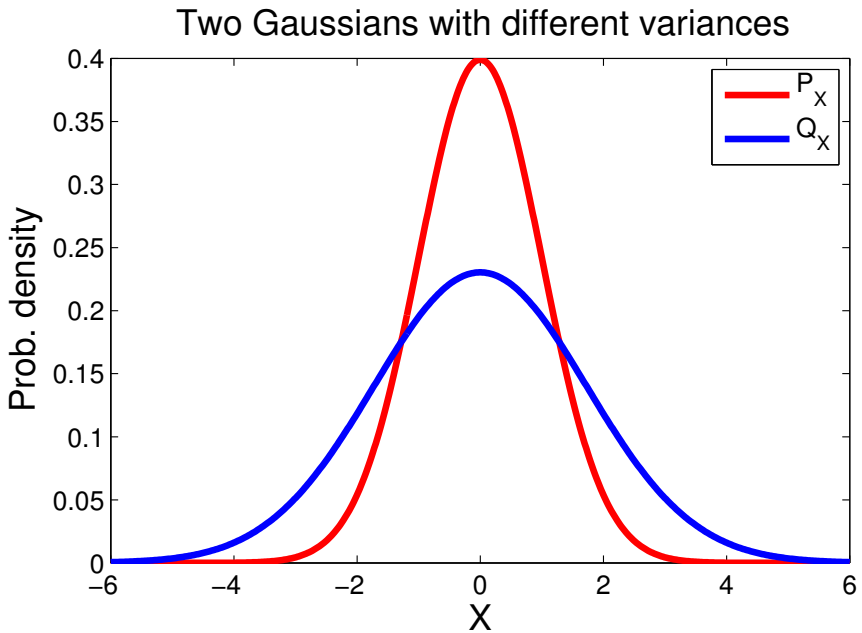
Feature mean difference

- 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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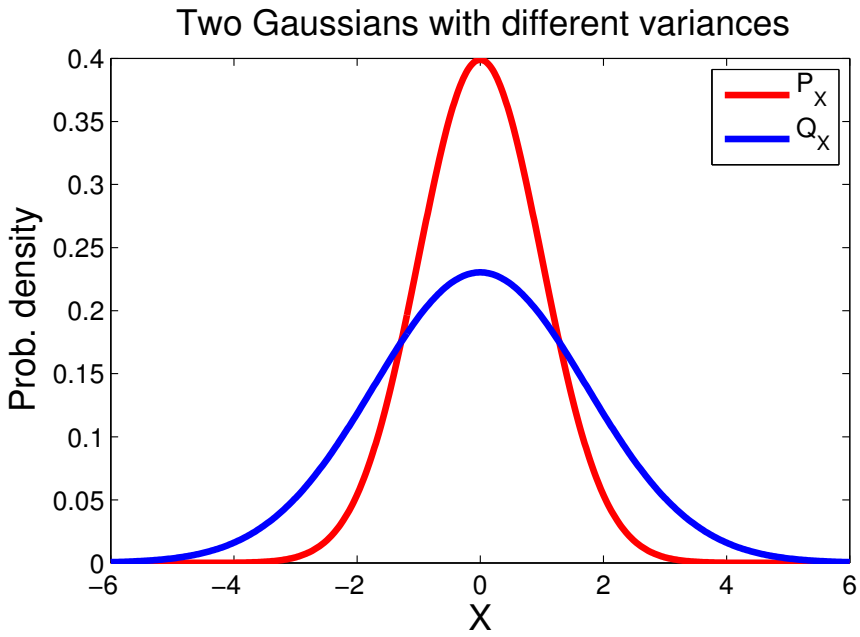
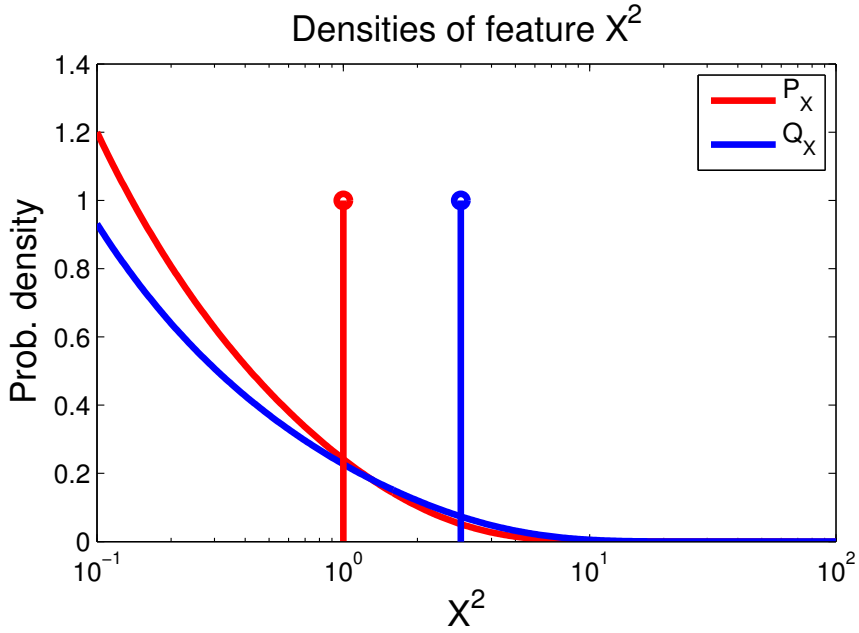
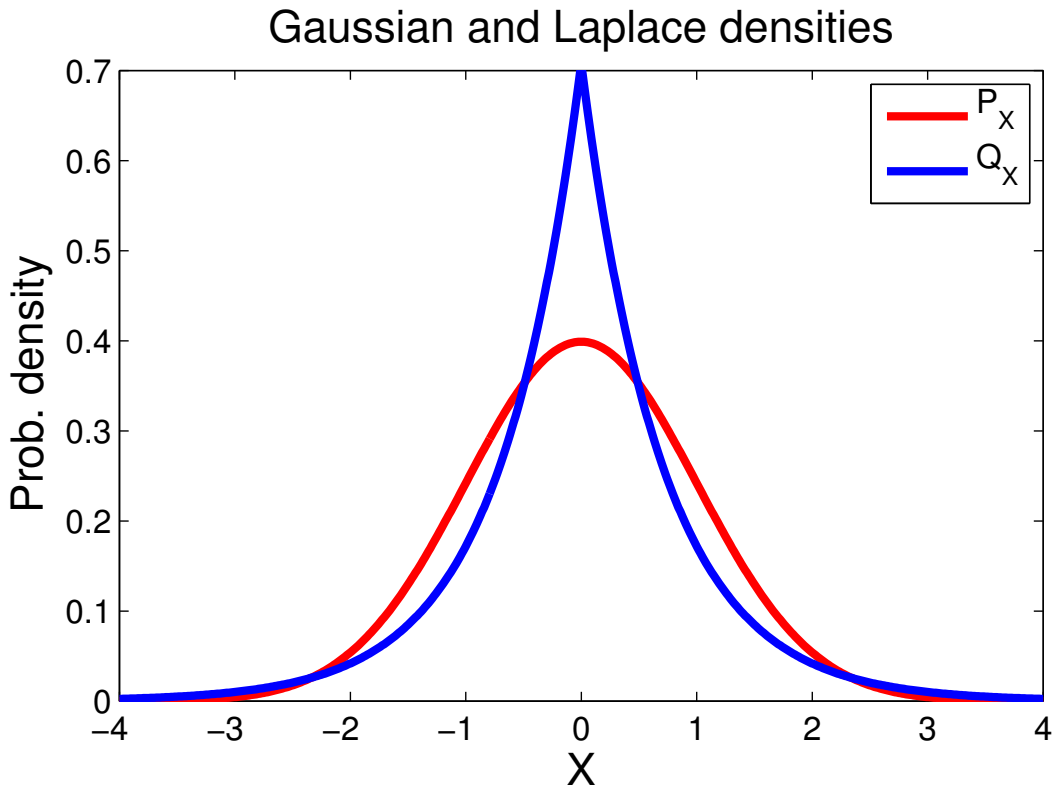




Feature mean difference

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



Infinitely many features using kernels

Kernels: dot products of features

Feature map $\varphi(x) \in \mathcal{F}$,

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

For positive definite k,

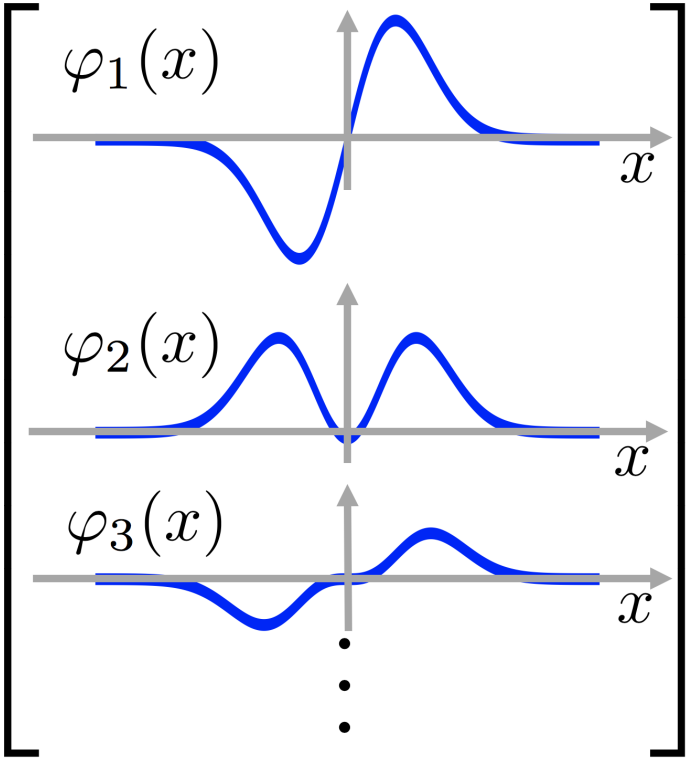
$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}}$$

Infinitely many features $\varphi(x)$, dot product in closed form!

Exponentiated quadratic kernel

$$k(x, x') = \exp\left(-\gamma \left\|x - x'\right\|^2\right)$$

$$\varphi(x) = \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \\ \vdots \end{bmatrix}$$



Features: Gaussian Processes for Machine learning, Rasmussen and Williams, Ch. 4.

Infinitely many features of *distributions*

Given P a Borel **probability measure** on $\mathcal{X}$, define feature map of probability P,

$$\mu_P = [\ldots \mathbf{E}_P [\varphi_i(X)] \ldots]$$

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

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

for $x \sim P$ and $y \sim Q$.

Fine print: feature map $\varphi(x)$ must be Bochner integrable for all probability measures considered. Always true if kernel bounded.

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The maximum mean discrepancy

The maximum mean discrepancy is the distance between **feature means**:

$$
\begin{aligned}
MMD^2(P, Q) &= \|\mu_P - \mu_Q\|_{\mathcal{F}}^2 \\
&= \langle \mu_P, \mu_P \rangle_{\mathcal{F}} + \langle \mu_Q, \mu_Q \rangle_{\mathcal{F}} - 2 \langle \mu_P, \mu_Q \rangle_{\mathcal{F}} \\
&= \underbrace{\mathbf{E}_P k(X, X')}_{\text{(a)}} + \underbrace{\mathbf{E}_Q k(Y, Y')}_{\text{(a)}} - 2 \underbrace{\mathbf{E}_{P,Q} k(X, Y)}_{\text{(b)}}
\end{aligned}
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\end{aligned}
$$

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

Illustration of MMD

- Dogs ($= P$) and fish ($= Q$) example revisited
- Each entry is one of $k(\text{dog}_i, \text{dog}_j)$, $k(\text{dog}_i, \text{fish}_j)$, or $k(\text{fish}_i, \text{fish}_j)$

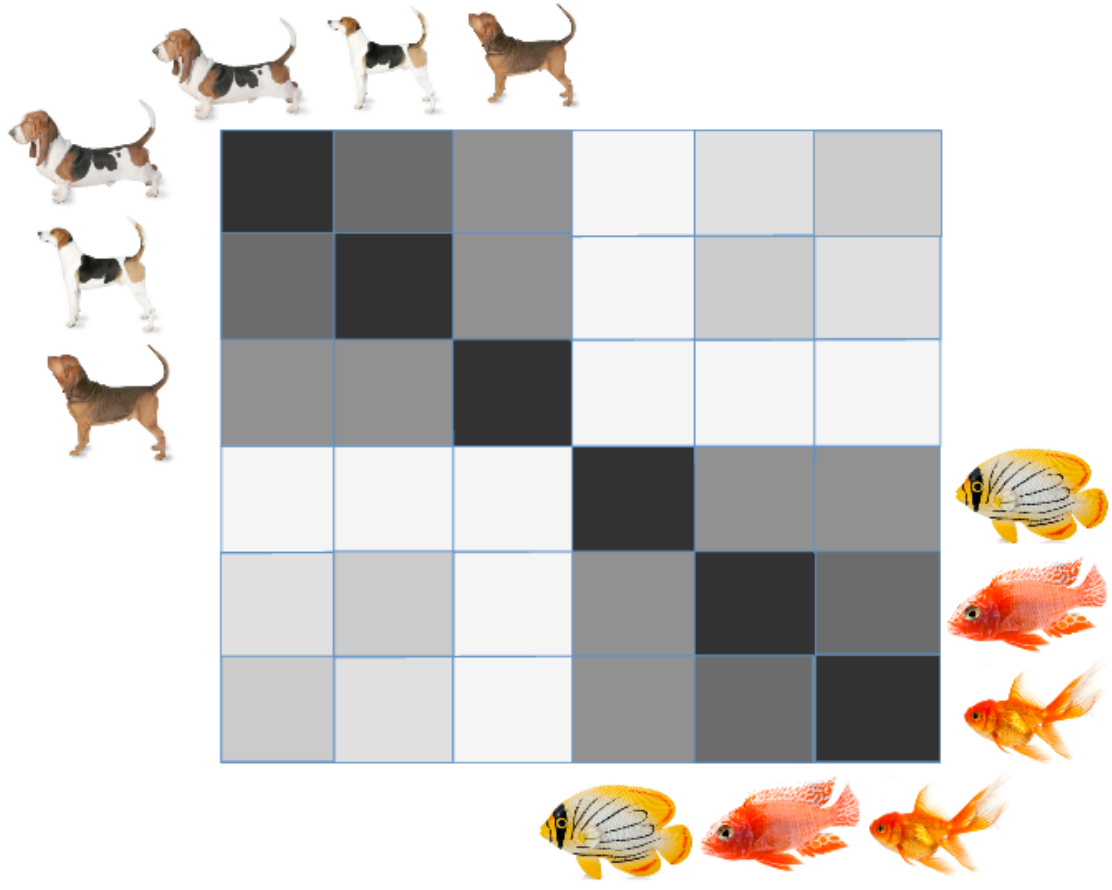
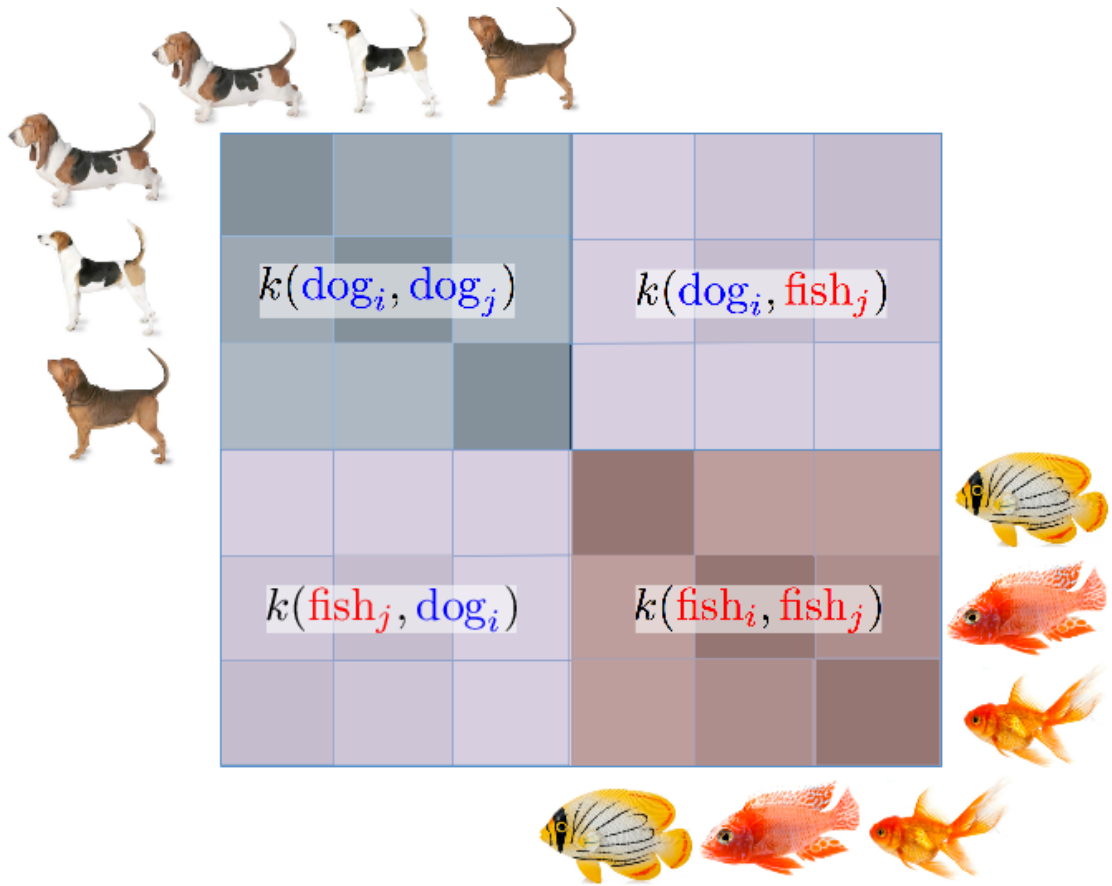


Illustration of MMD

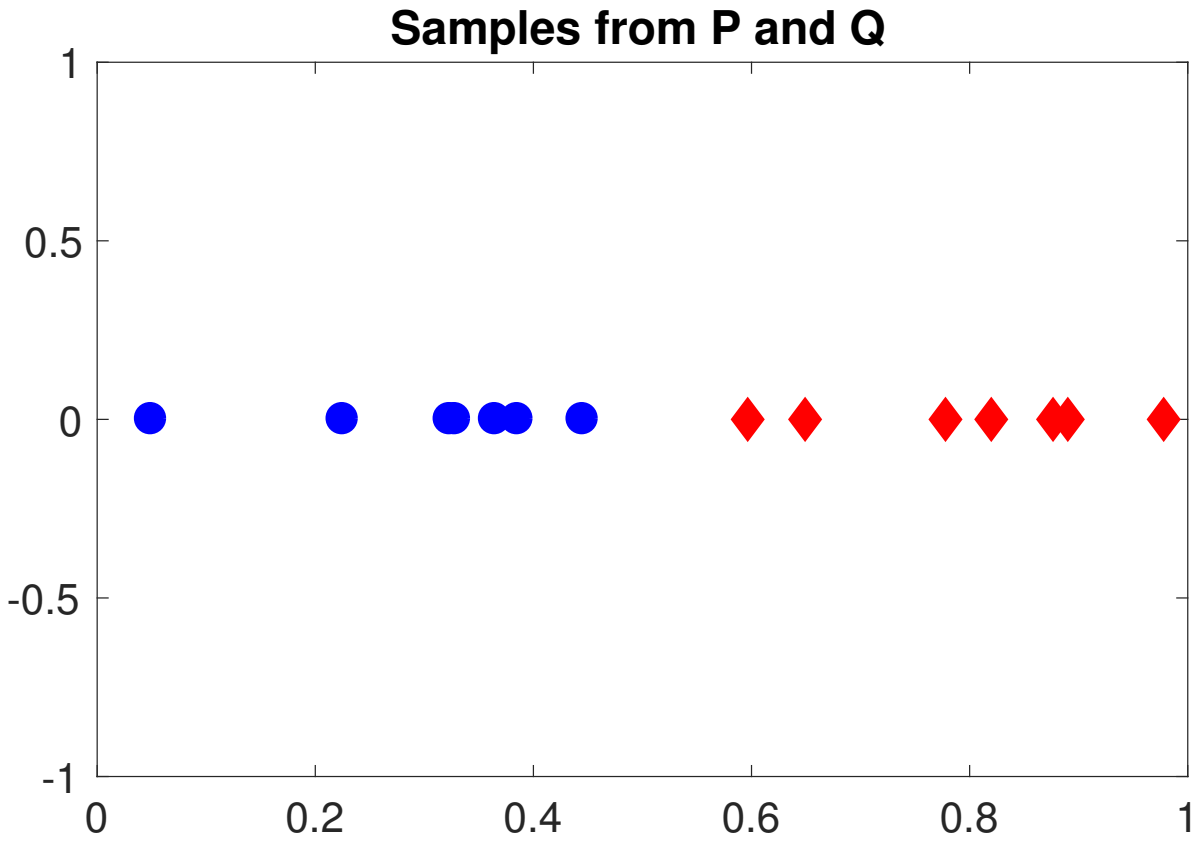
The maximum mean discrepancy:

$$\widehat{MMD}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} k(\text{dog}_i, \text{dog}_j) + \frac{1}{n(n-1)} \sum_{i \neq j} k(\text{fish}_i, \text{fish}_j) - \frac{2}{n^2} \sum_{i,j} k(\text{dog}_i, \text{fish}_j)$$



MMD as an integral probability metric

Are P and Q different?



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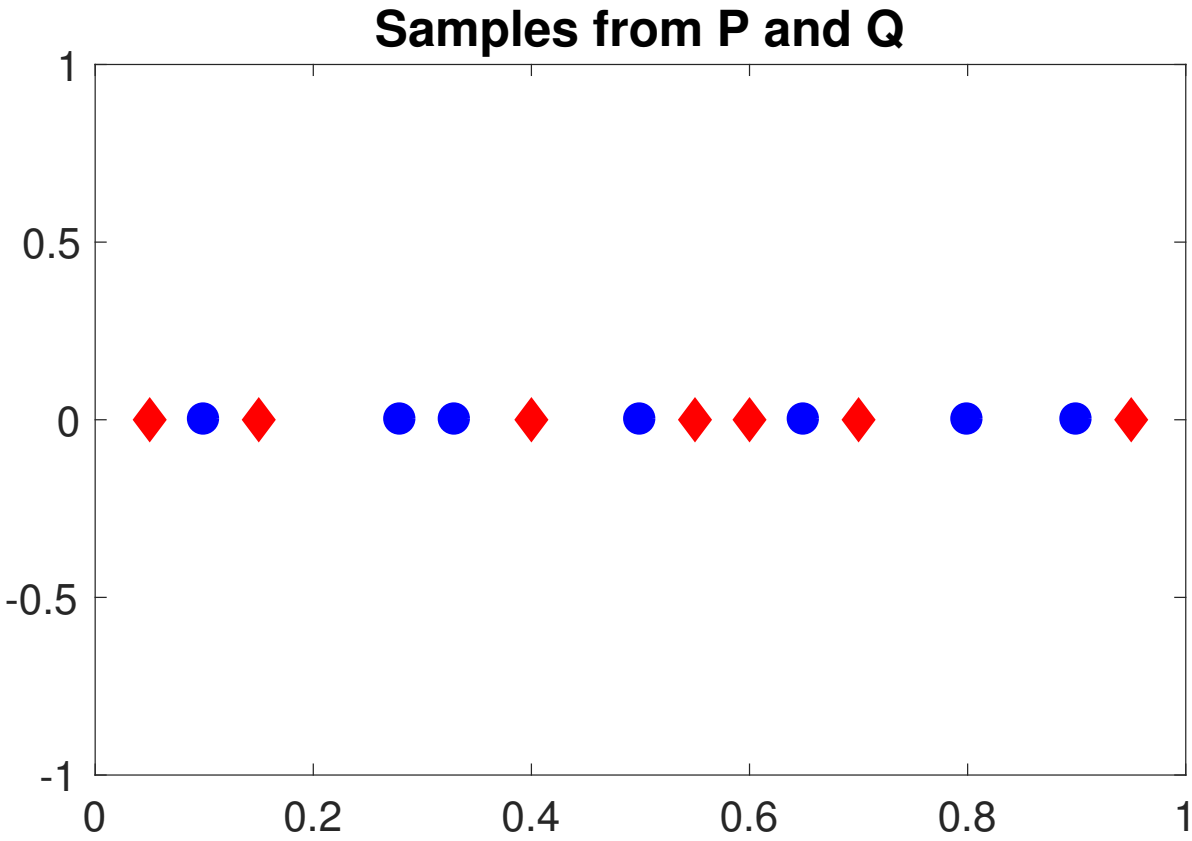
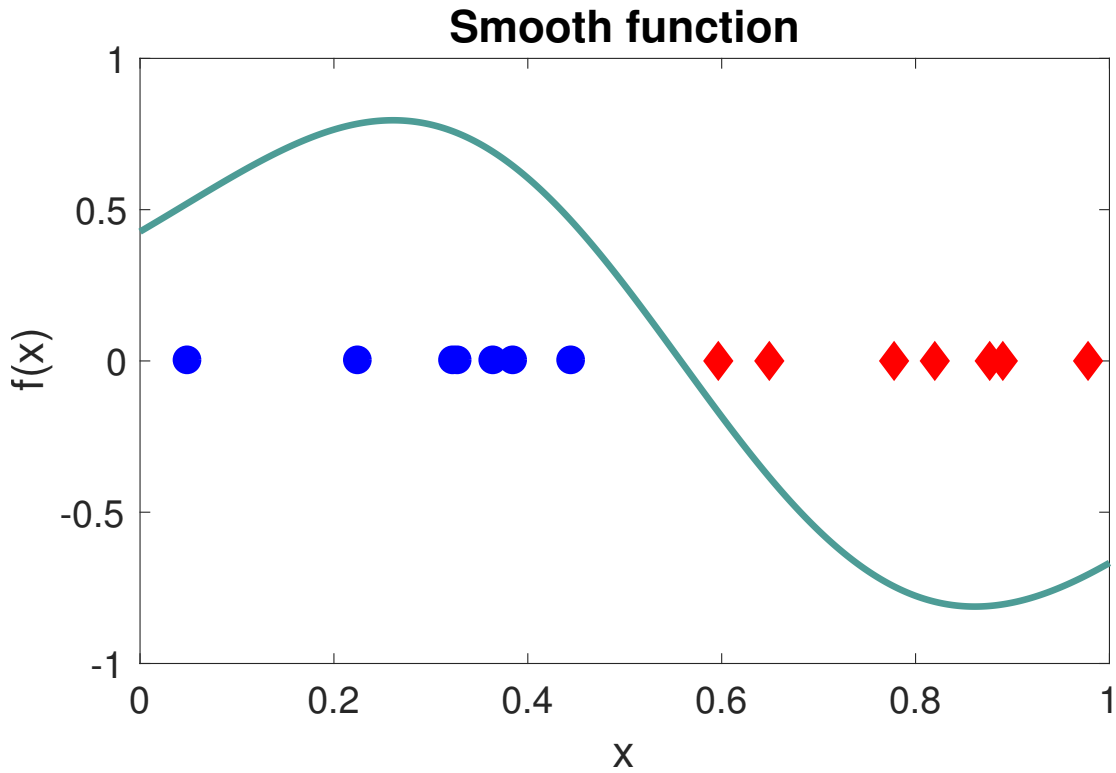


MMD as an integral probability metric

Integral probability metric:

Find a "well behaved function" $f(x)$ to maximize

$$\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y)$$



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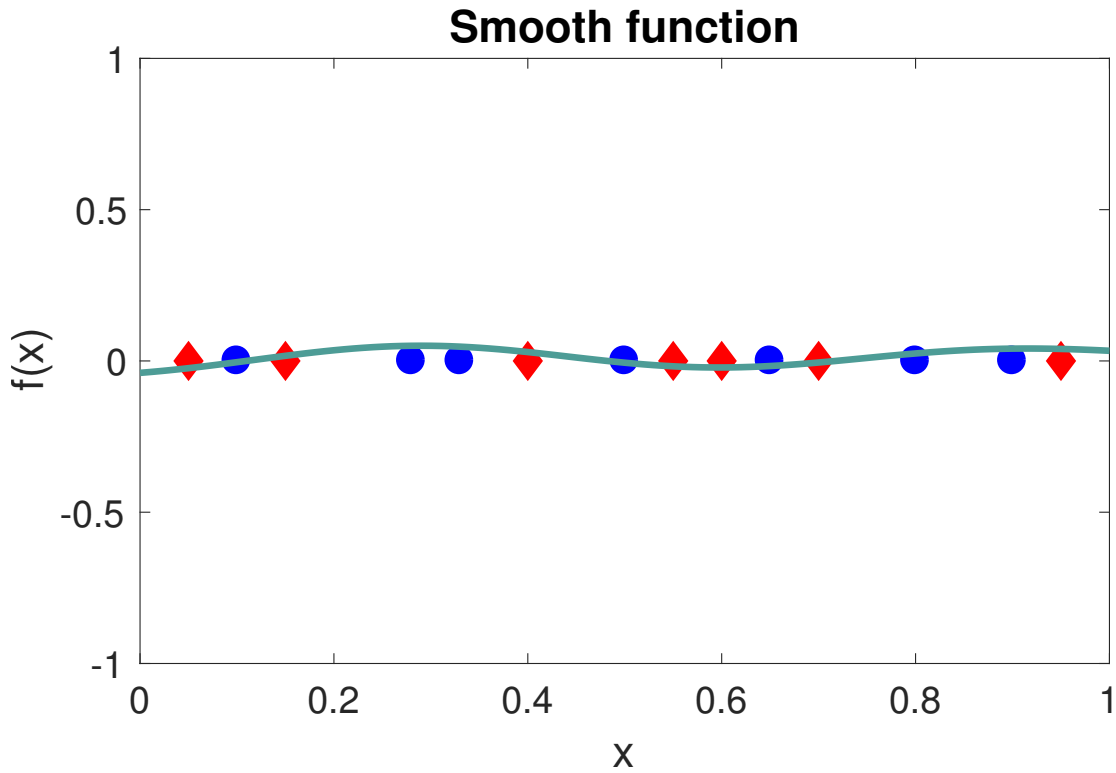

MMD as an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

$$MMD(P, Q; F) := \sup_{\|f\|_{\mathcal{F}} \leq 1} [\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y)]$$

$$(F = \text{unit ball in RKHS } \mathcal{F})$$

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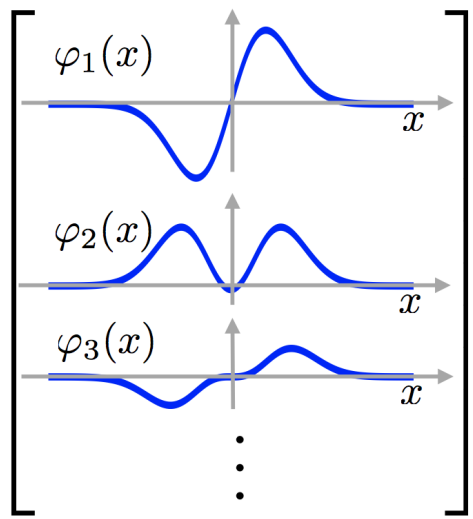
Functions are linear combinations of features:

$$f(x) = \langle f, \varphi(x) \rangle_{\mathcal{F}} = \sum_{\ell=1}^{\infty} f_\ell \varphi_\ell(x) = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix}^\top \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \varphi_3(x) \\ \vdots \end{bmatrix}$$



$$\|f\|_{\mathcal{F}}^2 := \sum_{i=1}^{\infty} f_i^2 \leq 1$$

MMD as an integral probability metric

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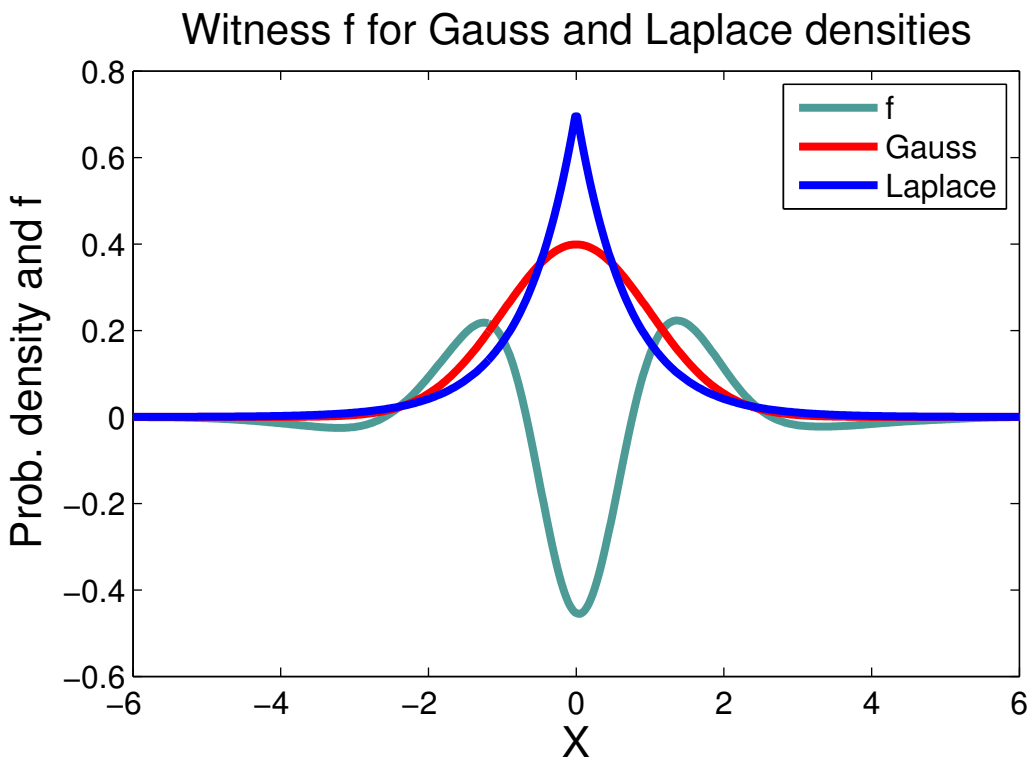

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For characteristic RKHS $\mathcal{F}$, $MMD(P, Q; F) = 0$ iff $P = Q$

Other choices for witness function class:

- Bounded continuous [Dudley, 2002]
- Bounded varation 1 (Kolmogorov metric) [Müller, 1997]
- Bounded Lipschitz (Wasserstein distances) [Dudley, 2002]

MMD as an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

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Expectations of functions are linear combinations of expected features

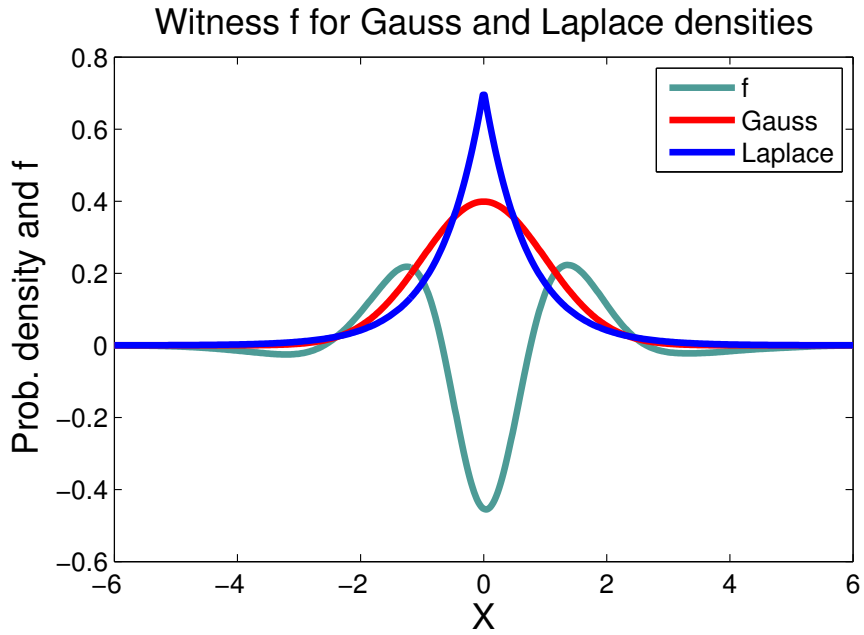
$$\mathbf{E}_P(f(X)) = \langle f, \mathbf{E}_P \varphi(X) \rangle_{\mathcal{F}} = \langle f, \mu_P \rangle_{\mathcal{F}}$$

(always true if kernel is bounded)

Integral prob. metric vs feature difference

The MMD:

$$MMD(P, Q; F)$$
$$= \sup_{||f||_{\mathcal{F}} \leq 1} [\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y)]$$



Integral prob. metric vs feature difference

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&= \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}}
\end{aligned}
$$

use

$$
\mathbf{E}_P f(X) = \langle \mu_P, f \rangle_{\mathcal{F}}
$$

Integral prob. metric vs feature difference

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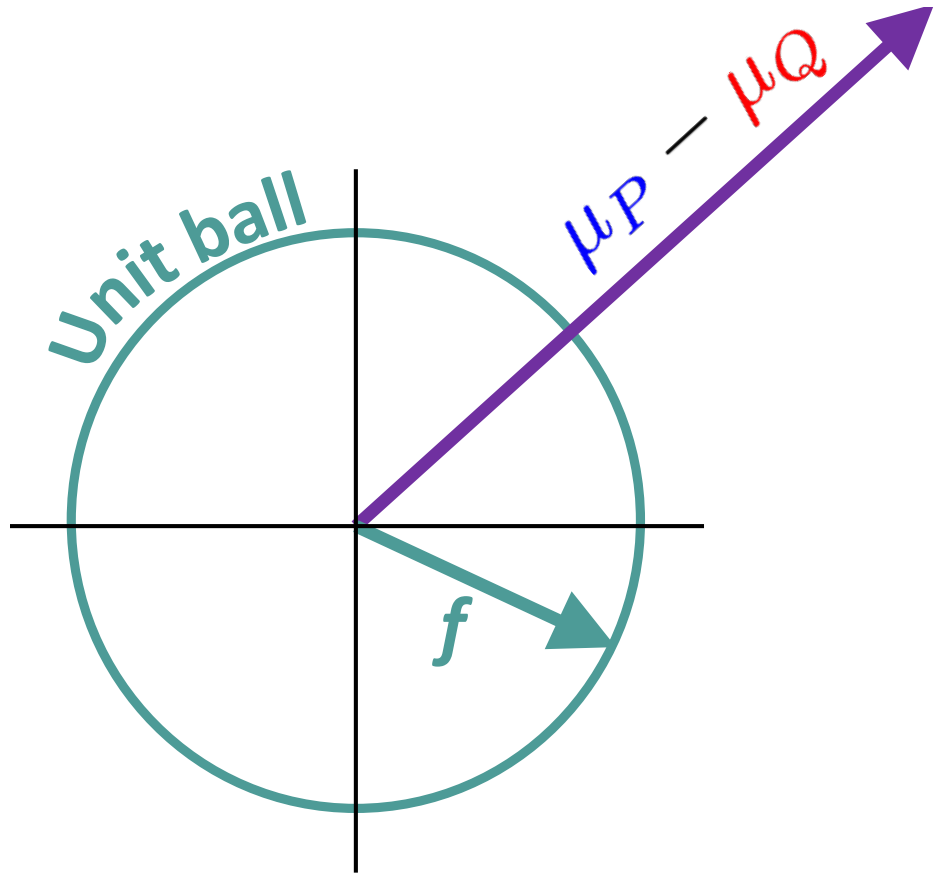

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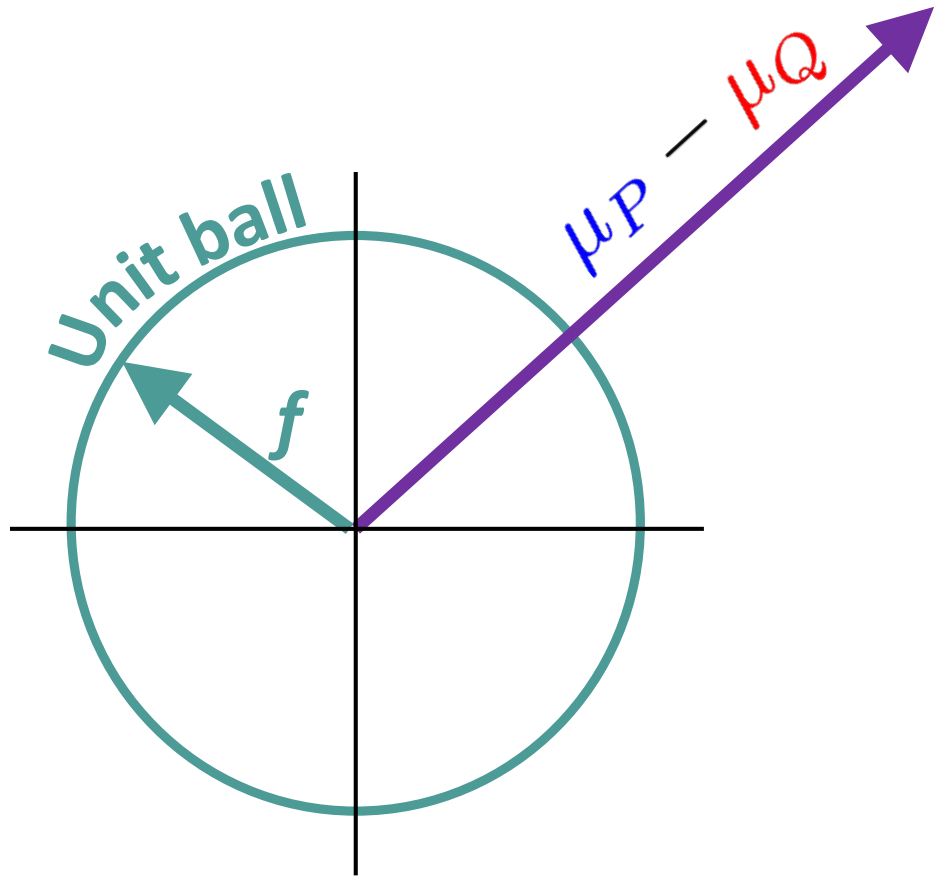

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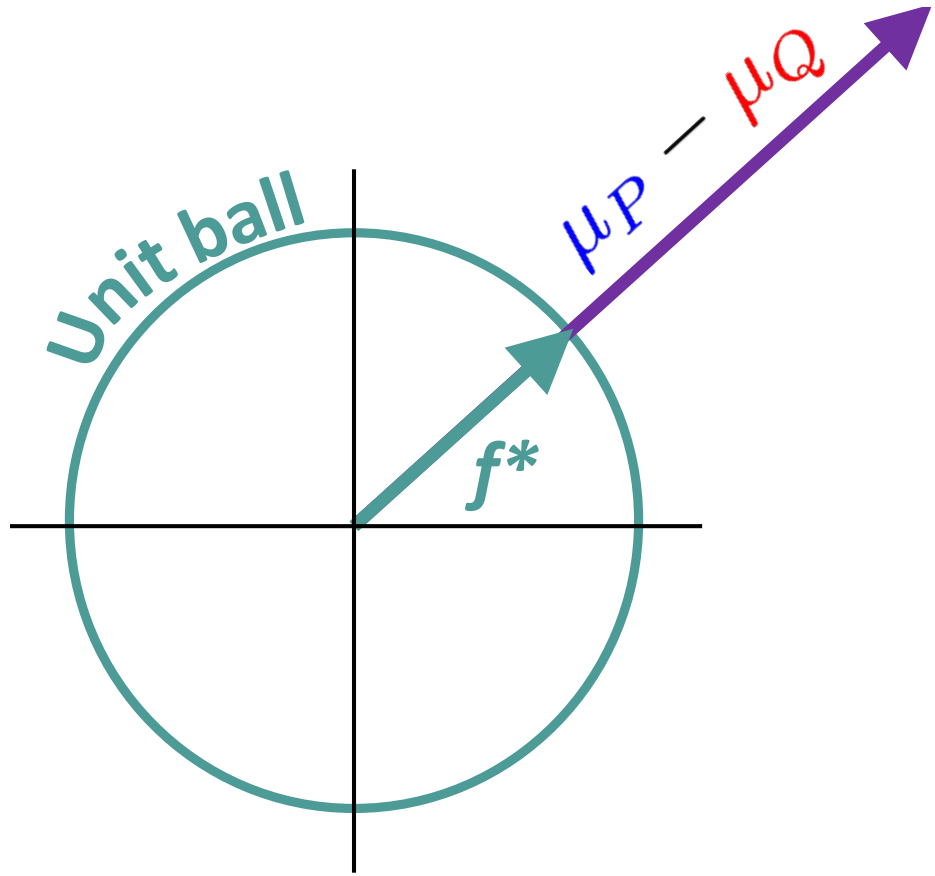

$$f^* = \frac{\mu_P - \mu_Q}{\|\mu_P - \mu_Q\|}$$

Integral prob. metric vs feature difference

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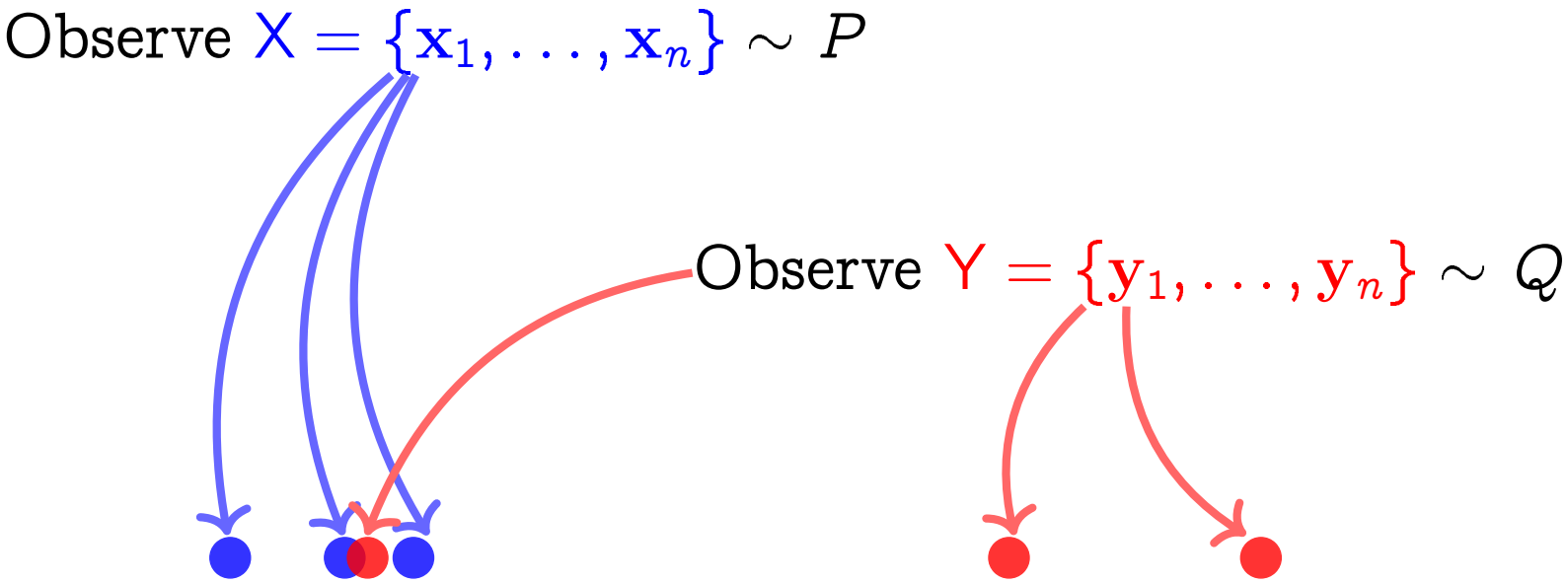
&= \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \\
&= \|\mu_P - \mu_Q\|
\end{aligned}
$$

Function view and feature view equivalent

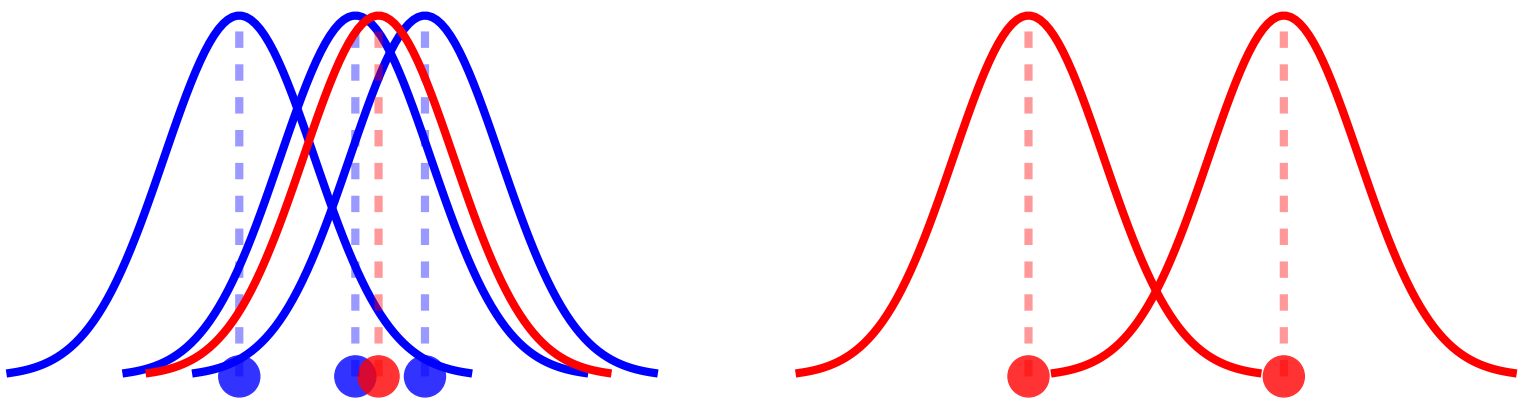
Construction of MMD witness

Construction of empirical witness function (proof: next slide!)



Construction of MMD witness

Construction of empirical witness function (proof: next slide!)



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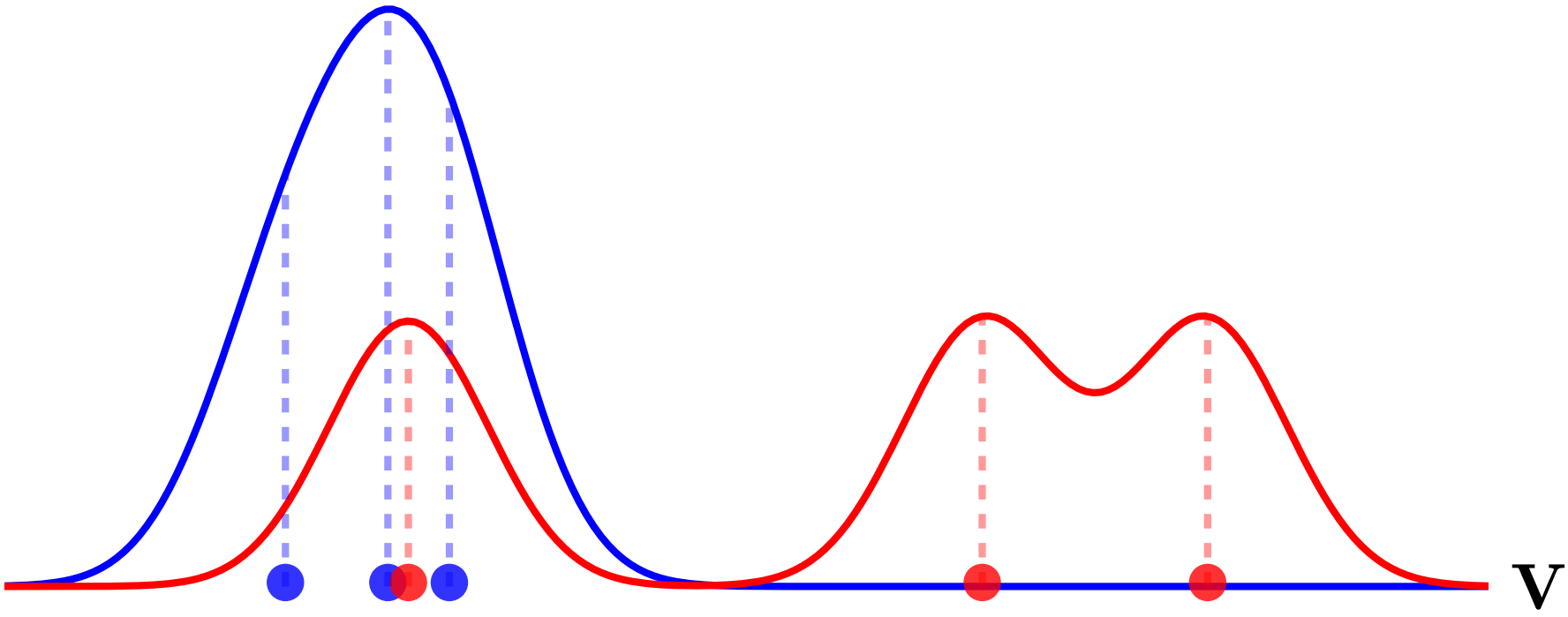

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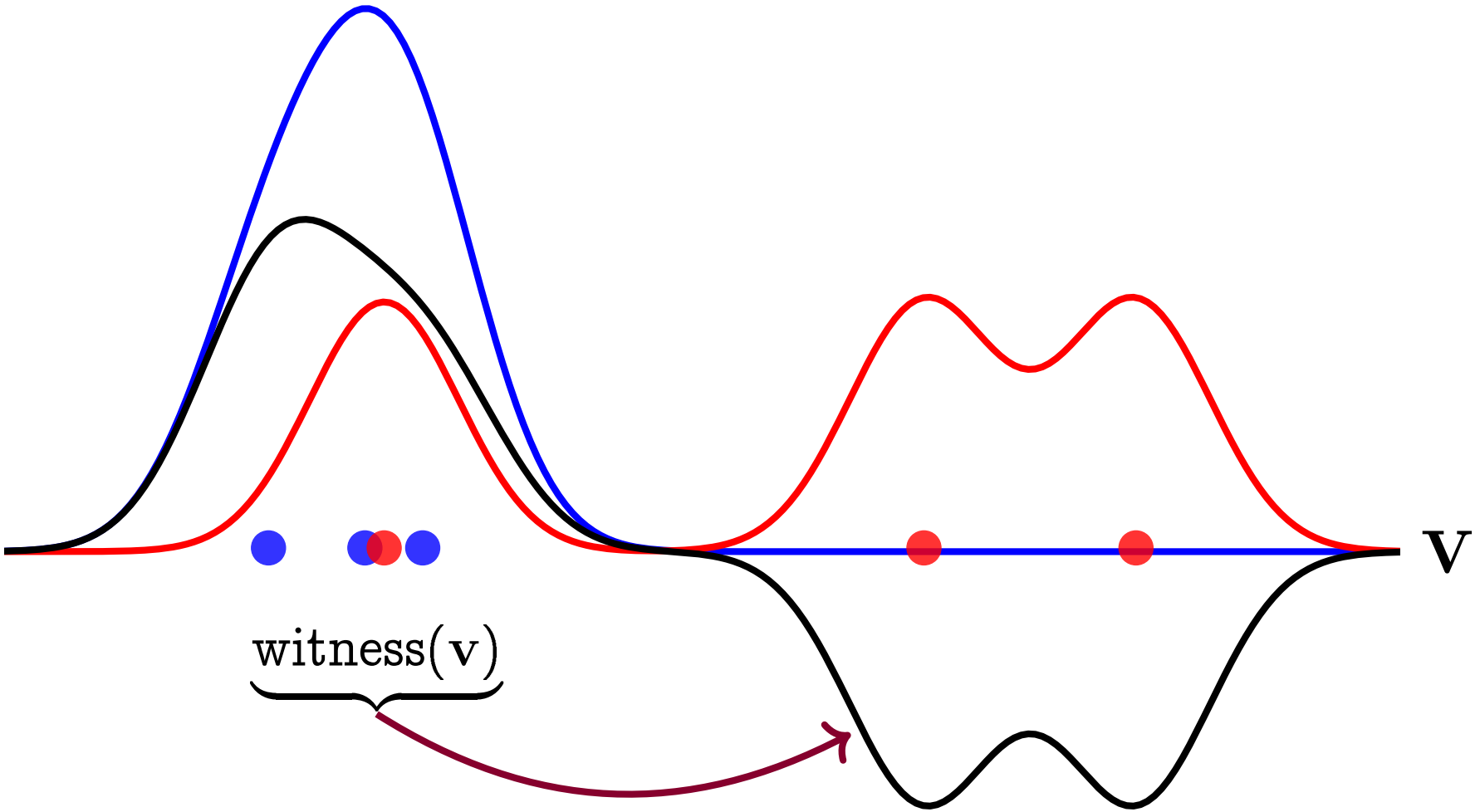

Derivation of empirical witness function

Recall the witness function expression

$$f^* \propto \mu_P - \mu_Q$$

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The empirical feature mean for P

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$$\begin{aligned} f^*(v) &= \langle f^*, \varphi(v) \rangle_{\mathcal{F}} \\ &\propto \langle \widehat{\mu}_P - \widehat{\mu}_Q, \varphi(v) \rangle_{\mathcal{F}} \end{aligned}$$

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Recall the witness function expression

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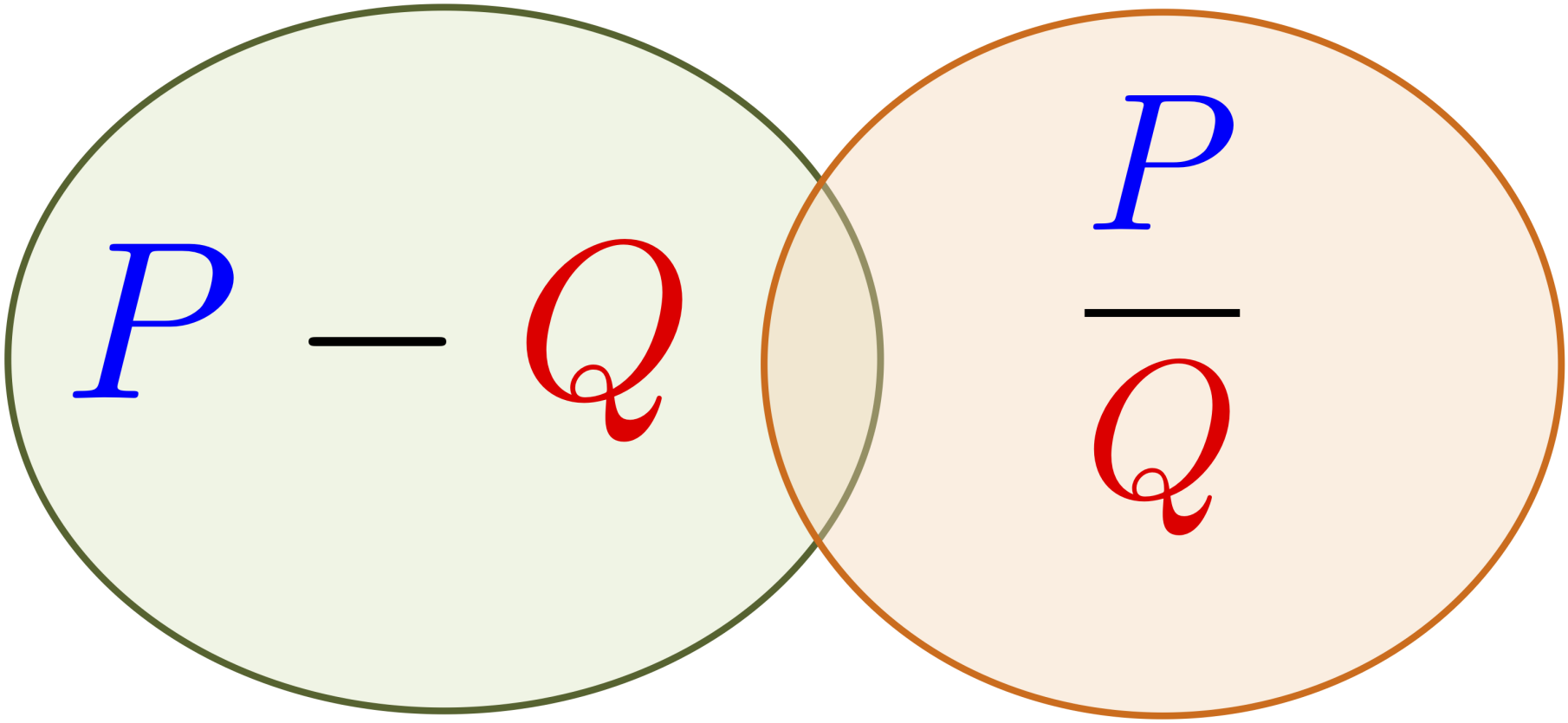
The empirical witness function at v

$$\begin{aligned} f^*(v) &= \langle f^*, \varphi(v) \rangle_{\mathcal{F}} \\ &\propto \langle \widehat{\mu}_P - \widehat{\mu}_Q, \varphi(v) \rangle_{\mathcal{F}} \\ &= \frac{1}{n} \sum_{i=1}^{n} k(x_i, v) - \frac{1}{n} \sum_{i=1}^{n} k(y_i, v) \end{aligned}$$

Don't need explicit feature coefficients $f^* := \begin{bmatrix} f_1^* & f_2^* & \dots \end{bmatrix}$

Interlude: divergence measures

Divergences



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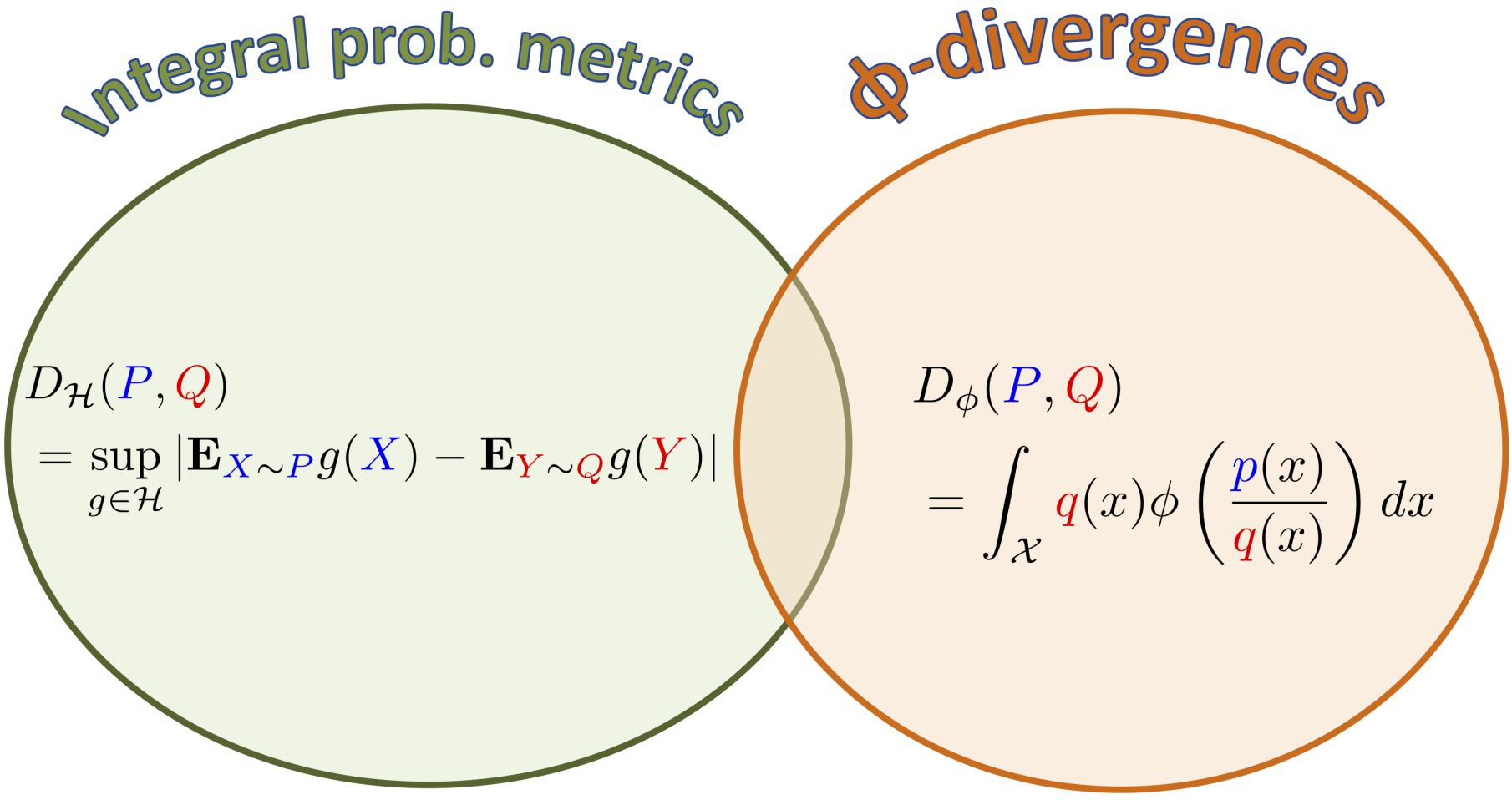
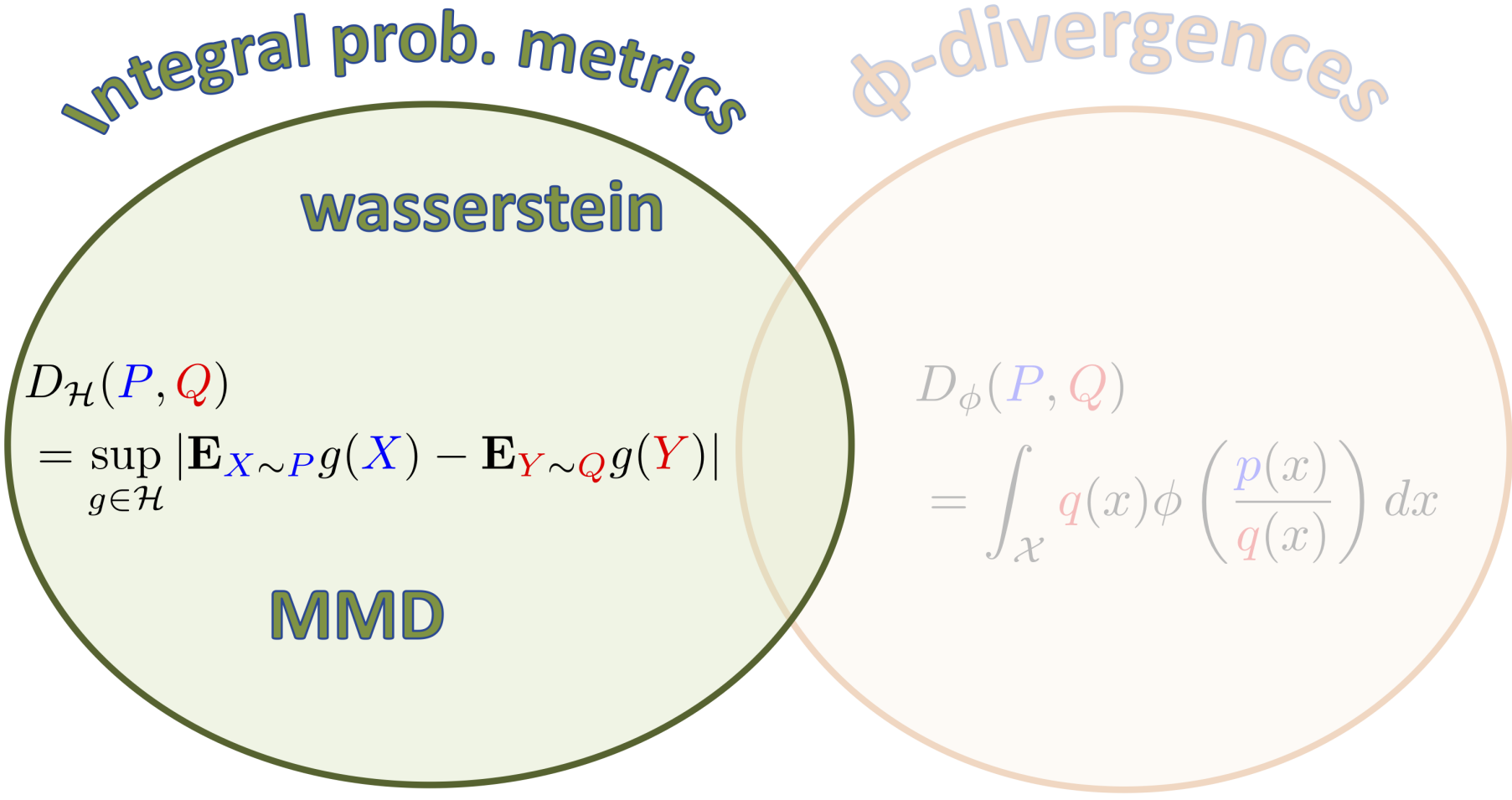
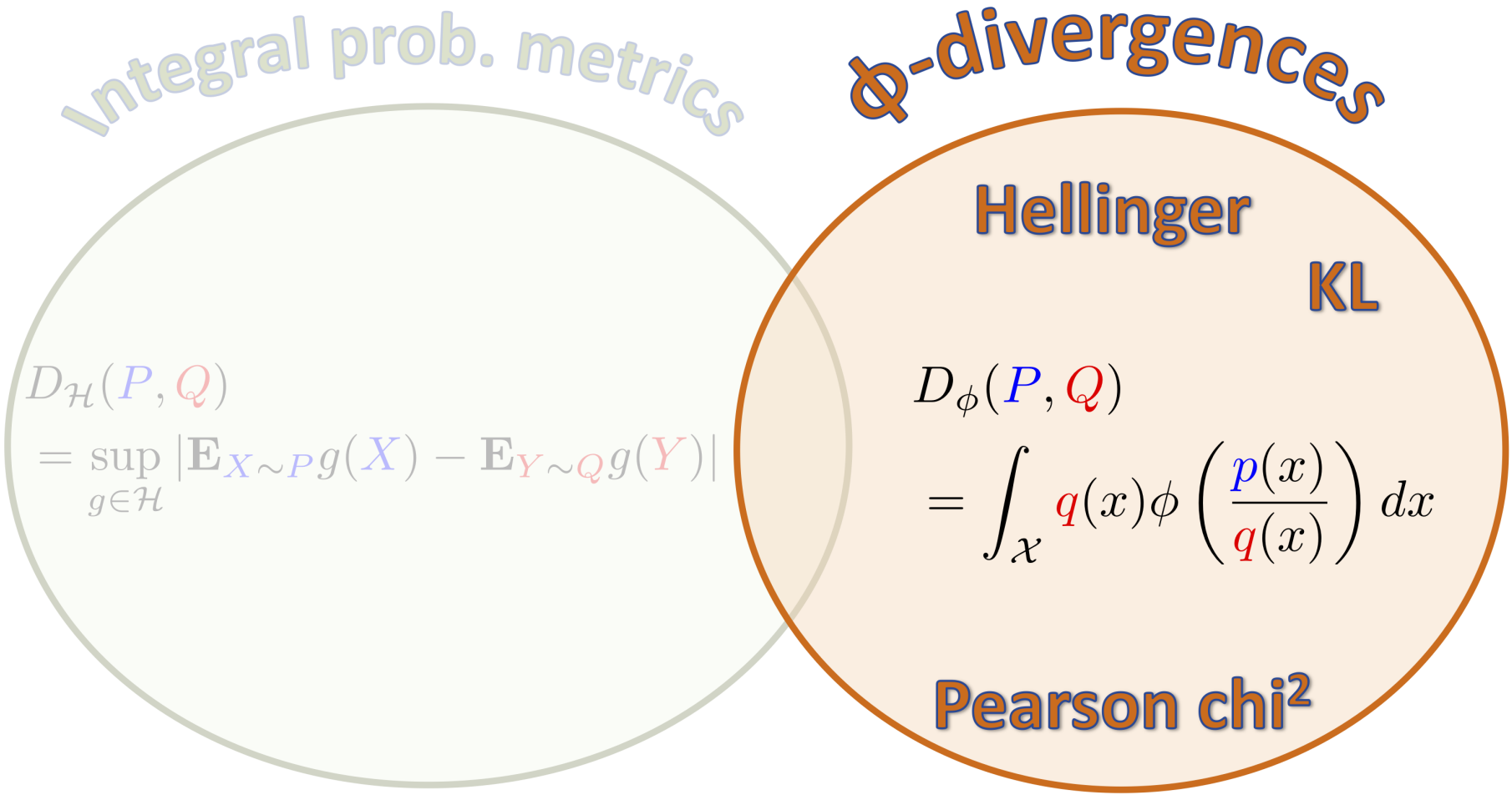


The integral probability metrics



The ϕ-divergences



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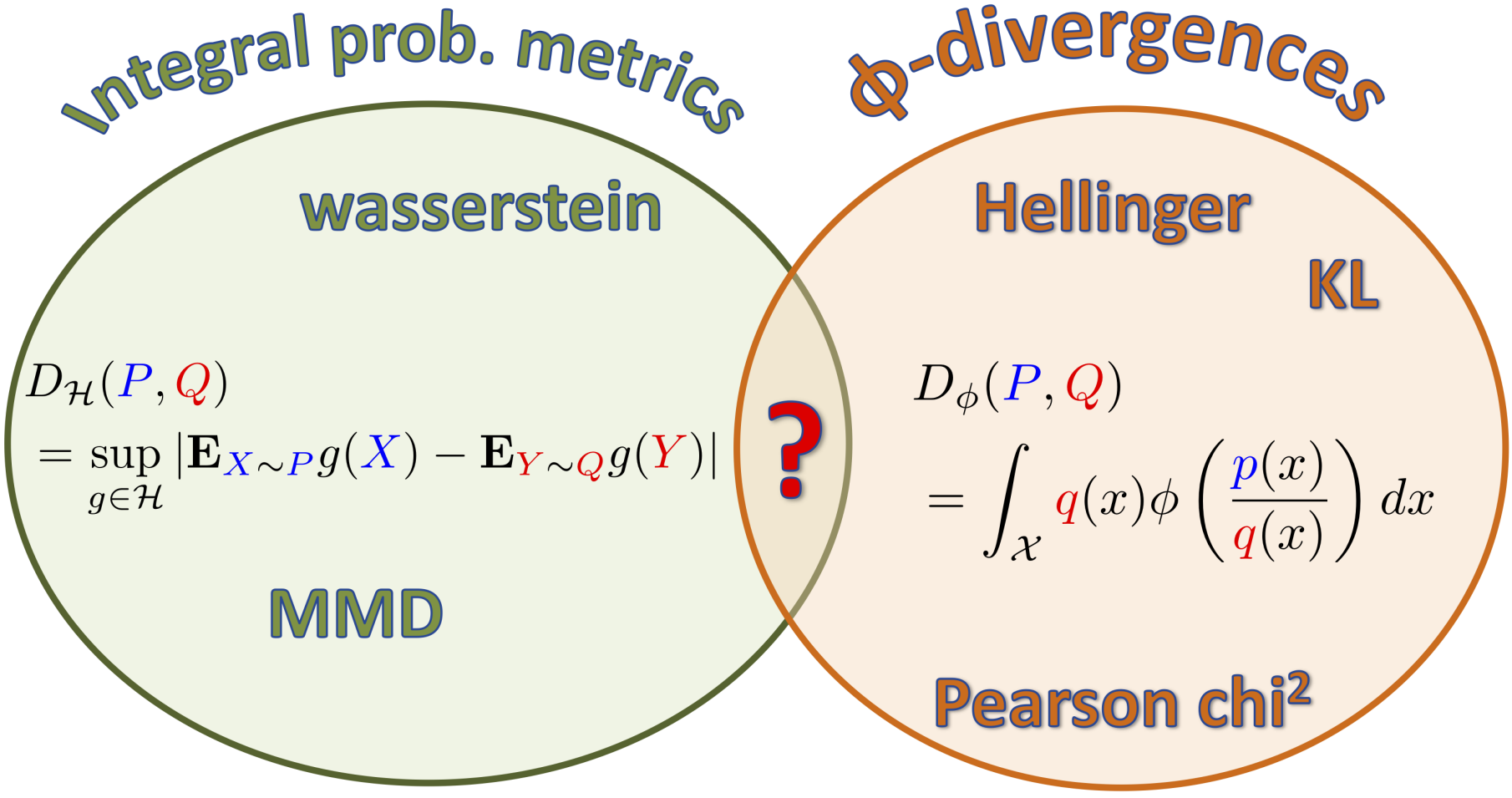
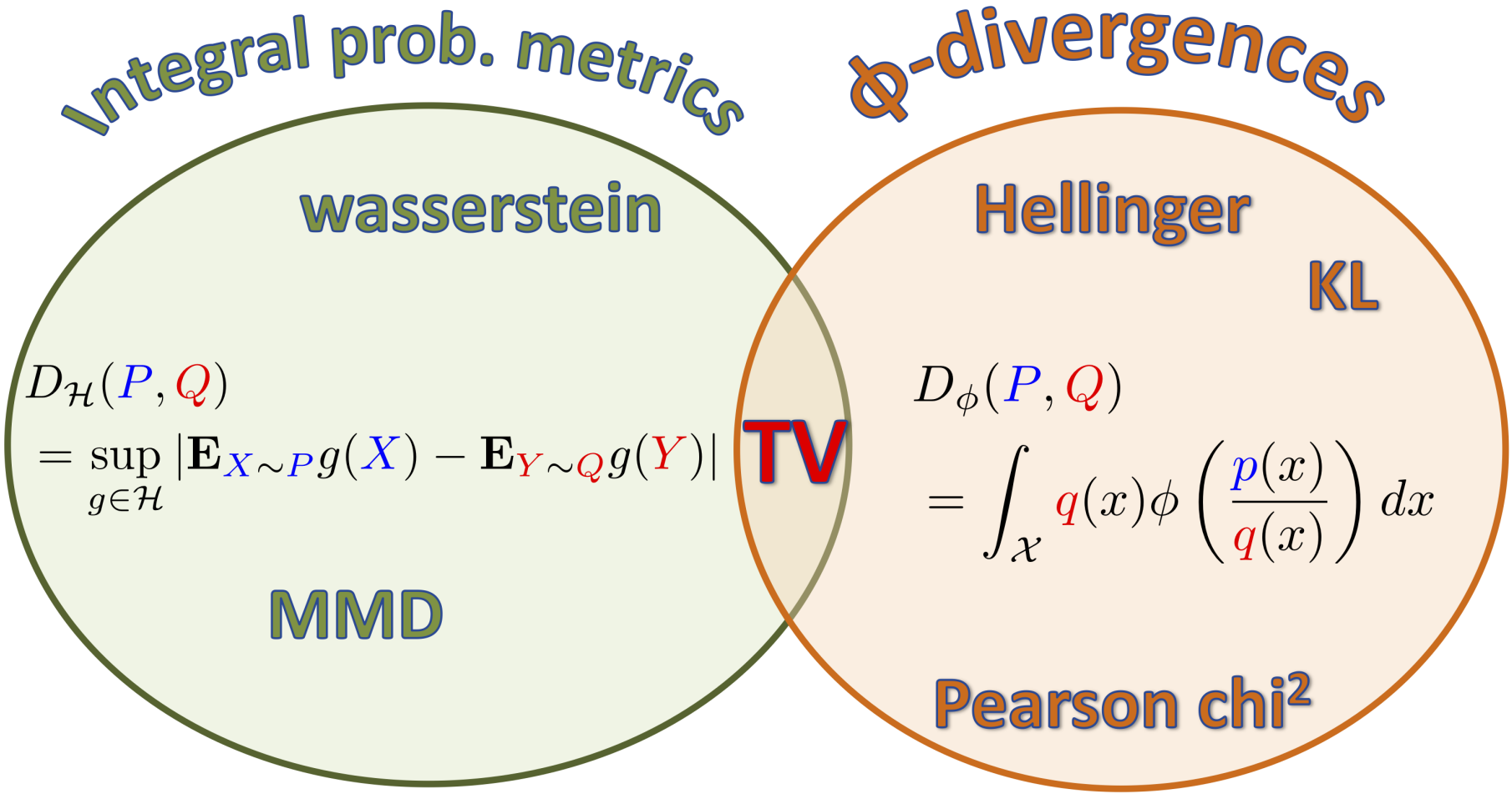


Divergences



Sriperumbudur, Fukumizu, G, Schoelkopf, Lanckriet, EJS (2012)

Two-Sample Testing with MMD

A statistical test using MMD

The empirical MMD:

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

How does this help decide whether $P = Q$?

A statistical test using MMD

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Perspective from statistical hypothesis testing:

- **Null hypothesis $\mathcal{H}_0$** when $P = Q$
  - should see $\widehat{MMD}^2$ "close to zero".
- **Alternative hypothesis $\mathcal{H}_1$** when $P \neq Q$
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Want Threshold c_α for $\widehat{MMD}^2$ to get false positive rate α

Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Draw $n = 200$ i.i.d samples from P and Q

- Laplace with different y-variance.
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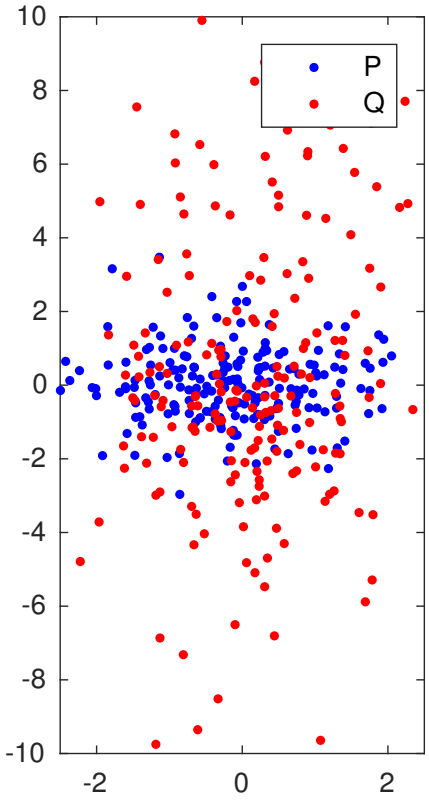

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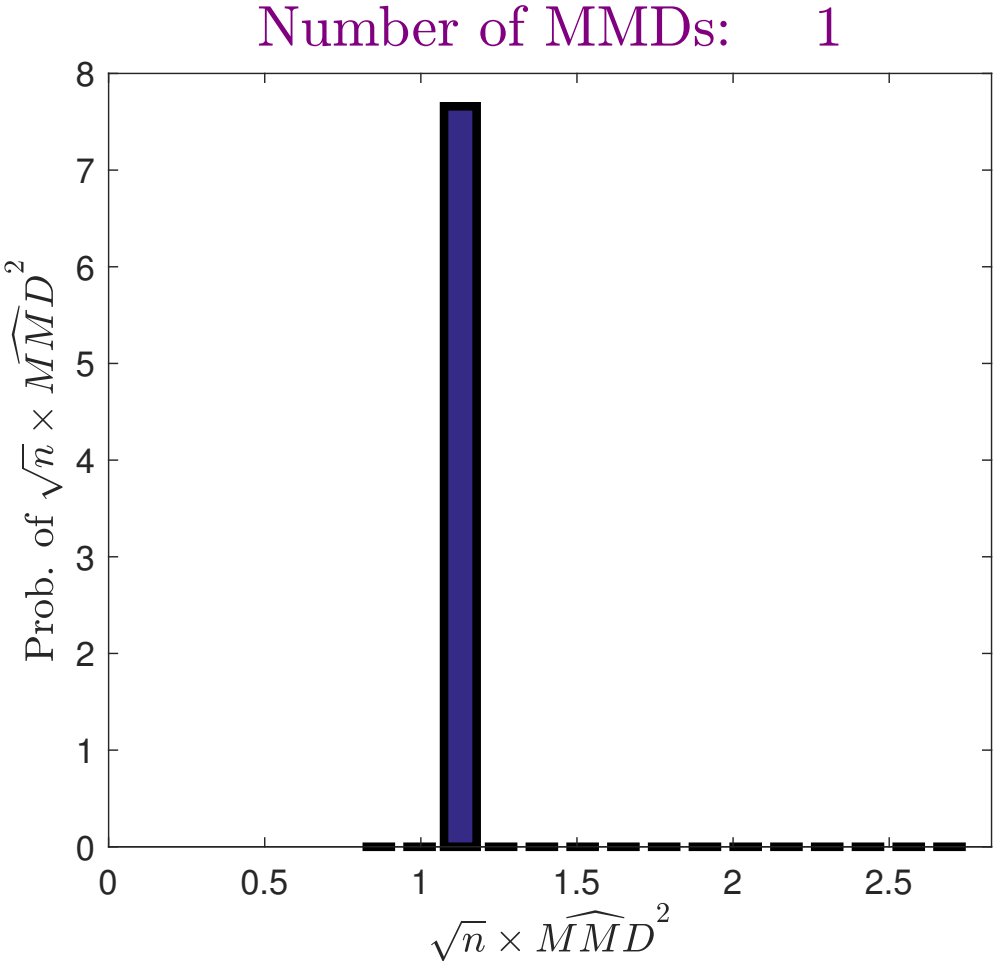
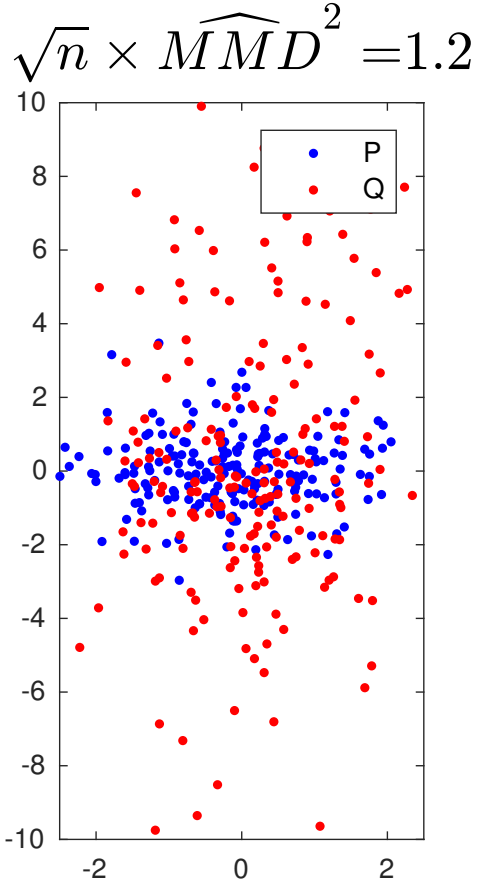
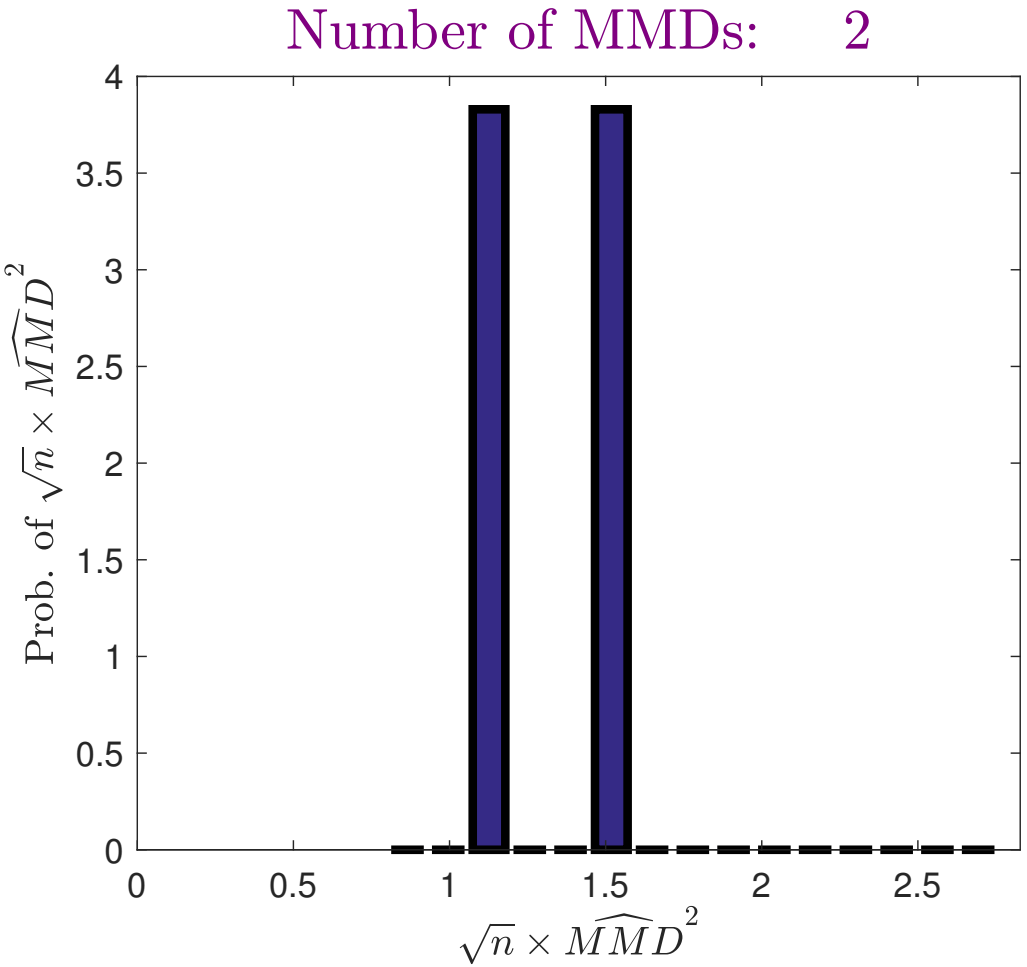


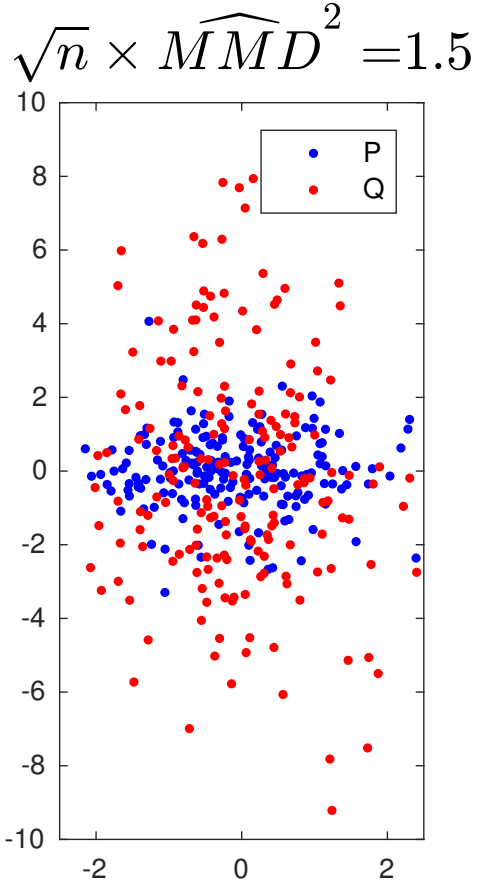


Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Draw $n = 200$ **new** samples from P and Q

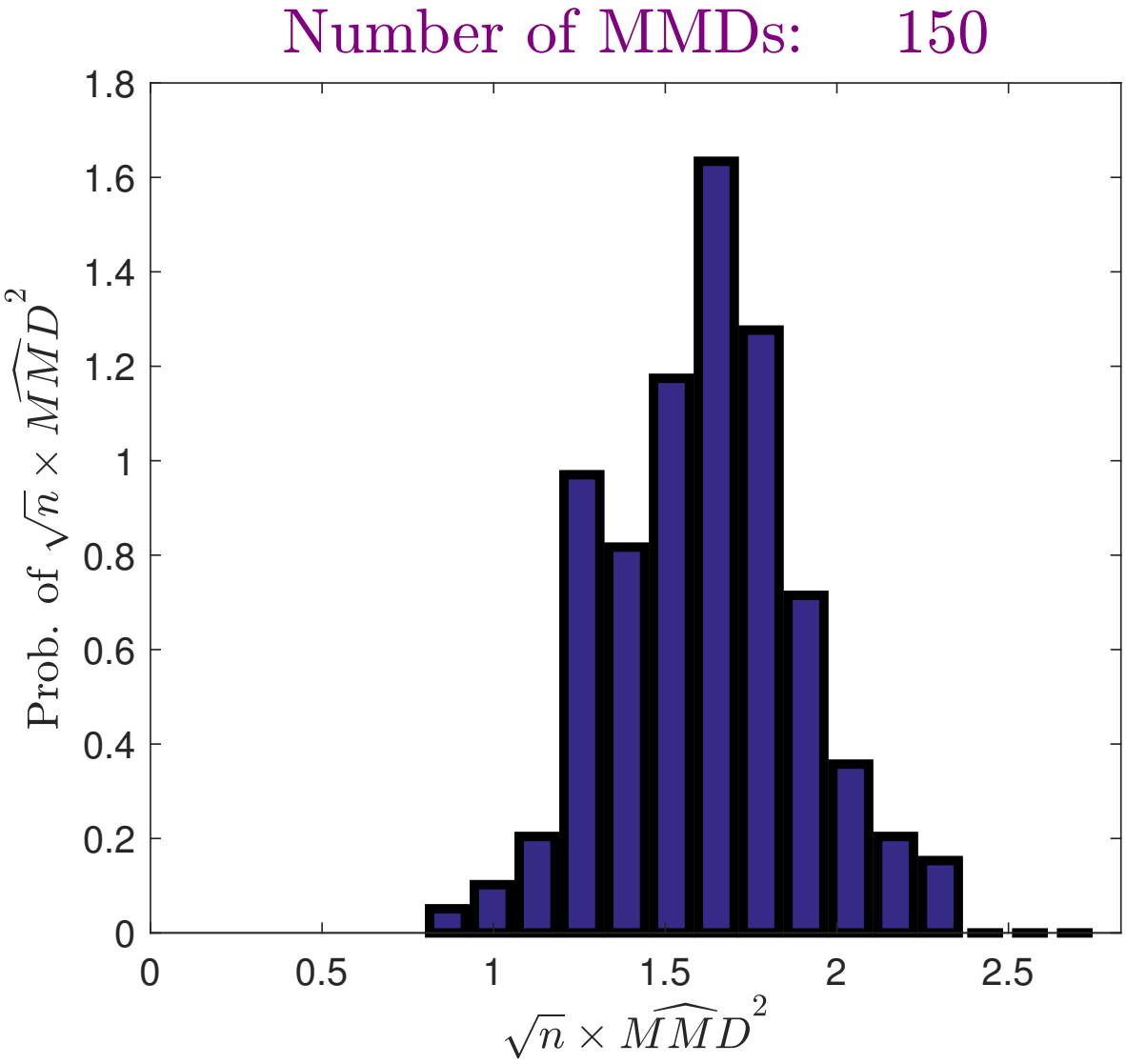
- Laplace with different y-variance.
- $\sqrt{n} \times \widehat{MMD}^2 = 1.5$





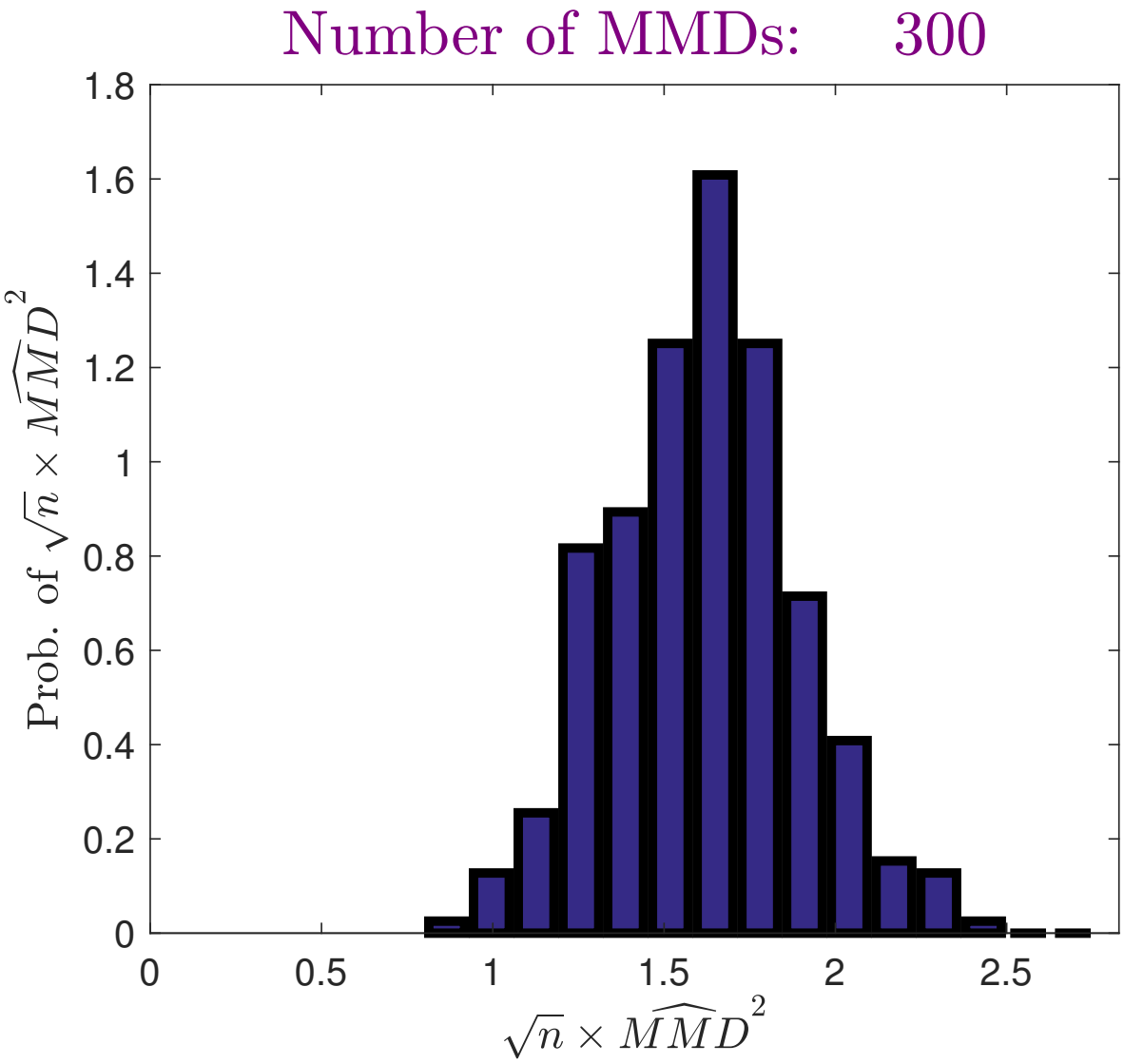
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 150 times ...



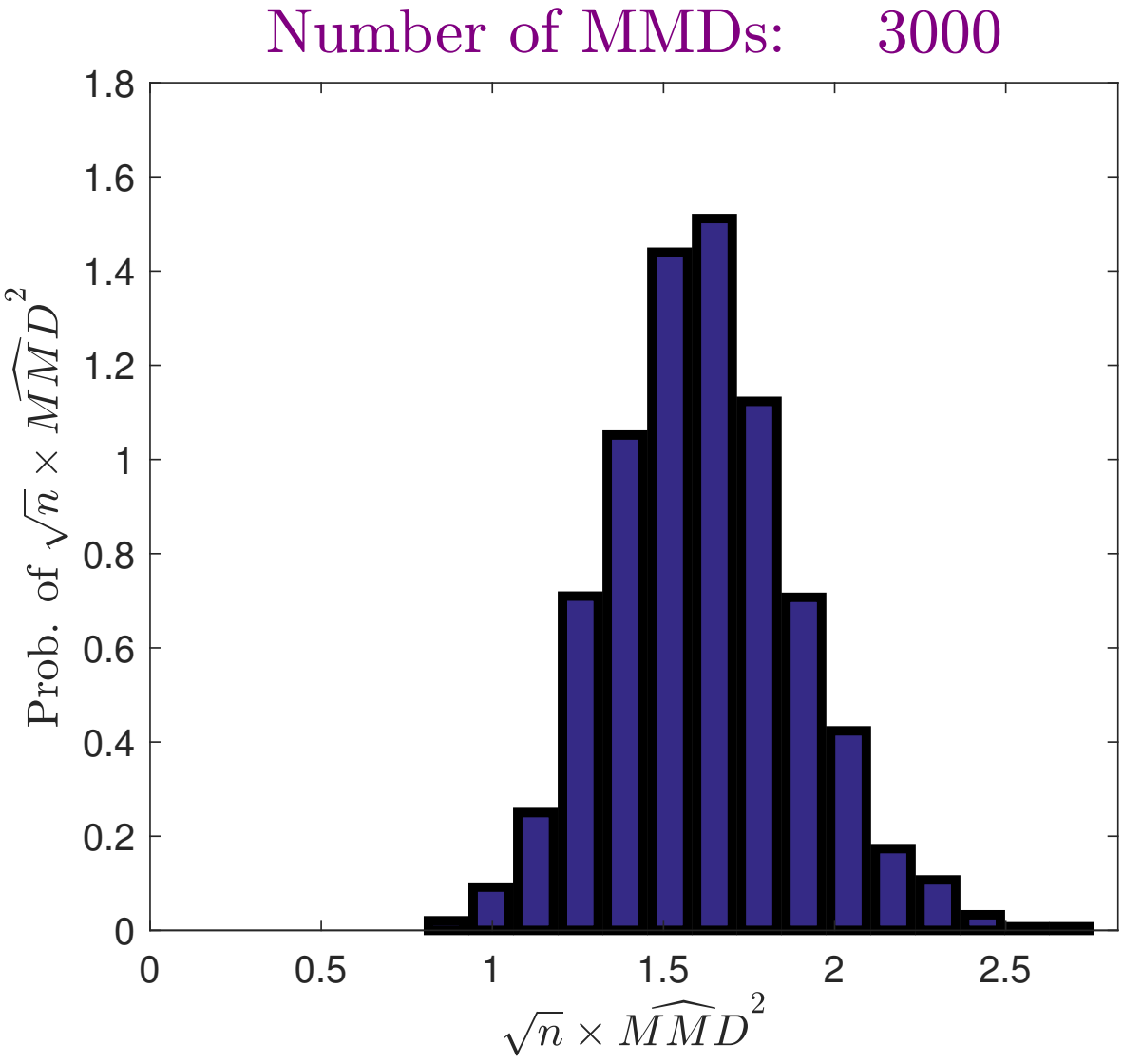
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 300 times ...



Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 3000 times ...

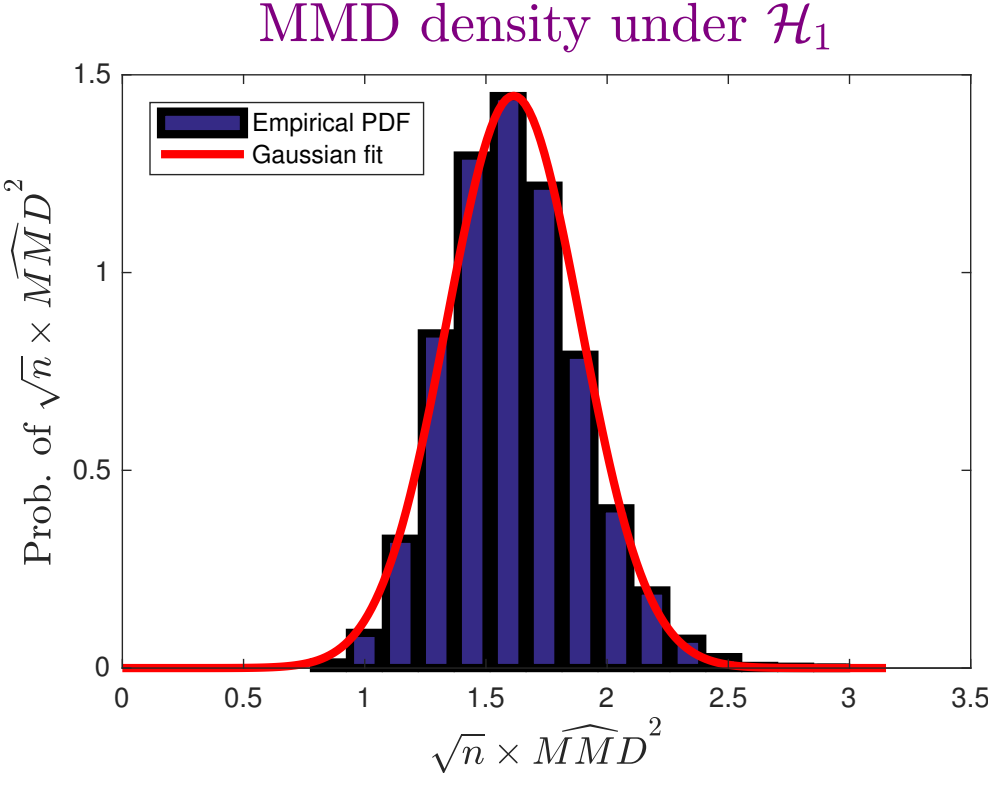


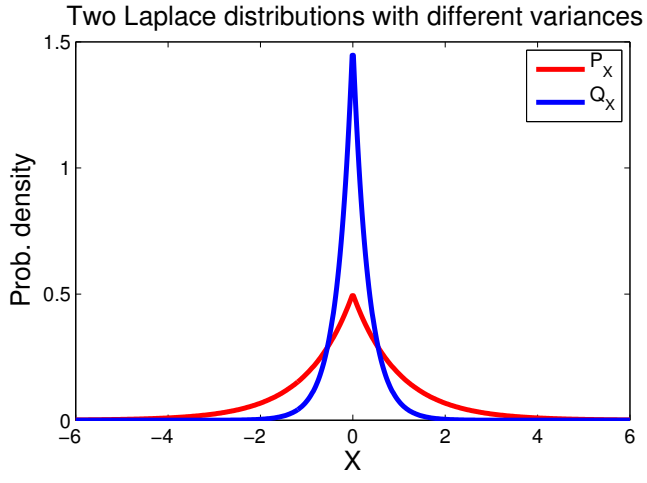
Asymptotics of $\widehat{MMD}^2$ when $P \neq Q$

When $P \neq Q$, statistic is asymptotically normal,

$$\frac{\widehat{\mathrm{MMD}}^2 - \mathrm{MMD}^2(P, Q)}{\sqrt{V_n(P, Q)}} \xrightarrow{D} \mathcal{N}(0, 1),$$

where variance $V_n(P, Q) = O\left(n^{-1}\right)$.



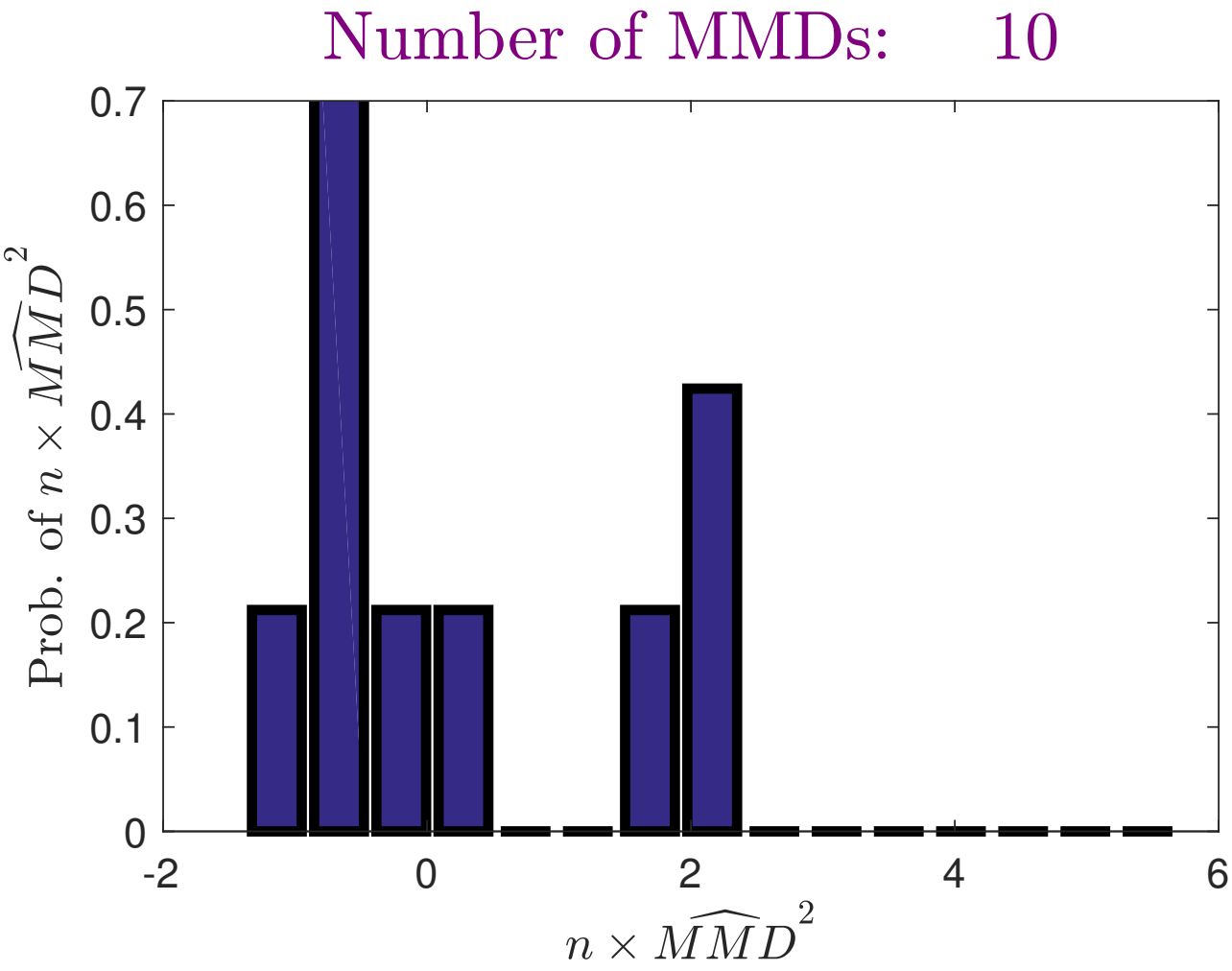


Behaviour of $\widehat{MMD}^2$ when $P = Q$

What happens when P and Q are the same?

Behaviour of $\widehat{MMD}^2$ when $P = Q$

- Case of $P = Q = \mathcal{N}(0, 1)$



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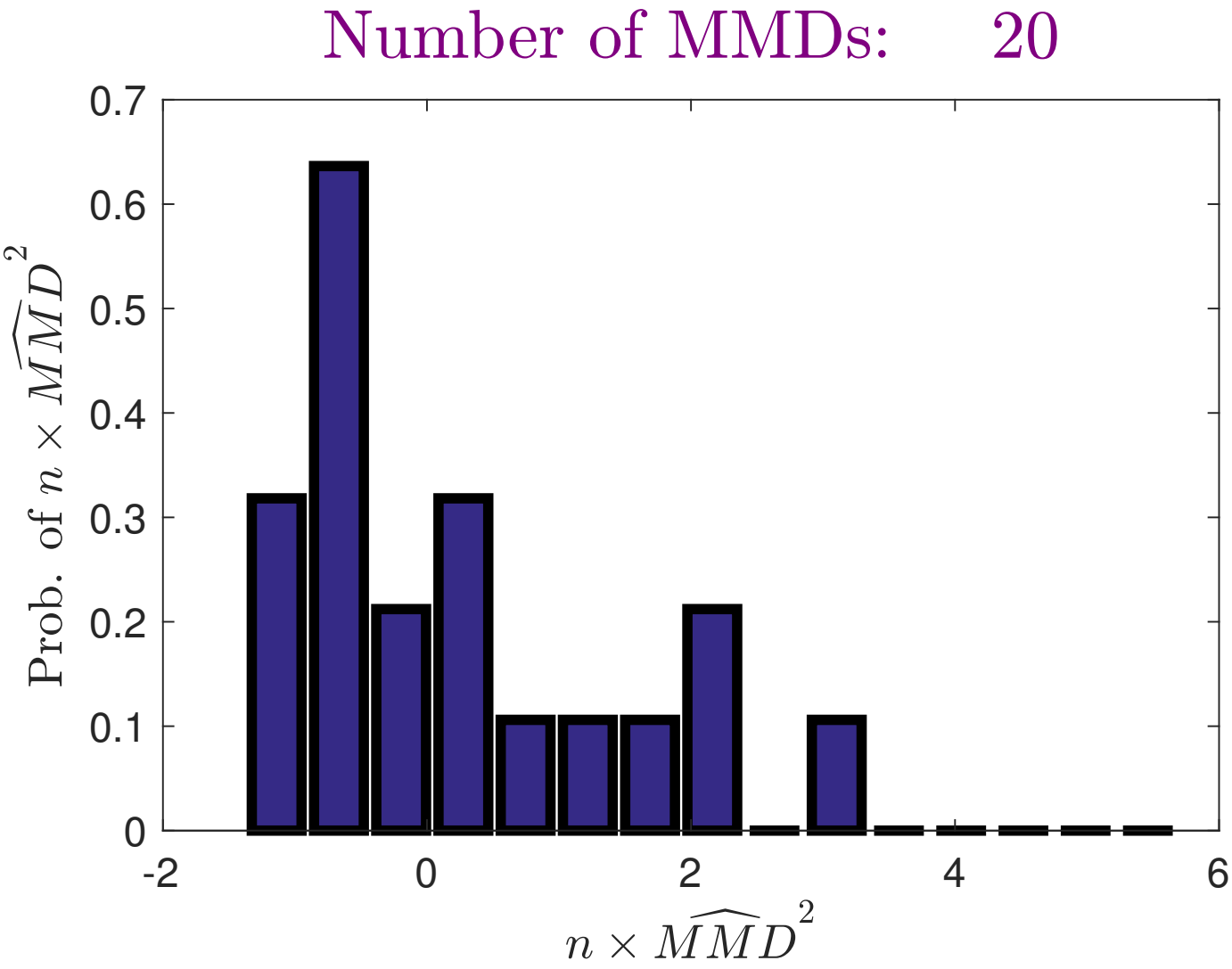

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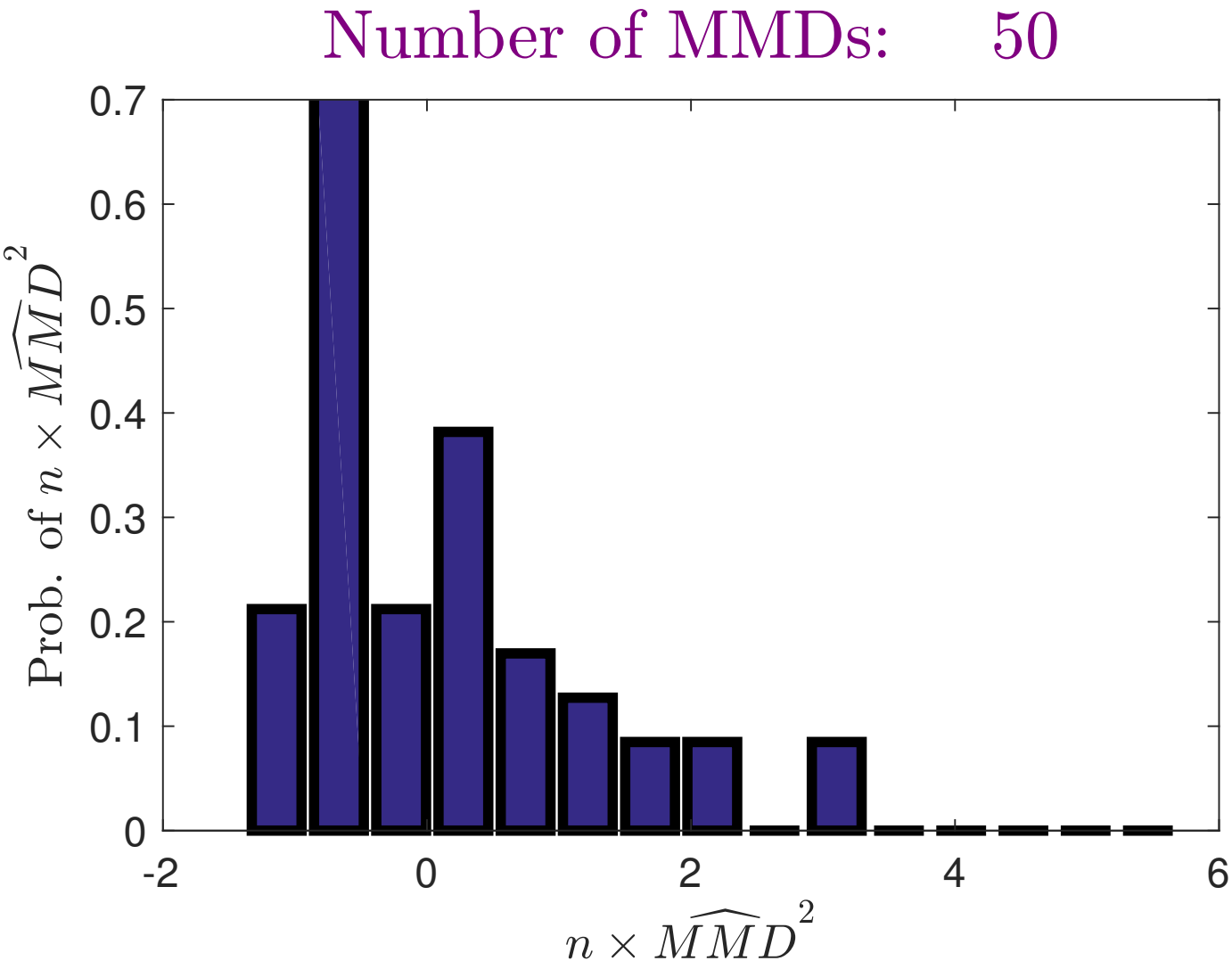

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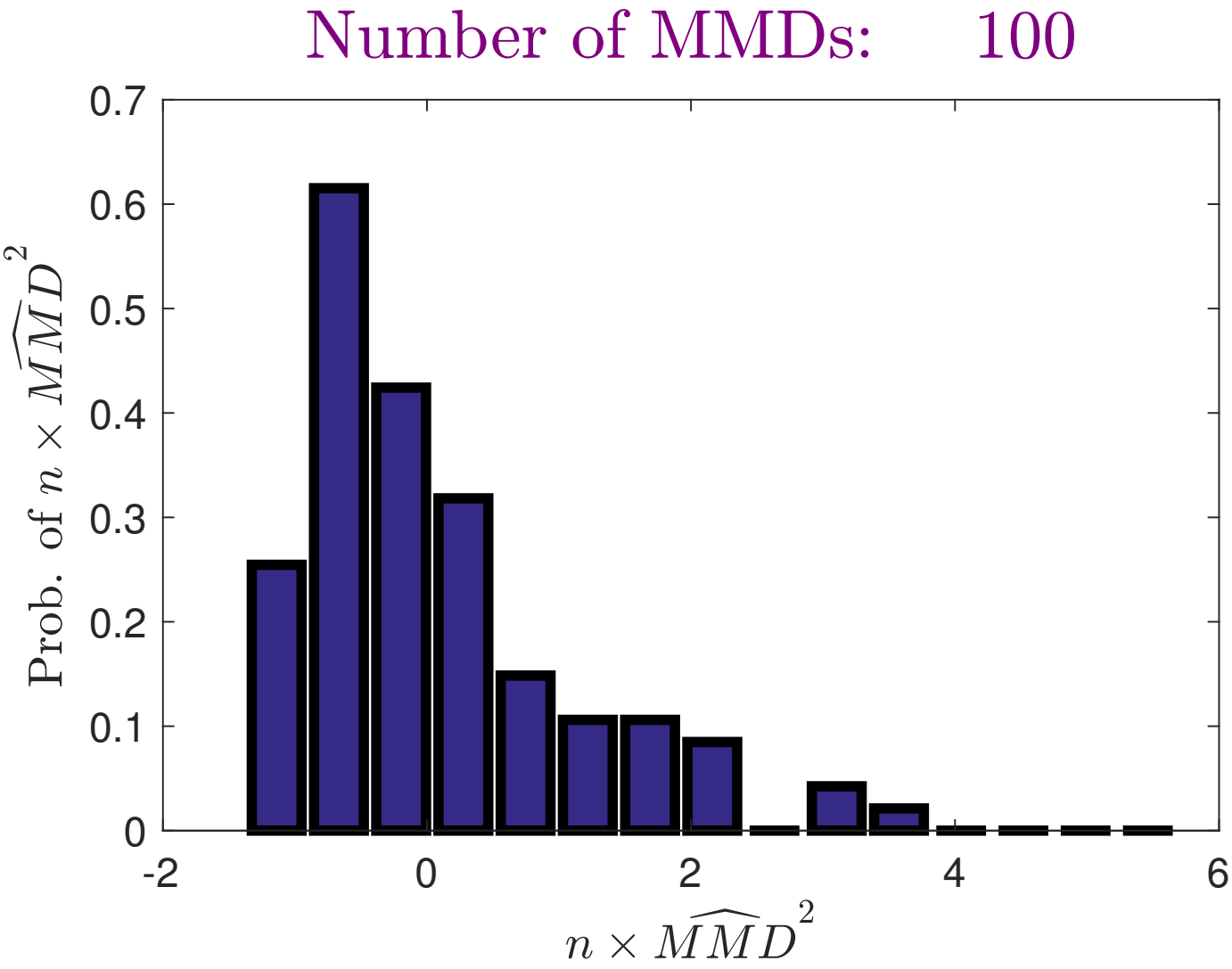

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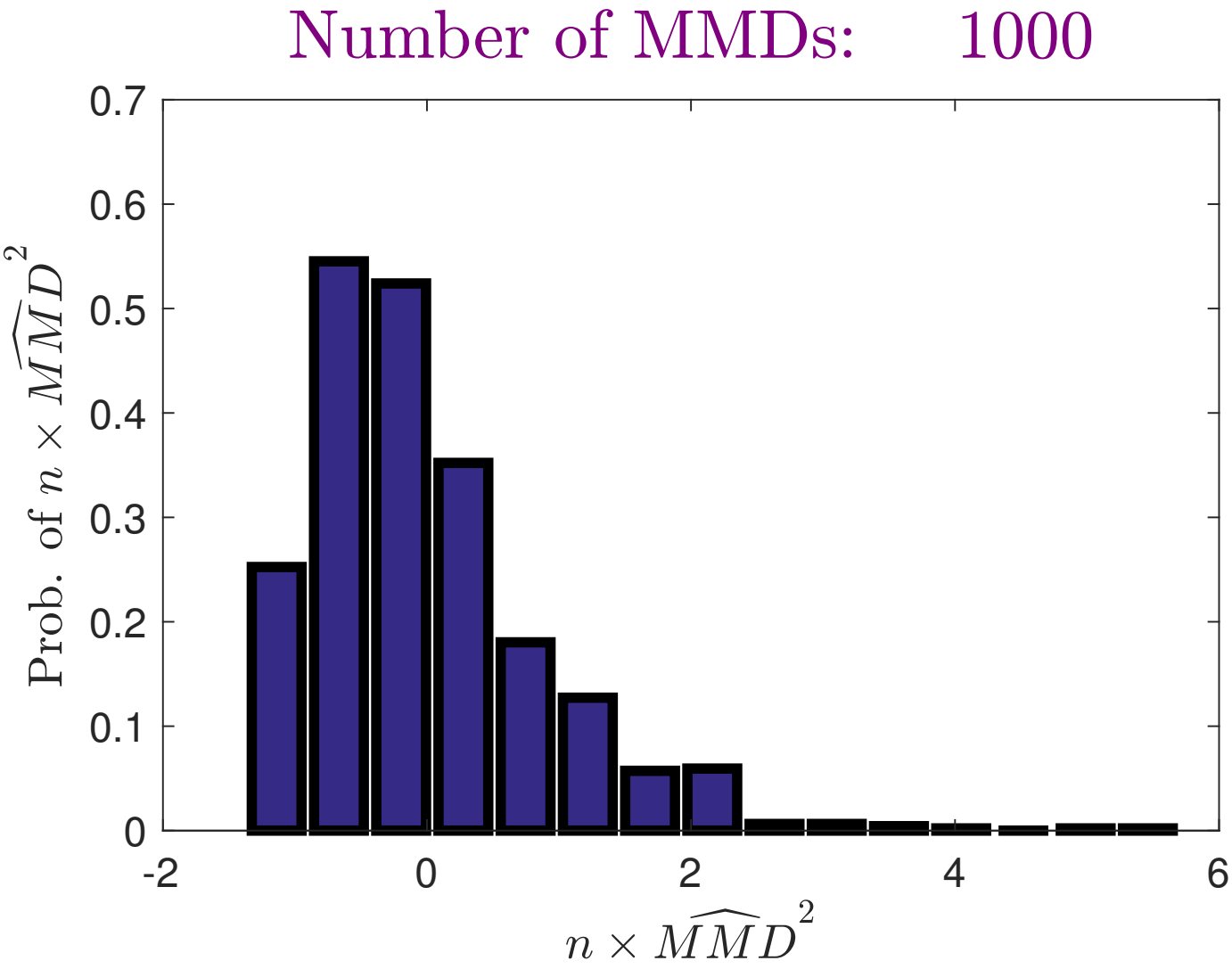
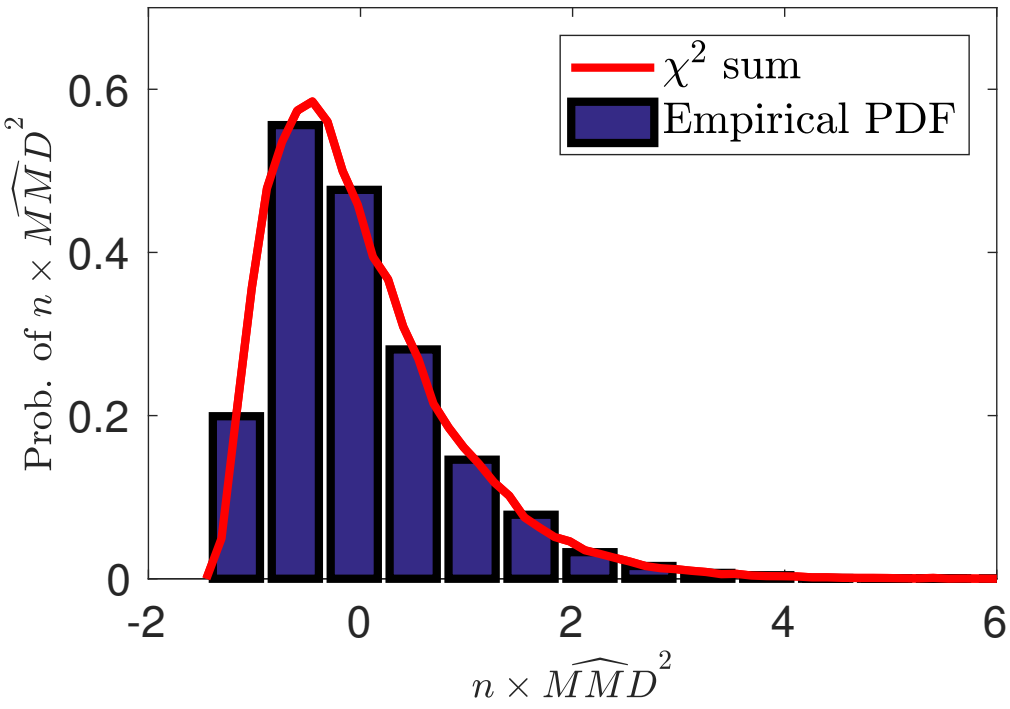


Asymptotics of $\widehat{MMD}^2$ when $P = Q$

Where $P = Q$, statistic has asymptotic distribution

$$n\widehat{\mathrm{MMD}}^2 \sim \sum_{l=1}^{\infty} \lambda_l \left[z_l^2 - 2\right]$$

MMD density under $\mathcal{H}_0$



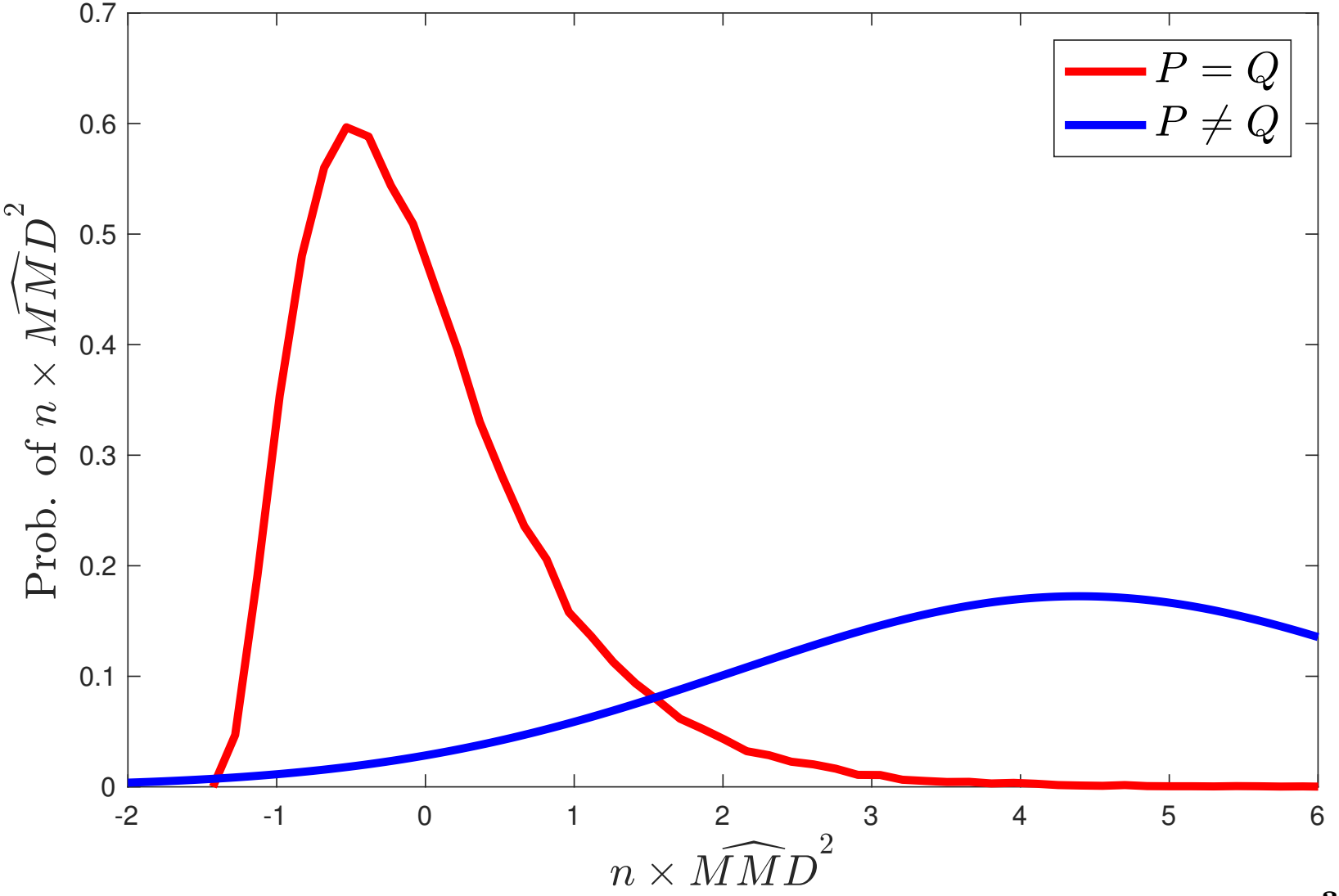
where

$$\lambda_i \psi_i(x') = \int_{\mathcal{X}} \underbrace{\tilde{k}(x, x')}_{\text{centred}} \psi_i(x) dP(x)$$

$$z_l \sim \mathcal{N}(0, 2) \quad \text{i.i.d.}$$

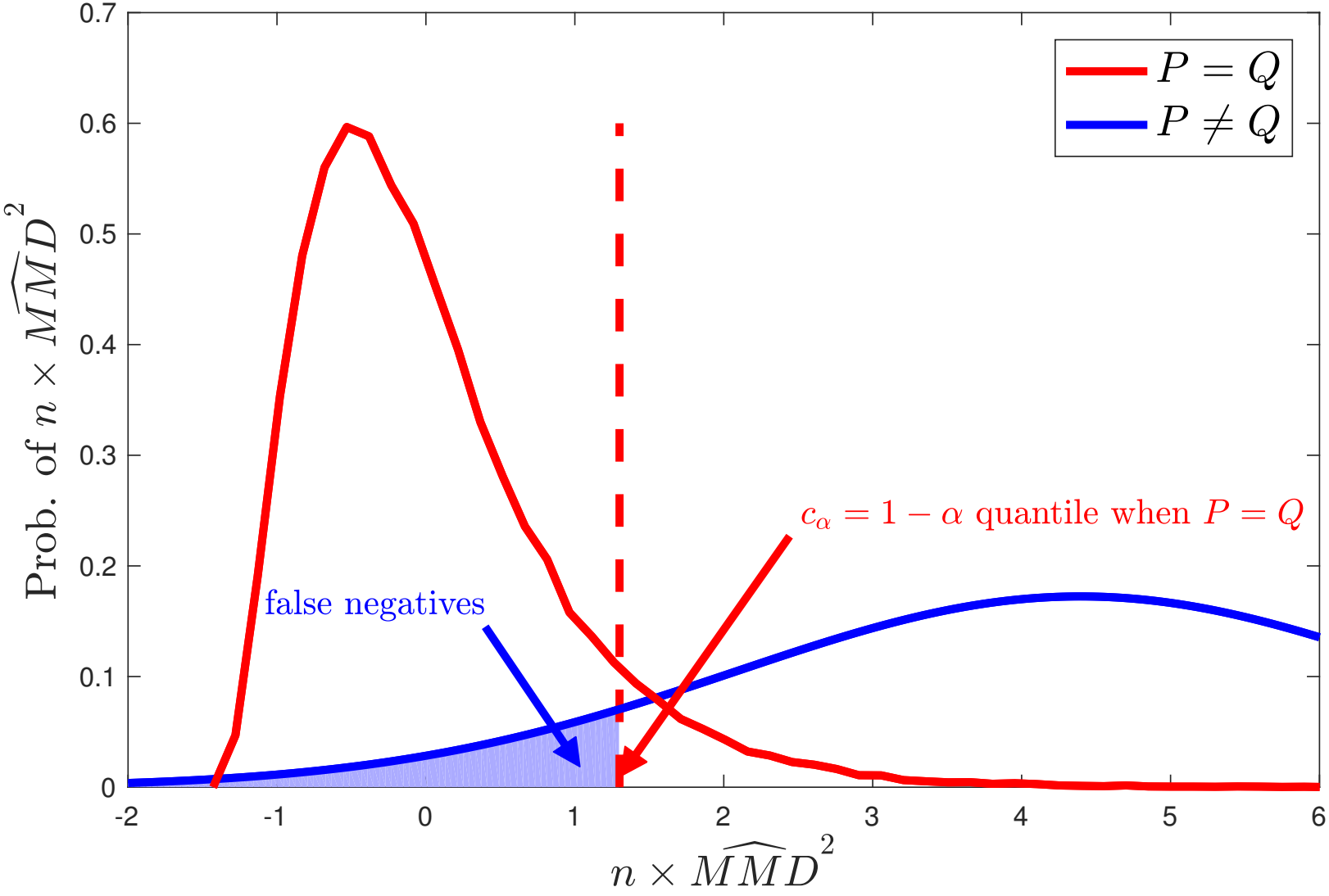
A statistical test

A summary of the asymptotics:



A statistical test

Test construction: (G., Borgwardt, Rasch, Schoelkopf, and Smola, JMLR 2012)



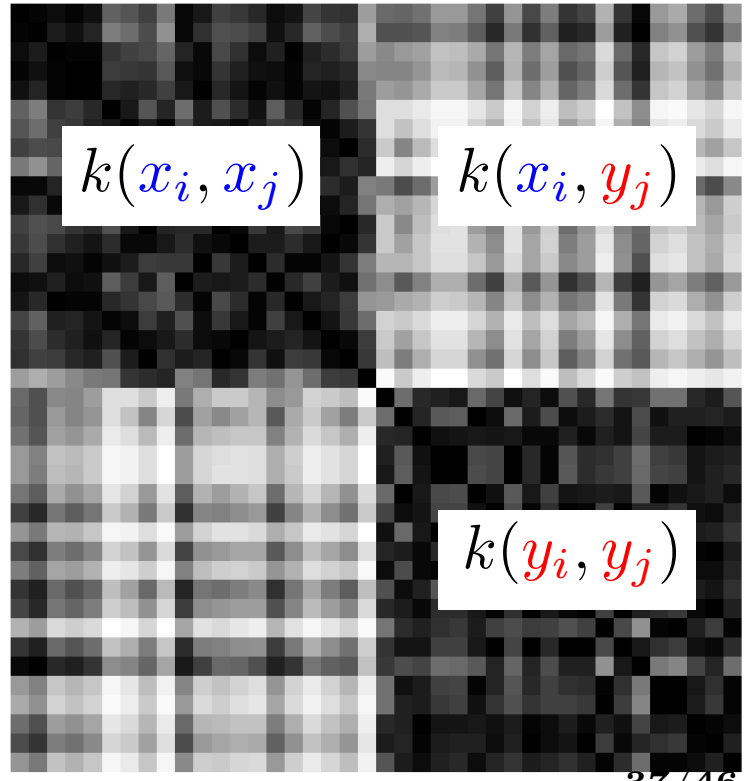
How do we get test threshold c_α?

Original empirical MMD for dogs and fish:

$X = [$  $\dots]$

$Y = [$  $\dots]$

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

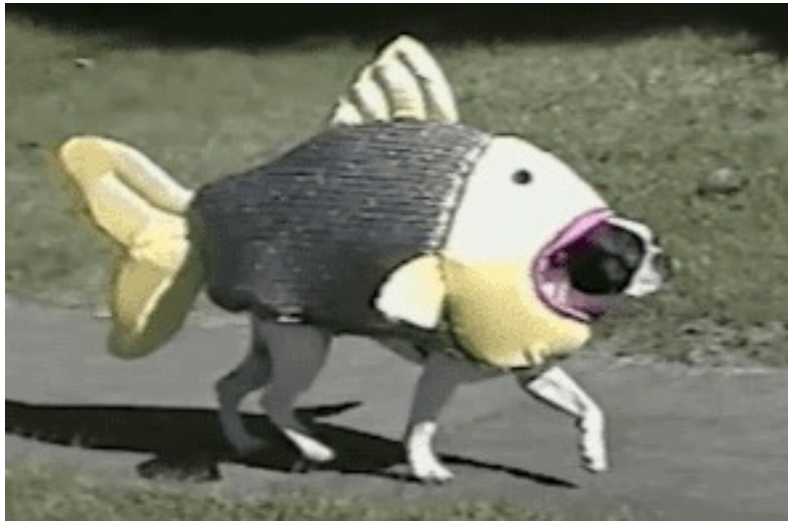


How do we get test threshold c_α?

Permuted dog and fish samples (**merdogs**):

$\widetilde{X} = [$  $\ldots\ ]$

$\widetilde{Y} = [$  $\ldots\ ]$



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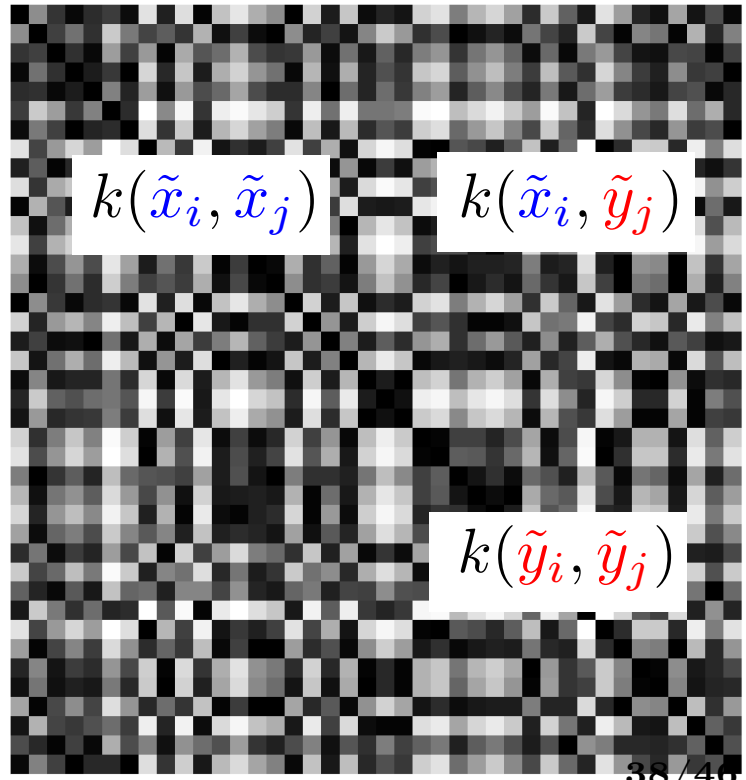
$$\widehat{MMD}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} k(\tilde{x}_i, \tilde{x}_j) + \frac{1}{n(n-1)} \sum_{i \neq j} k(\tilde{y}_i, \tilde{y}_j) - \frac{2}{n^2} \sum_{i,j} k(\tilde{x}_i, \tilde{y}_j)$$



Permutation simulates $P = Q$

How to choose the best kernel: optimising the kernel parameters

The best test for the job

- A test's power depends on $k(x, x')$, P, and Q (and n)
- With characteristic kernel, MMD test has power $\to 1$ as $n \to \infty$ for any (fixed) problem
  - But, for many P and Q, will have terrible power with reasonable n!

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  - But, for many P and Q, will have terrible power with reasonable n!
- You *can* choose a good kernel for a given problem
- You *can't* get one kernel that has good finite-sample power for all problems
  - No one test can have all that power

Choosing a kernel for the test

- Simple choice: exponentiated quadratic

$$k(x, y) = \exp\left(-\frac{1}{2\sigma^2}\|x - y\|^2\right)$$

- *Characteristic:* for any σ: for any P and Q, power $\to 1$ as $n \to \infty$

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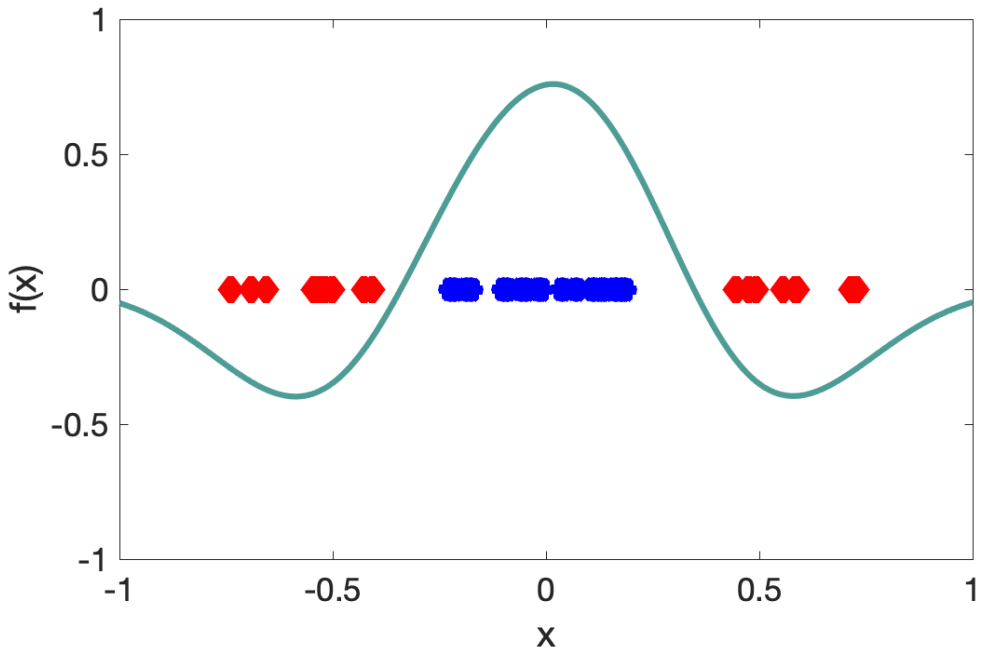

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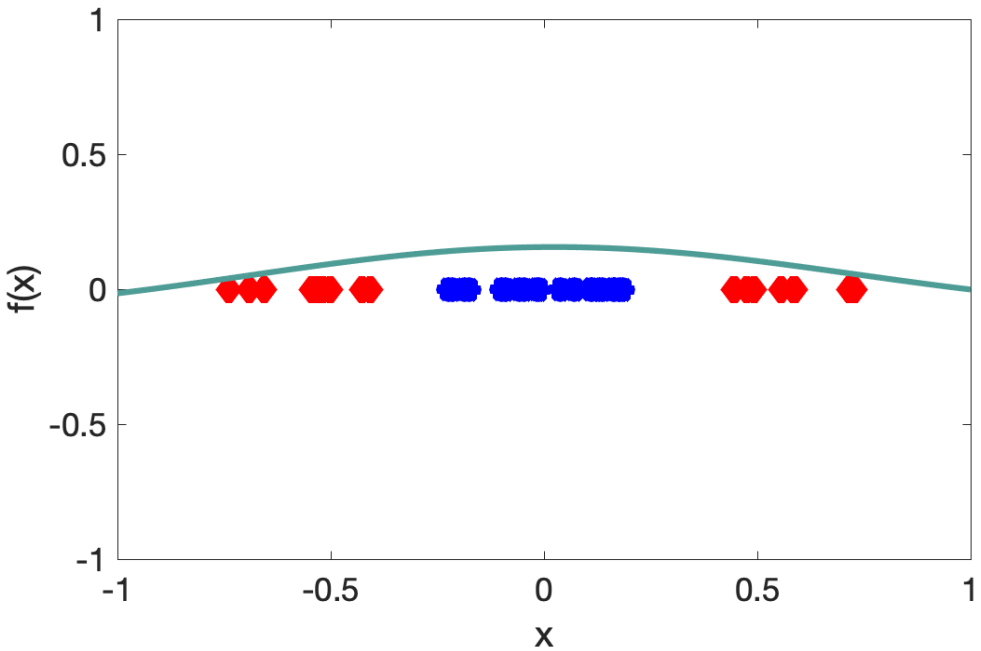

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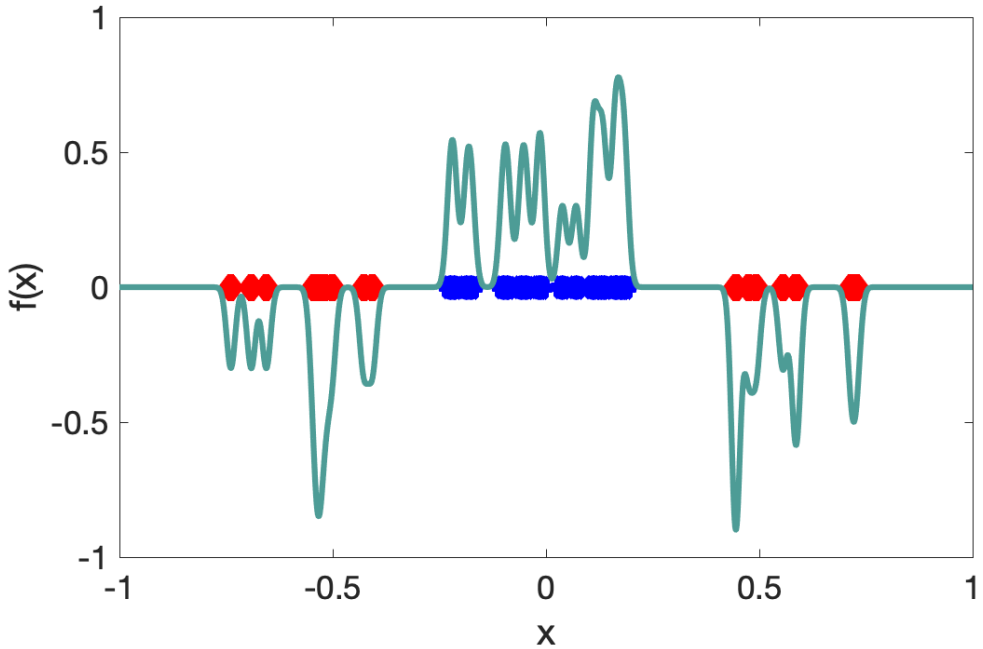

Choosing a kernel for the test

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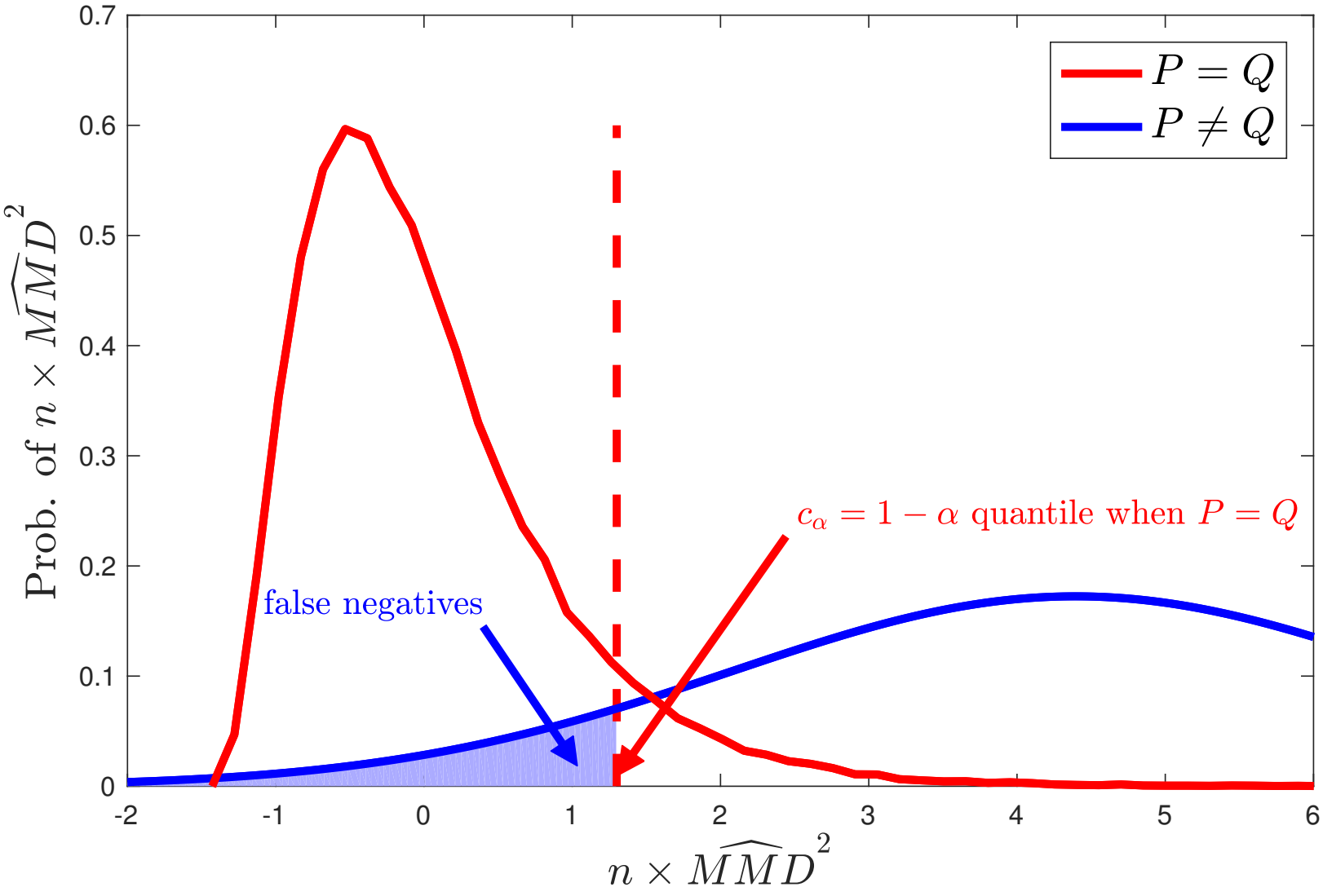
- *Characteristic:* for any σ: for any P and Q, power $\to 1$ as $n \to \infty$
- But choice of σ is very important for finite n...
- ...and some problems (e.g. images) might have no good choice for σ

Graphical illustration

- Maximising test power same as minimizing false negatives



Optimizing kernel for test power

The power of our test ($\Pr_1$ denotes probability under $P \neq Q$):

$$\Pr_1 \left(n \widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha \right)$$

Optimizing kernel for test power

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$$\Pr_1\left(n\widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha\right)$$
$$\to \Phi\left(\frac{\mathrm{MMD}^2(P,Q)}{\sqrt{V_n(P,Q)}} - \frac{c_\alpha}{n\sqrt{V_n(P,Q)}}\right)$$

where

- Φ is the CDF of the standard normal distribution.
- $\hat{c}_\alpha$ is an estimate of c_α test threshold.

Optimizing kernel for test power

The power of our test ($\Pr_1$ denotes probability under $P \neq Q$):

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For large n, second term negligible!

Optimizing kernel for test power

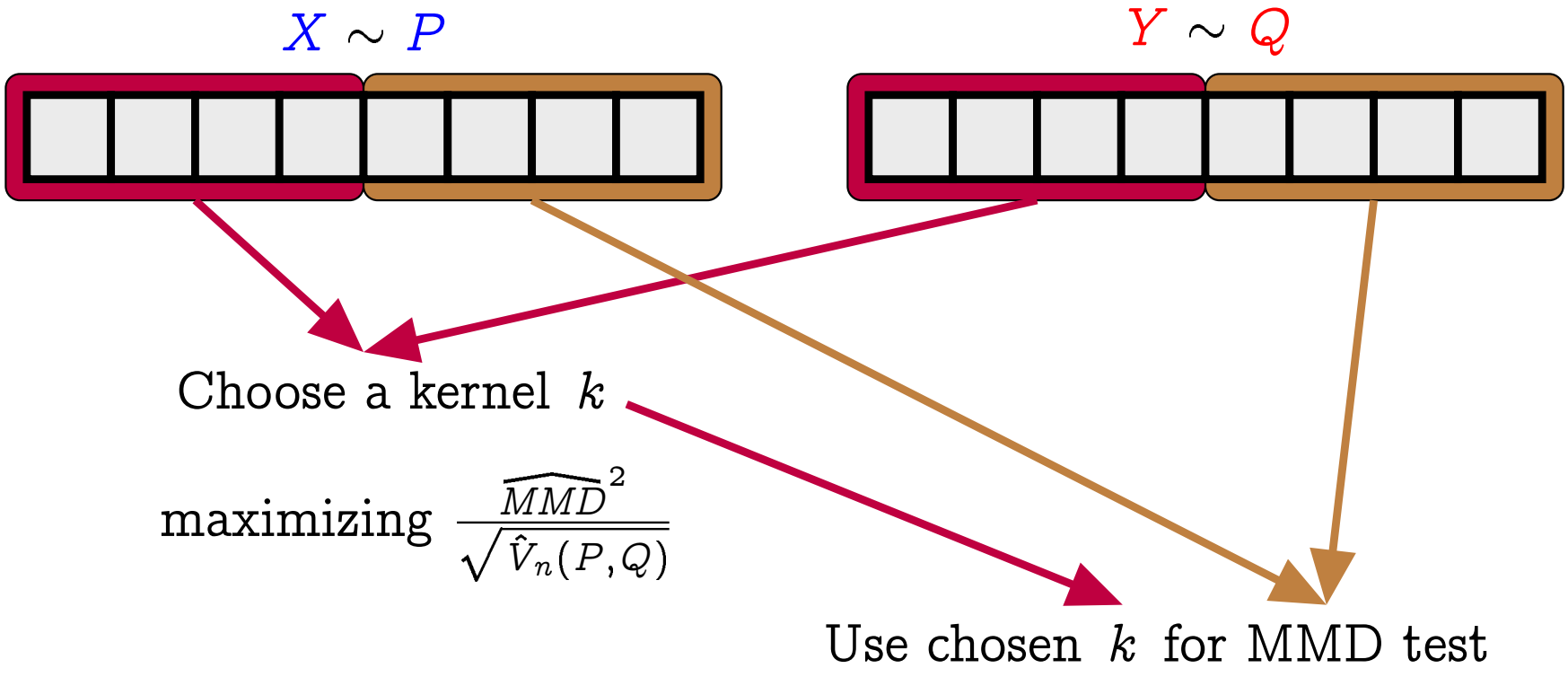
The power of our test ($\Pr_1$ denotes probability under $P \neq Q$):

$$\Pr_1\left(n\widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha\right)$$
$$\to \Phi\left(\frac{\mathrm{MMD}^2(P,Q)}{\sqrt{V_n(P,Q)}} - \frac{c_\alpha}{n\sqrt{V_n(P,Q)}}\right)$$

To maximize test power, maximize

$$\frac{\mathrm{MMD}^2(P,Q)}{\sqrt{V_n(P,Q)}}$$

Data splitting

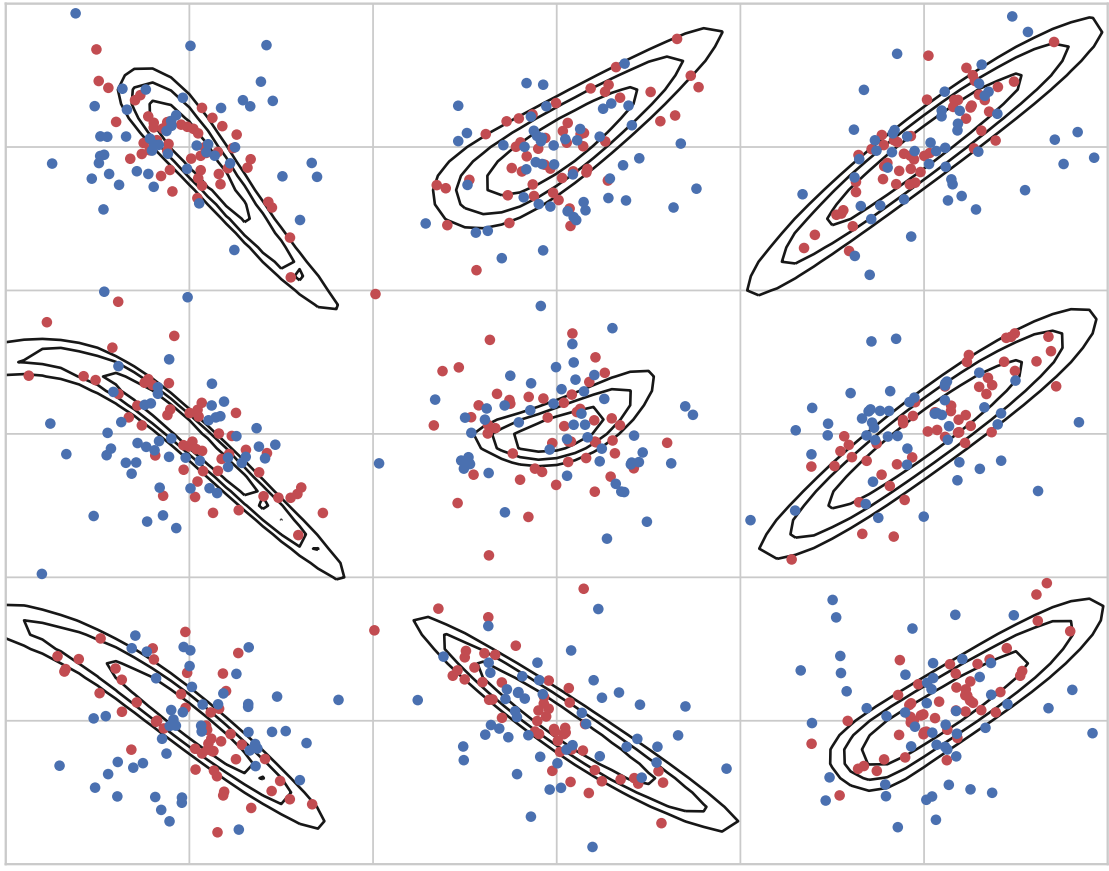


Learning a kernel helps a lot

Kernel with deep learned features:

$$k_\theta(x, y) = [(1 - \epsilon)\kappa(\Phi_\theta(x), \Phi_\theta(y)) + \epsilon]\, q(x, y)$$

κ and q are Gaussian kernels



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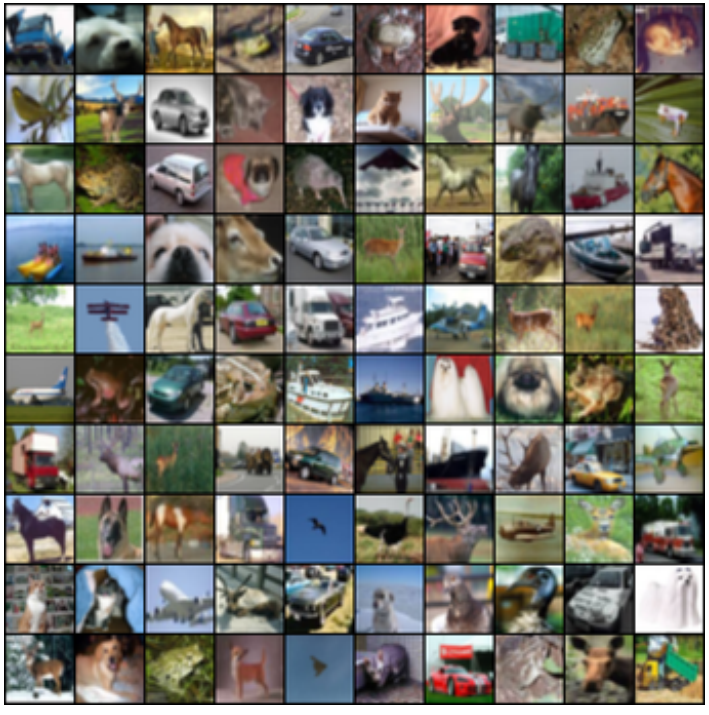
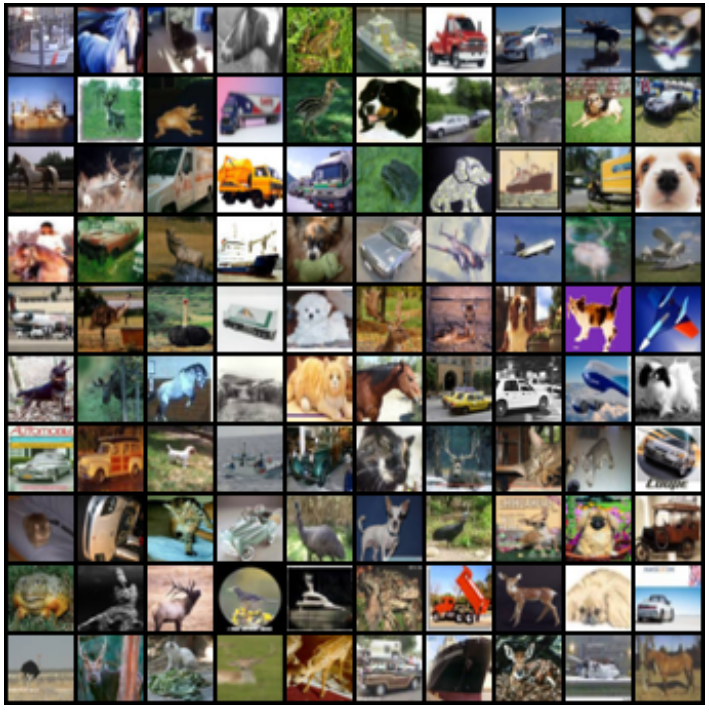
- CIFAR-10 vs CIFAR-10.1, **null rejected 75% of time**



CIFAR-10 test set (Krizhevsky 2009)

$X \sim P$



CIFAR-10.1 (Recht+ ICML 2019)

$Y \sim Q$

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κ and q are Gaussian kernels

- CIFAR-10 vs CIFAR-10.1, **null rejected 75% of time**

Accepted to ICML 2020

Questions?

- A brief introduction to RKHS
- Maximum Mean Discrepancy (MMD)...
  - ...as a difference in feature means
  - ...as an integral probability metric
    (not just a technicality!)
- A statistical test based on the MMD