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

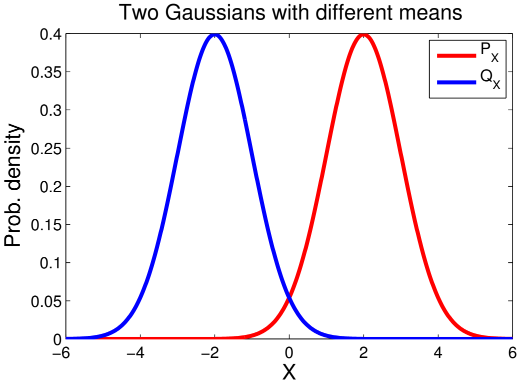
- Maximum Mean Discrepancy (MMD)...
  - ...as a difference in feature means
  - ...as an integral probability metric (not just a technicality!)

- A statistical test based on the MMD

- Next slides: training generative adversarial networks with MMD
  - Gradient regularisation and data adaptivity

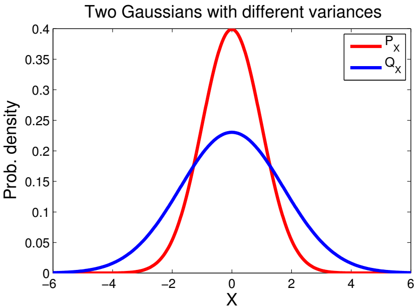
Feature mean difference

- 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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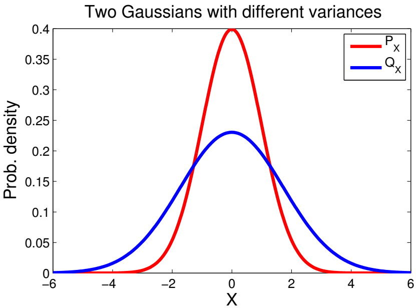
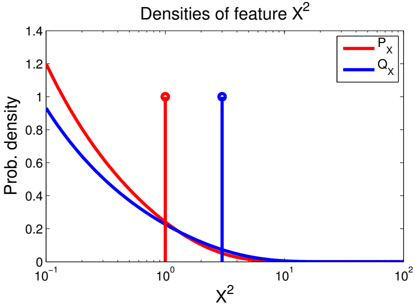


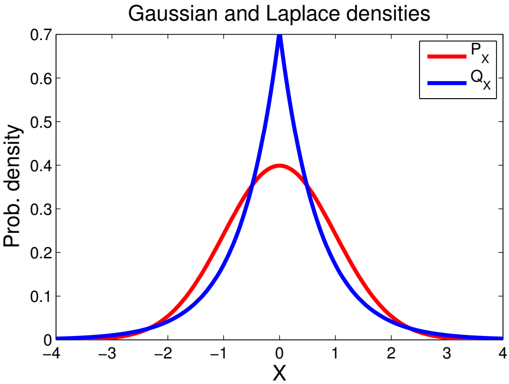
Two Gaussians with different variances



Densities of feature X^2

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,

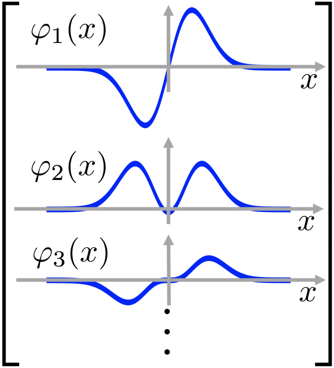
$$k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}}$$

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

Exponentiated quadratic kernel

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

$$\varphi(x) =$$



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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The maximum mean discrepancy

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

$$
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&= \underbrace{\mathbf{E}_P k(X, X')}_{\text{(a)}} + \underbrace{\mathbf{E}_Q k(Y, Y')}_{\text{(a)}} - 2\underbrace{\mathbf{E}_{P,Q} k(X, Y)}_{\text{(b)}}
\end{aligned}
$$

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

Illustration of MMD

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

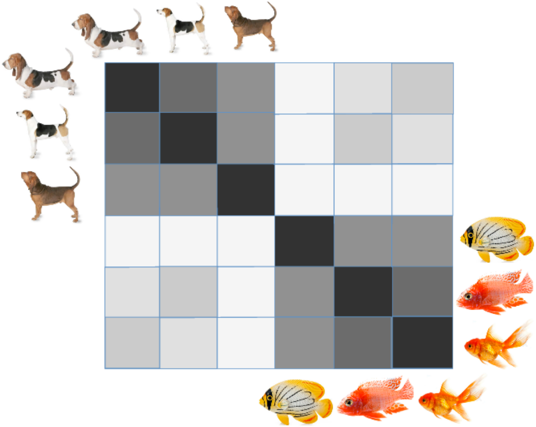
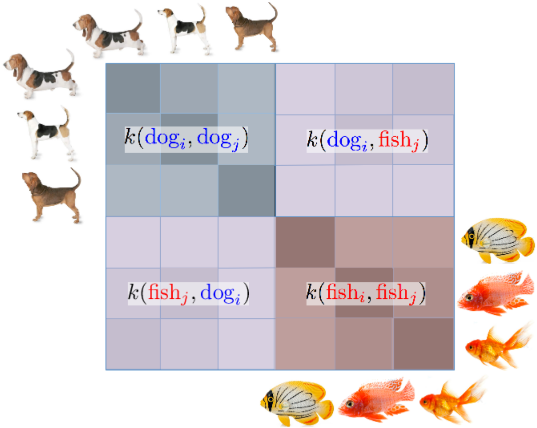


Illustration of MMD

The maximum mean discrepancy:

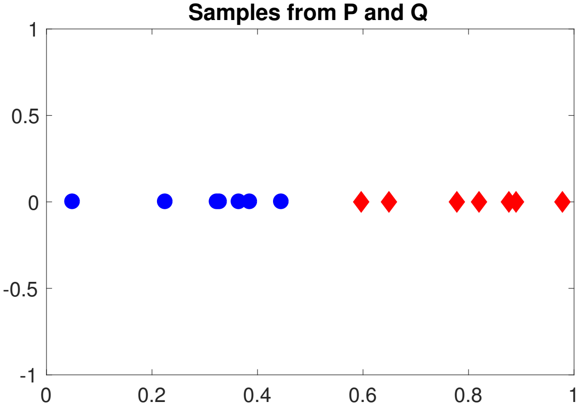
$$\widehat{MMD}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} k(\text{dog}_i, \text{dog}_j) + \frac{1}{n(n-1)} \sum_{i \neq j} k(\text{fish}_i, \text{fish}_j) - \frac{2}{n^2} \sum_{i,j} k(\text{dog}_i, \text{fish}_j)$$



$k(\text{dog}_i, \text{dog}_j)$
$k(\text{dog}_i, \text{fish}_j)$
$k(\text{fish}_j, \text{dog}_i)$
$k(\text{fish}_i, \text{fish}_j)$

MMD as an integral probability metric

Are P and Q different?



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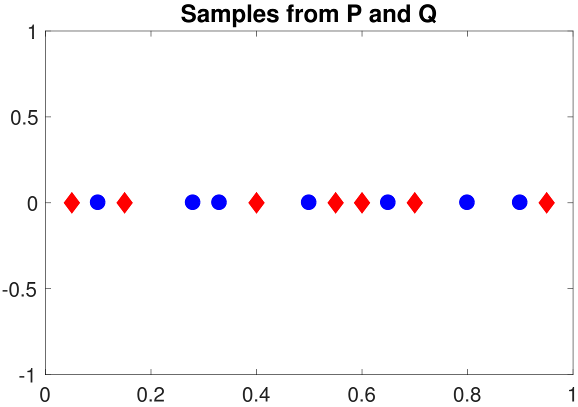
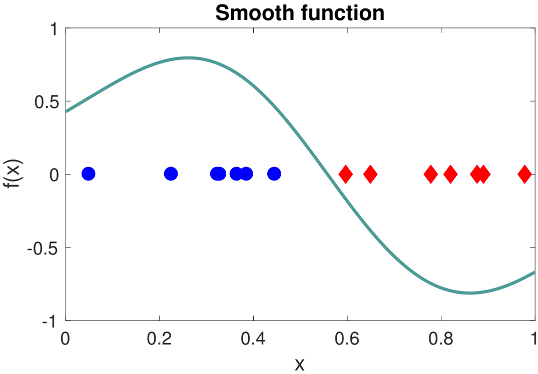


MMD as an integral probability metric

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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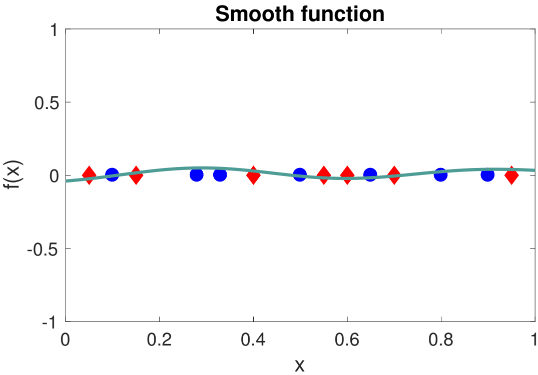

MMD as an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

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

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

MMD as an integral probability metric

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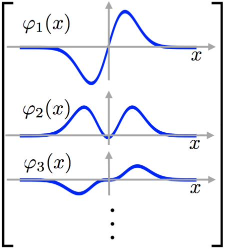
Functions are linear combinations of features:

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



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

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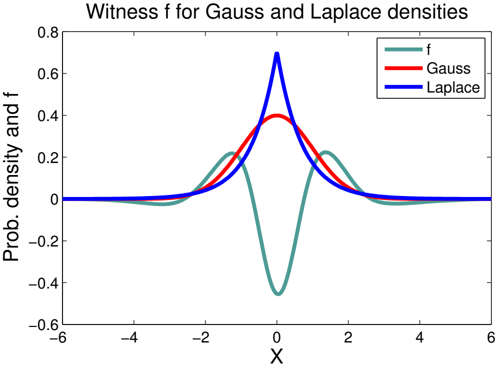

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For characteristic RKHS $\mathcal{F}$, $MMD(P, Q; F) = 0$ iff $P = Q$

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

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:

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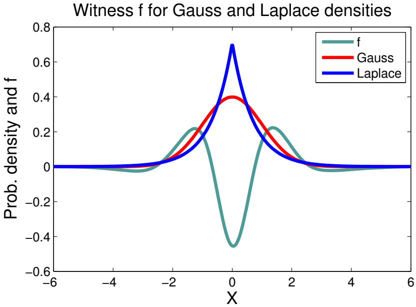

Integral prob. metric vs feature difference

The MMD:

use

$$\begin{aligned} & MMD(P, Q; F) \\ = & \sup_{\|f\|_{\mathcal{F}} \leq 1} \left[\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y) \right] \\ = & \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \end{aligned}$$

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

Integral prob. metric vs feature difference

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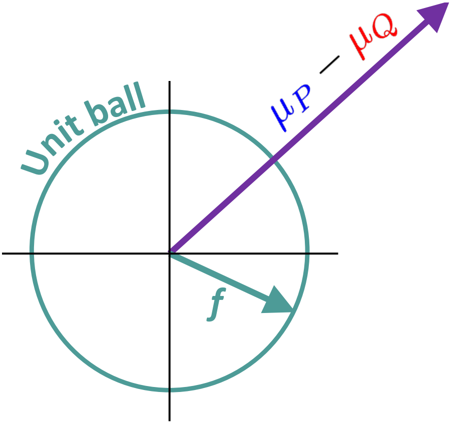

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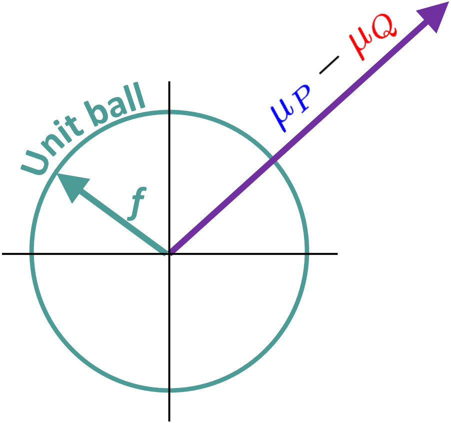

Integral prob. metric vs feature difference

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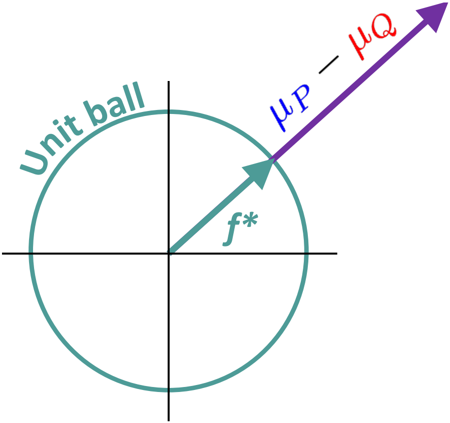

$$f^* = \frac{\mu_P - \mu_Q}{\|\mu_P - \mu_Q\|}$$

Integral prob. metric vs feature difference

The MMD:

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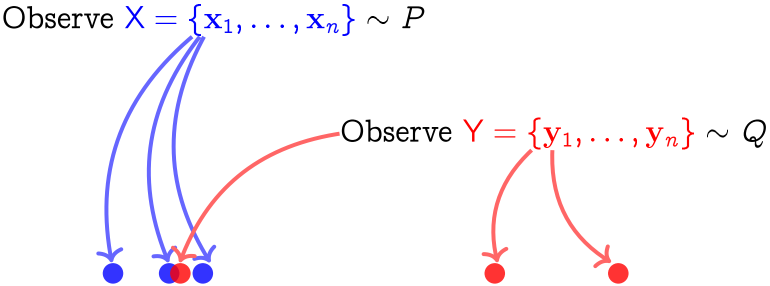
&= \sup_{\|f\|_{\mathcal{F}} \leq 1} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \\
&= \|\mu_P - \mu_Q\|
\end{aligned}
$$

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

Construction of MMD witness

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

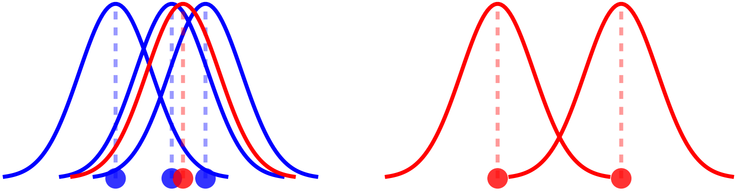


Observe $\mathsf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \sim P$

Observe $\mathsf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_n\} \sim Q$

Construction of MMD witness

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



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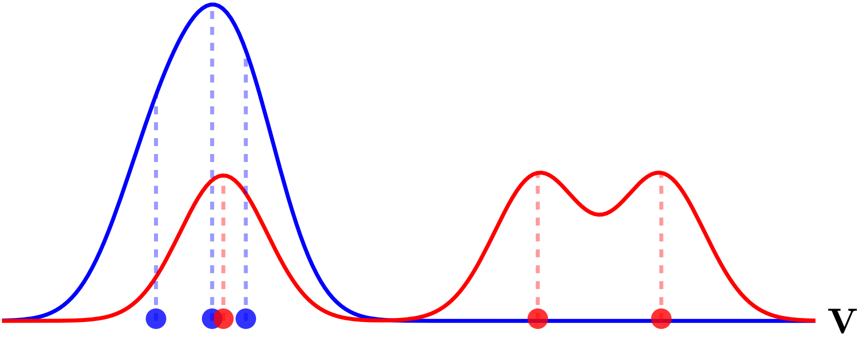

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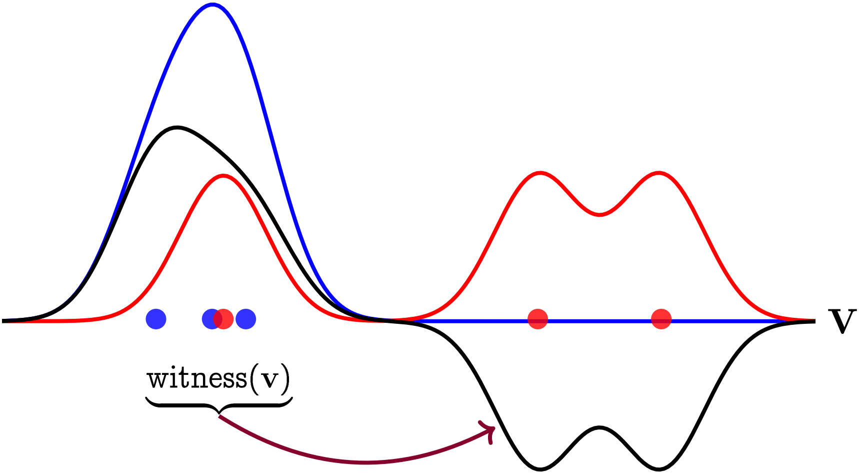

Derivation of empirical witness function

Recall the witness function expression

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

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The empirical witness function at v

$$f^*(v) = \langle f^*, \varphi(v) \rangle_{\mathcal{F}}$$

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Derivation of empirical witness function

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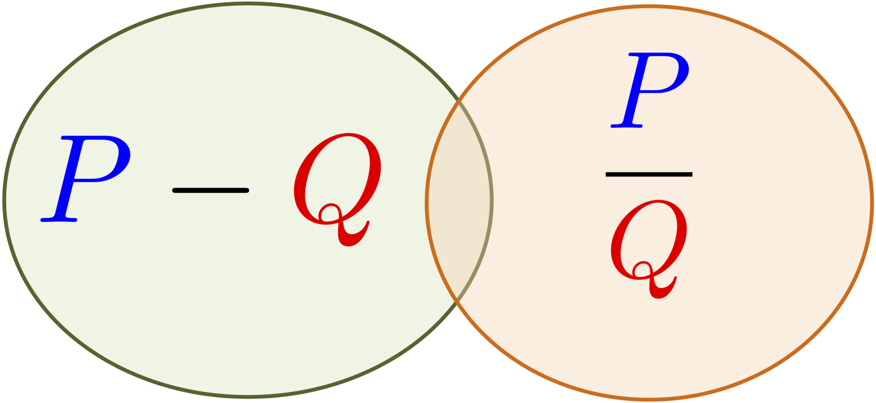
The empirical witness function at v

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

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

Interlude: divergence measures

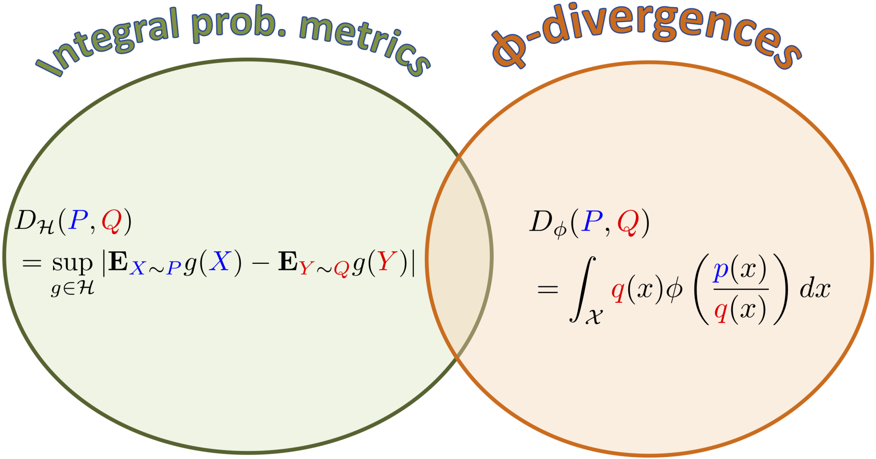
Divergences



$P - Q$

$$\frac{P}{Q}$$

Divergences



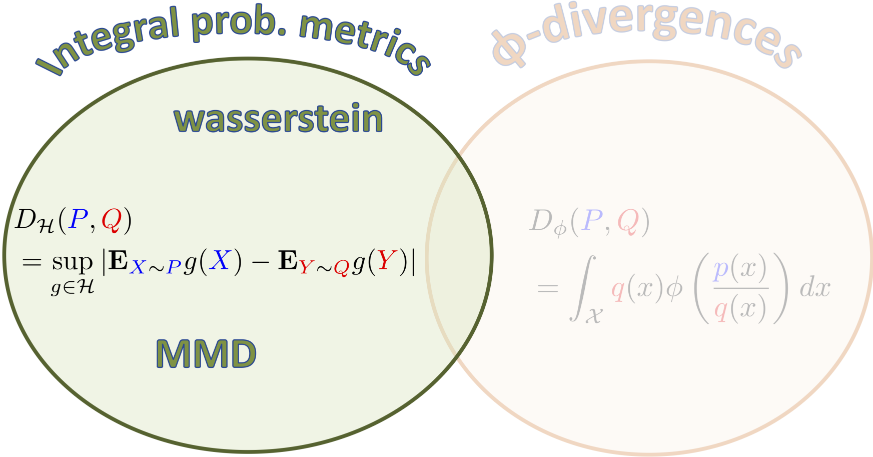
Integral prob. metrics

ϕ-divergences

$$D_{\mathcal{H}}(P,Q) = \sup_{g\in\mathcal{H}} \left|\mathbf{E}_{X\sim P}\, g(X) - \mathbf{E}_{Y\sim Q}\, g(Y)\right|$$

$$D_{\phi}(P,Q) = \int_{\mathcal{X}} q(x)\phi\left(\frac{p(x)}{q(x)}\right) dx$$

The integral probability metrics



Integral prob. metrics

wasserstein

$$D_{\mathcal{H}}(P,Q) = \sup_{g\in\mathcal{H}} \left|\mathbf{E}_{X\sim P}\, g(X) - \mathbf{E}_{Y\sim Q}\, g(Y)\right|$$

MMD

ϕ-divergences

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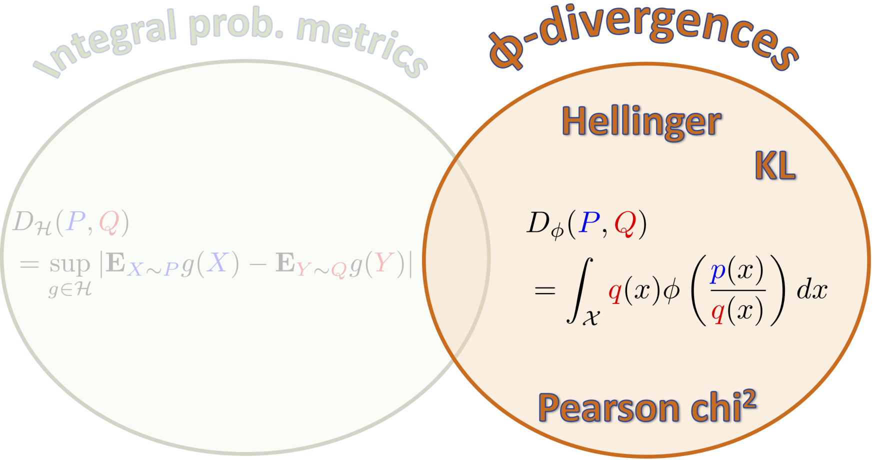
The ϕ-divergences



Integral prob. metrics

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ϕ-divergences

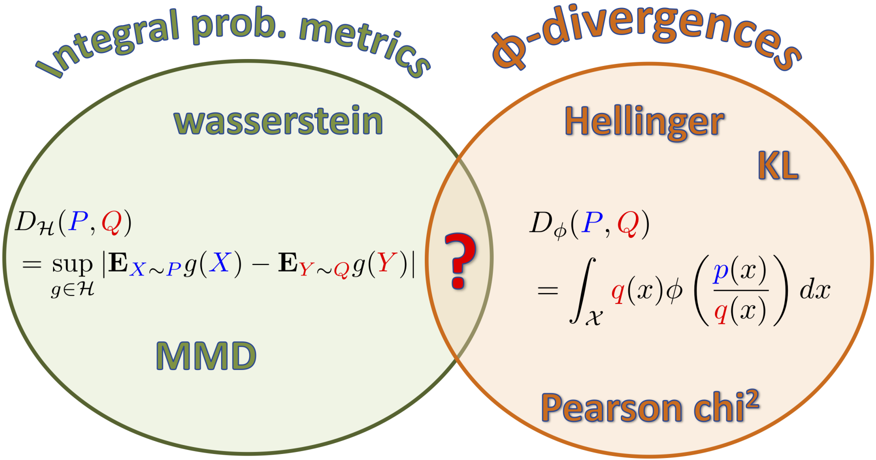
Hellinger

KL

$$D_\phi(P,Q) = \int_{\mathcal{X}} q(x)\phi\left(\frac{p(x)}{q(x)}\right)dx$$

Pearson chi²

Divergences



Integral prob. metrics

wasserstein

$$D_{\mathcal{H}}(P,Q) = \sup_{g\in\mathcal{H}} \left|\mathbf{E}_{X\sim P}\,g(X) - \mathbf{E}_{Y\sim Q}\,g(Y)\right|$$

MMD

?

ϕ-divergences

Hellinger

KL

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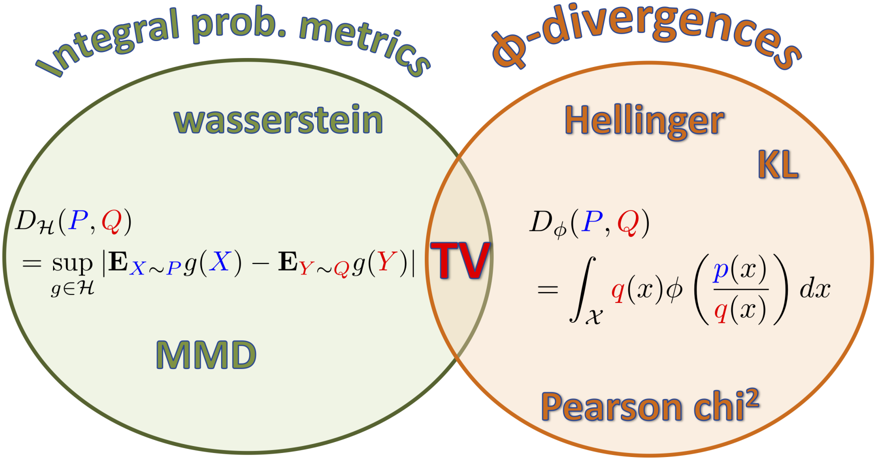
Pearson chi²

Divergences



Integral prob. metrics

ϕ-divergences

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KL

$$D_{\mathcal{H}}(P,Q) = \sup_{g\in\mathcal{H}} \left|\mathbf{E}_{X\sim P}\, g(X) - \mathbf{E}_{Y\sim Q}\, g(Y)\right|$$

TV

$$D_{\phi}(P,Q) = \int_{\mathcal{X}} q(x)\phi\left(\frac{p(x)}{q(x)}\right) dx$$

MMD

Pearson chi²

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

Two-Sample Testing with MMD

A statistical test using MMD

The empirical MMD:

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

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

A statistical test using MMD

The empirical MMD:

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

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 $P \neq Q$
  - should see $\widehat{MMD}^2$ "far from zero"

A statistical test using MMD

The empirical MMD:

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

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 $P \neq Q$
  - should see $\widehat{MMD}^2$ “far from zero”

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.
- $\sqrt{n} \times \widehat{MMD}^2 = 1.2$

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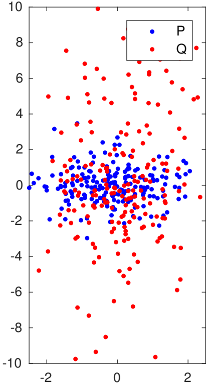

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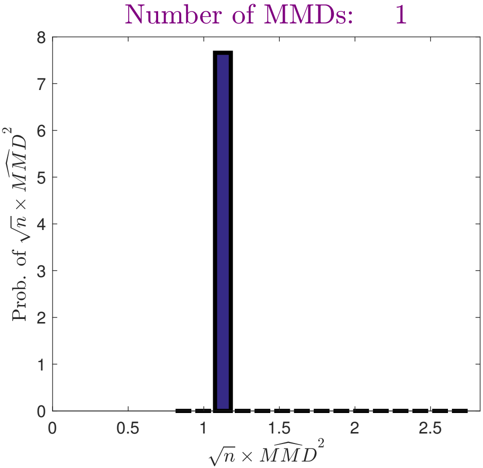
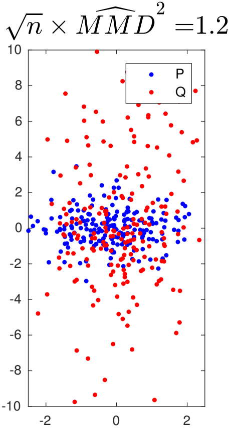
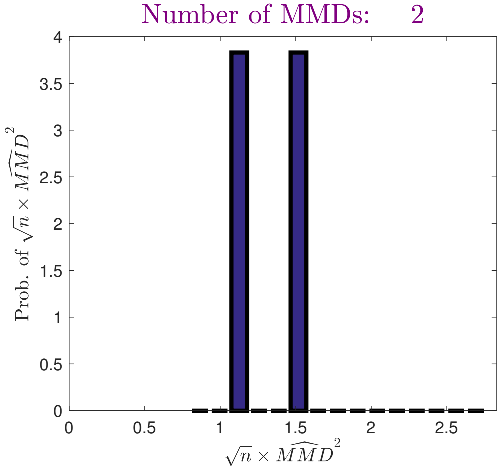


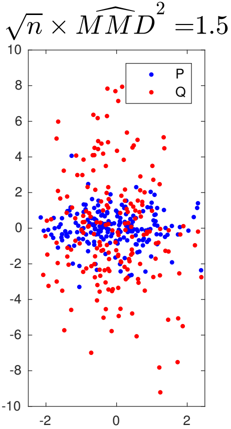


Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

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

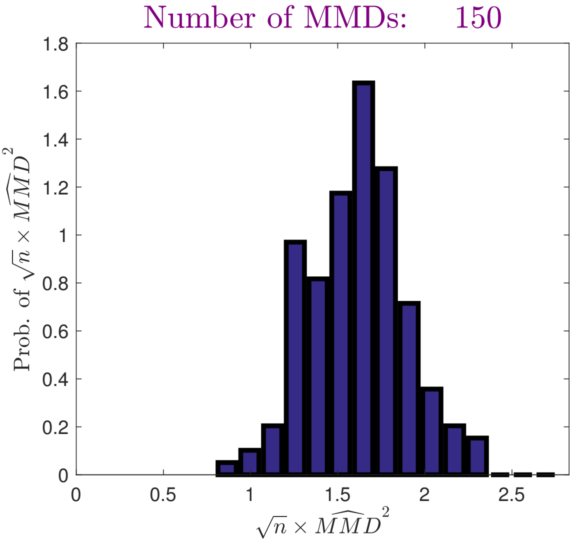
- Laplace with different y-variance.
- $\sqrt{n} \times \widehat{MMD}^2 = 1.5$





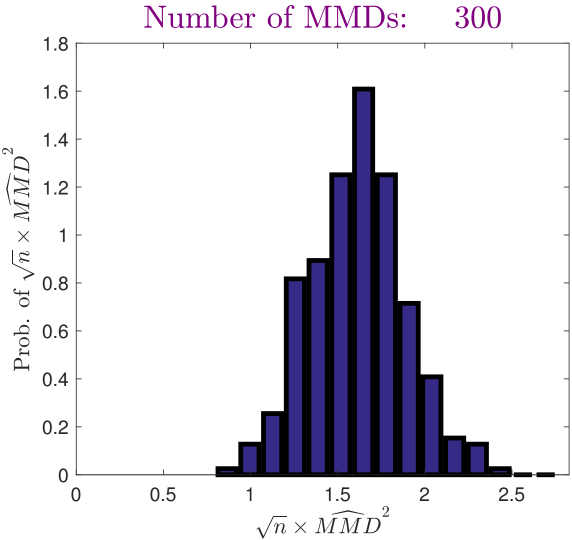
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 150 times . . .



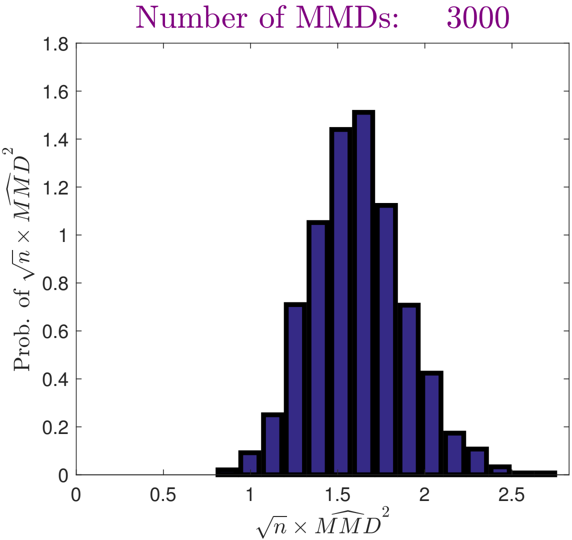
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 300 times . . .



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

Repeat this 3000 times ...

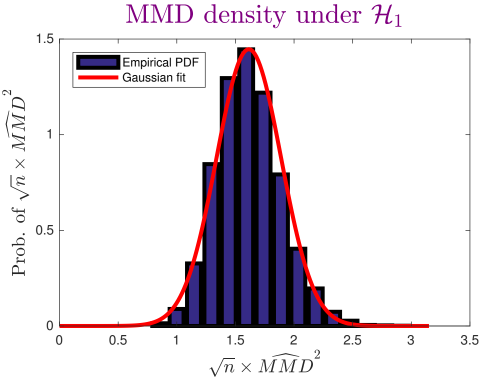


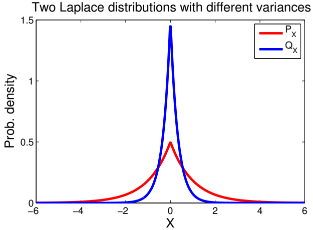
Asymptotics of $\widehat{MMD}^2$ when $P \neq Q$

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



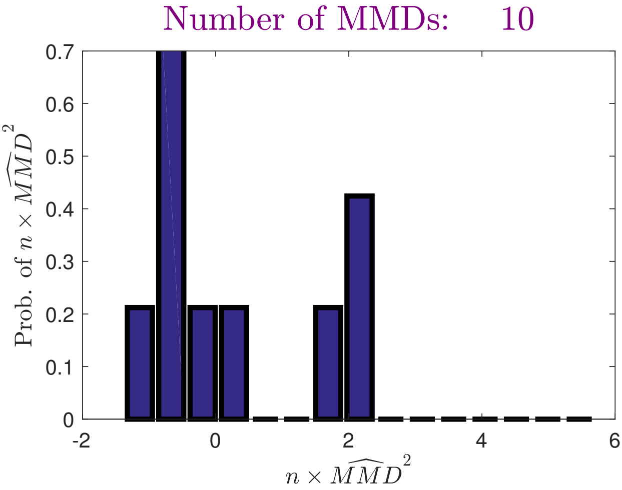


Behaviour of $\widehat{MMD}^2$ when $P = Q$

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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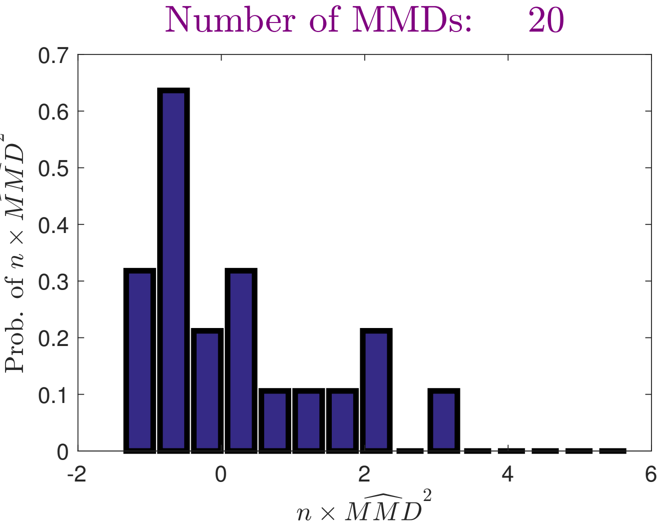

Behaviour of $\widehat{MMD}^2$ when $P = Q$

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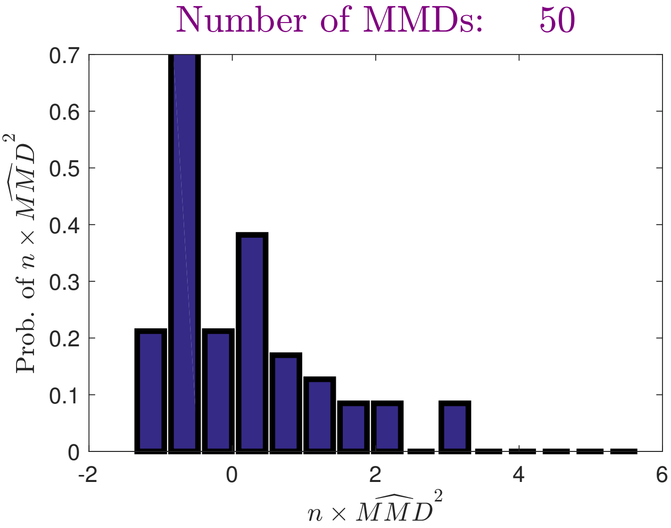

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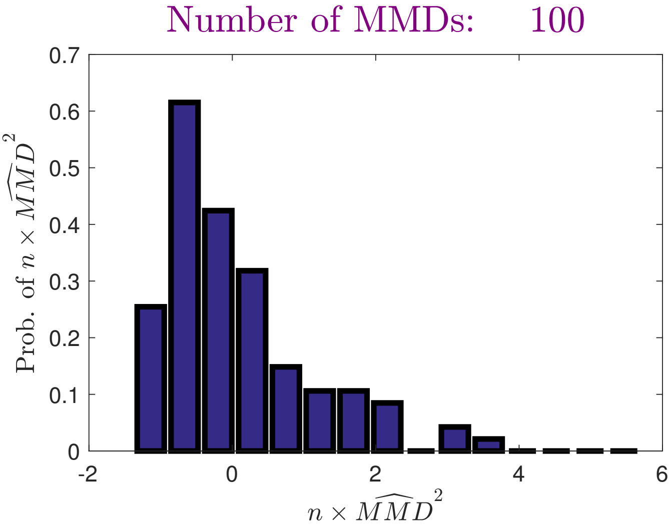

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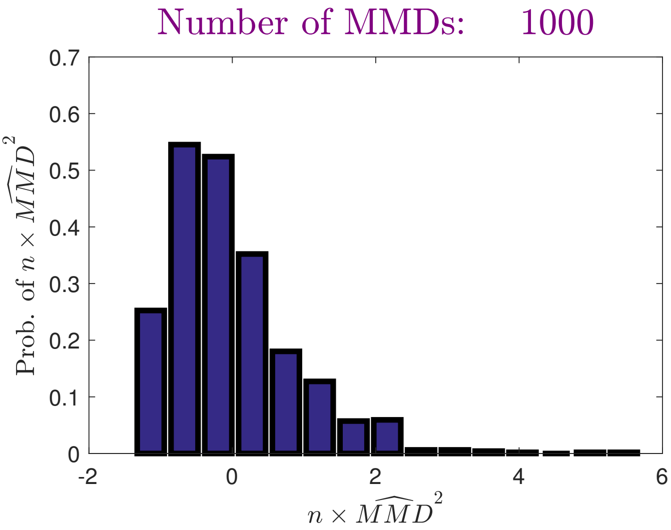
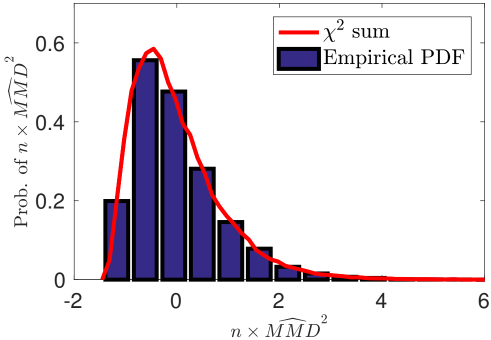


Asymptotics of $\widehat{MMD}^2$ when $P = Q$

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 $\mathcal{H}_0$



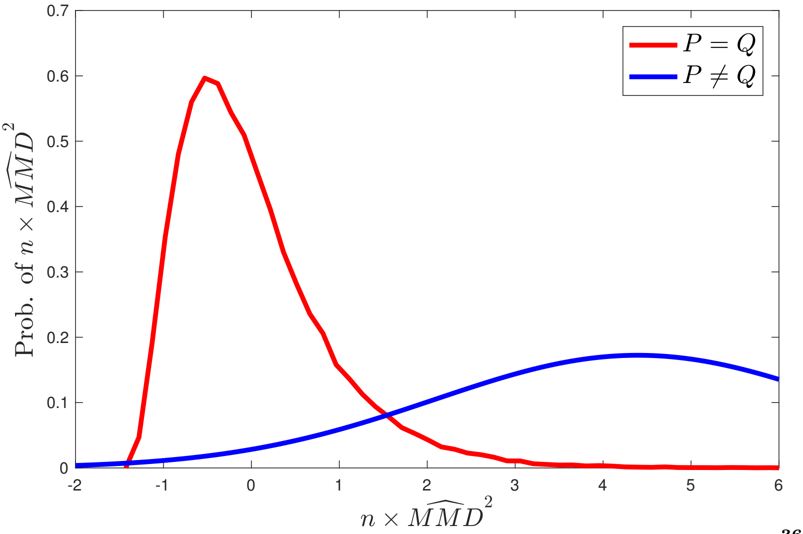
where

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

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

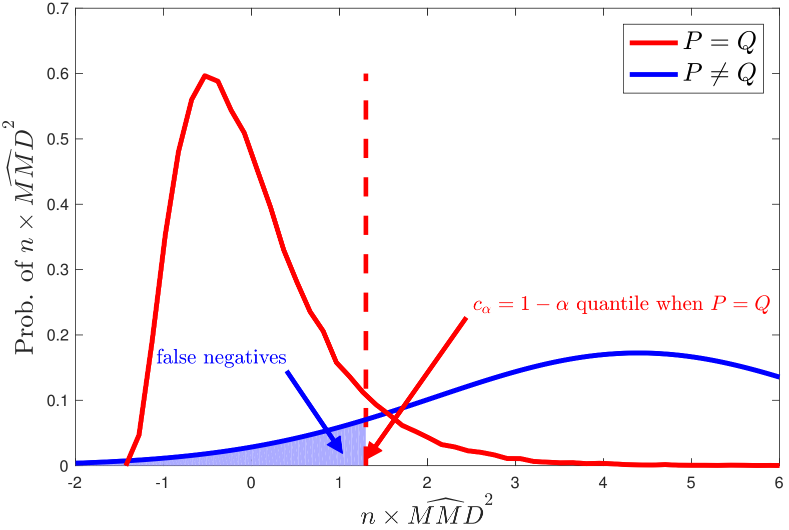
A statistical test

A summary of the asymptotics:



A statistical test

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



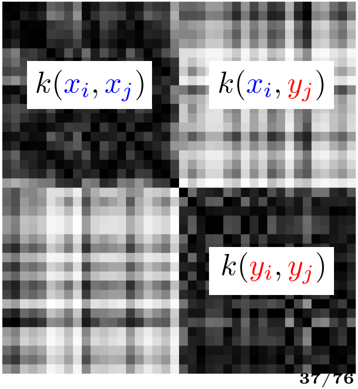
How do we get test threshold c_α?

Original empirical MMD for dogs and fish:

$X = [$ $\ldots]$

$Y = [$ $\ldots]$

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

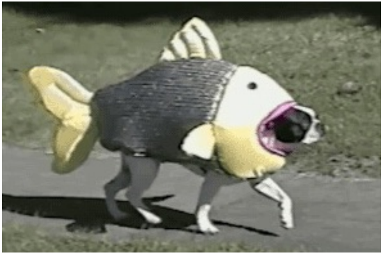


How do we get test threshold c_α?

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

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

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



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$\dots]$

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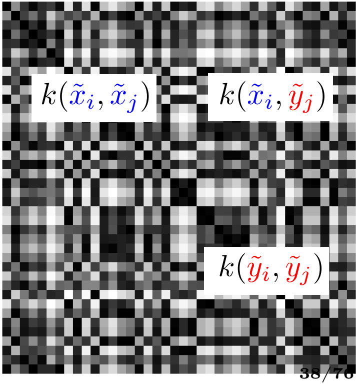

Permutation simulates

$P = Q$

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 → 1 as $n \to \infty$ for any (fixed) problem
  - But, for many P and Q, will have terrible power with reasonable n!

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!
- 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 → 1 as $n \to \infty$

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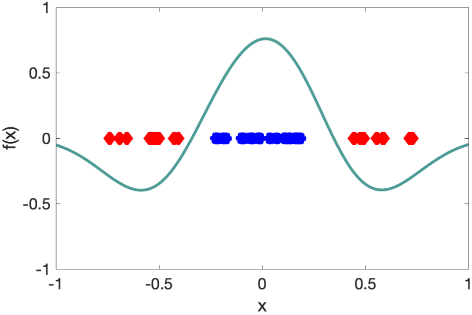

Choosing a kernel for the test

- Simple choice: exponentiated quadratic

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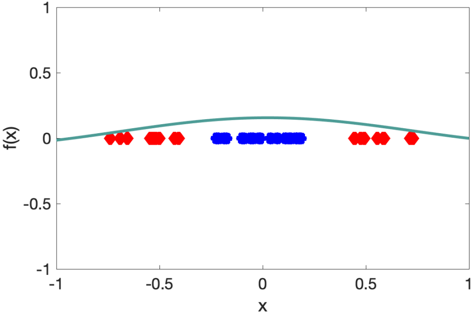

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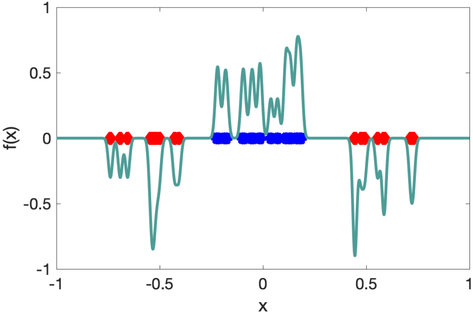

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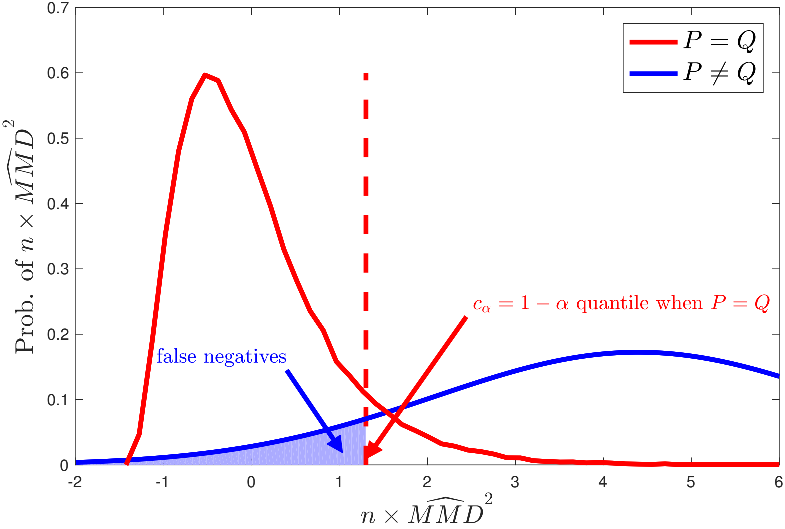
- *Characteristic:* for any σ: for any P and Q, power $\to 1$ as $n \to \infty$
- But choice of σ is very important for finite n...
- ...and some problems (e.g. images) might have no good choice for σ

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

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

$$
\begin{aligned}
&\mathrm{Pr}_1\left(n\widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha\right) \\
&\to \Phi\left(\frac{\mathrm{MMD}^2(P,Q)}{\sqrt{V_n(P,Q)}} - \frac{c_\alpha}{n\sqrt{V_n(P,Q)}}\right)
\end{aligned}
$$

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 $P \neq Q$):

$$\Pr_1\left(n\widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha\right)$$
$$\to \Phi\left(\underbrace{\frac{\mathrm{MMD}^2(P,Q)}{\sqrt{V_n(P,Q)}}}_{O(n^{1/2})} - \underbrace{\frac{c_\alpha}{n\sqrt{V_n(P,Q)}}}_{O(n^{-1/2})}\right)$$

For large n, second term negligible!

Optimizing kernel for test power

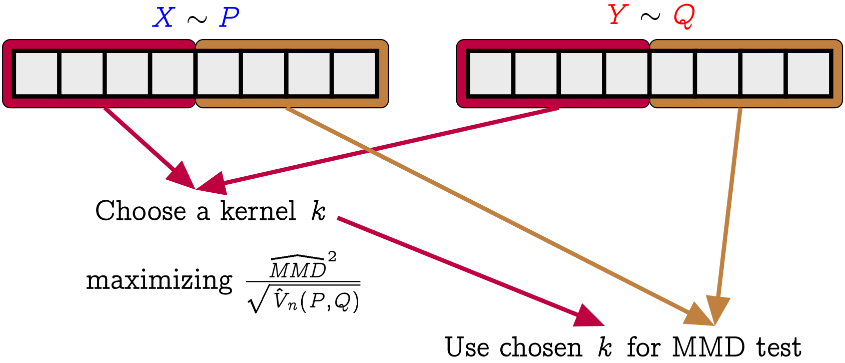
The power of our test ($\Pr_1$ denotes probability under $P \neq Q$):

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

To maximize test power, maximize

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

Data splitting



$X \sim P$

$Y \sim Q$

Choose a kernel k

maximizing $\frac{\widehat{MMD}^2}{\sqrt{\hat{V}_n(P,Q)}}$

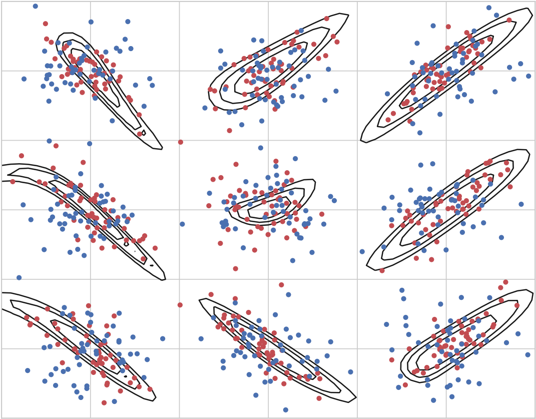
Use chosen k for MMD test

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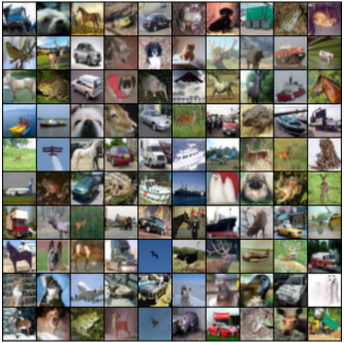
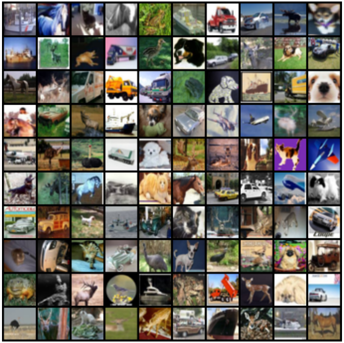
- CIFAR-10 vs CIFAR-10.1, **null rejected 75% of time**



CIFAR-10 test set (Krizhevsky 2009)

$X \sim P$



CIFAR-10.1 (Recht+ ICML 2019)

$Y \sim Q$

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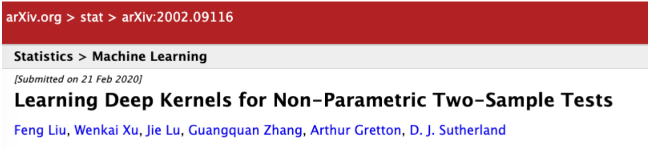


arXiv.org > stat > arXiv:2002.09116

Statistics > Machine Learning

[Submitted on 21 Feb 2020]

Learning Deep Kernels for Non-Parametric Two-Sample Tests

Feng Liu, Wenkai Xu, Jie Lu, Guangquan Zhang, Arthur Gretton, D. J. Sutherland

Accepted to ICML 2020

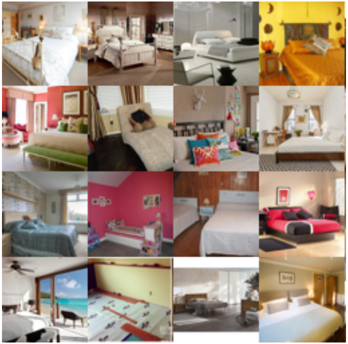
Questions?

- 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

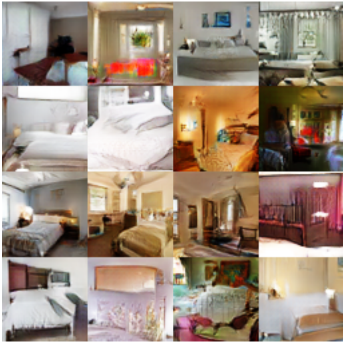
MMD for GAN training

Training implicit generative models

- **Have:** One collection of samples X from unknown distribution P.
- **Goal:** generate samples Q that look like P



LSUN bedroom samples P

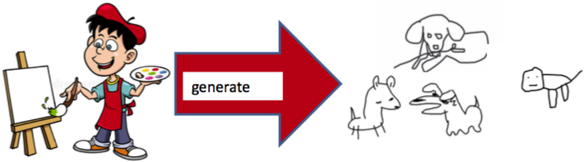


Generated Q, MMD GAN

Using a critic $D(P, Q)$ to train a GAN

(Binkowski, Sutherland, Arbel, G., ICLR 2018),
(Arbel, Sutherland, Binkowski, G., NeurIPS 2018)

Visual notation: GAN setting



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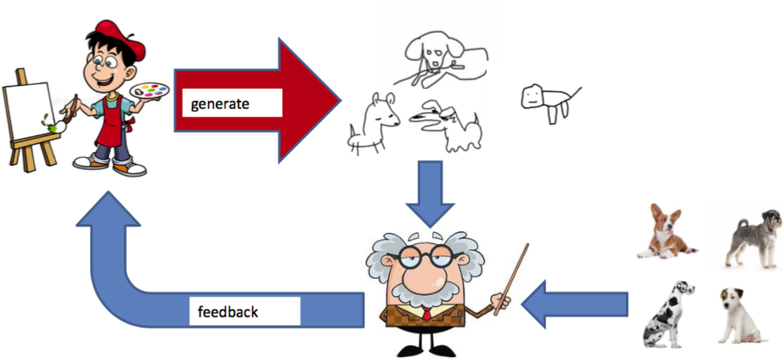
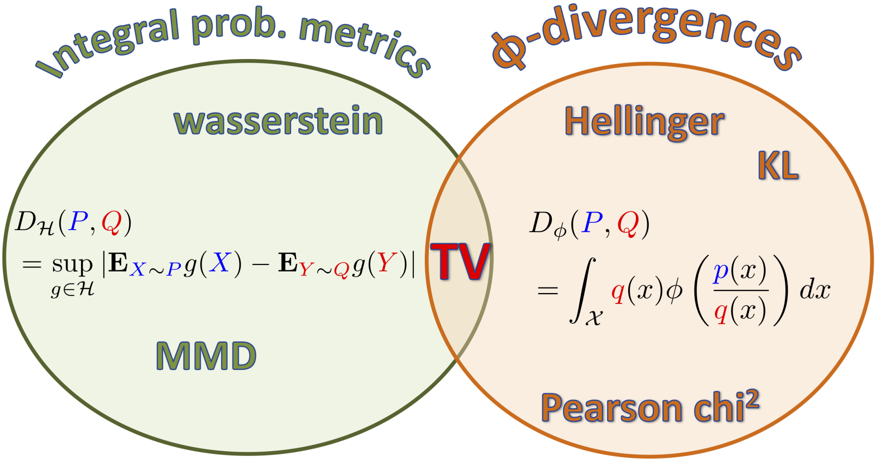


Critic functions



Integral prob. metrics

ϕ-divergences

wasserstein

$$D_{\mathcal{H}}(P, Q) = \sup_{g \in \mathcal{H}} \left| \mathbf{E}_{X \sim P} g(X) - \mathbf{E}_{Y \sim Q} g(Y) \right|$$

MMD

TV

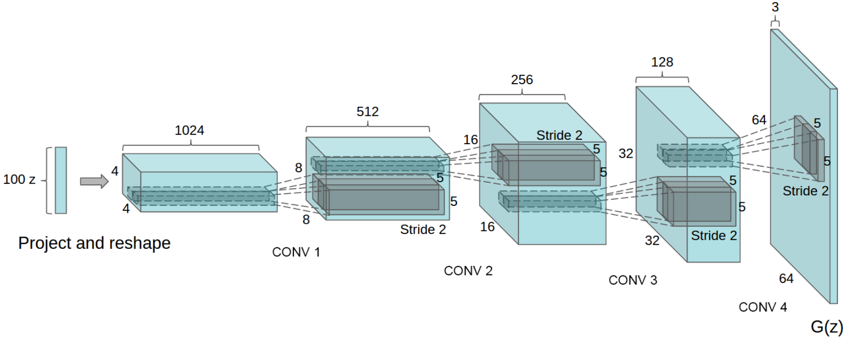
Hellinger

KL

$$D_{\phi}(P, Q) = \int_{\mathcal{X}} q(x) \phi\left(\frac{p(x)}{q(x)}\right) dx$$

Pearson chi²

What I *won't* cover: the generator



Radford, Metz, Chintala, ICLR 2016

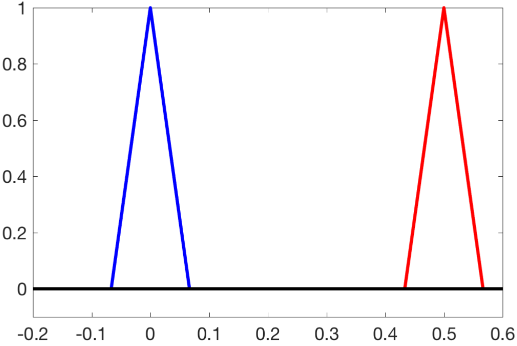
F-divergence as critic

An unhelpful critic? Jensen-Shannon,

Goodfellow et al. (NeurIPS 2014), Arjovsky and Bottou [ICLR 2017]

$$D_{JS}(P, Q) = \frac{1}{2} D_{KL}\left(p, \frac{p+q}{2}\right) + \frac{1}{2} D_{KL}\left(q, \frac{p+q}{2}\right)$$

$$D_{JS}(P, Q) = \log 2$$



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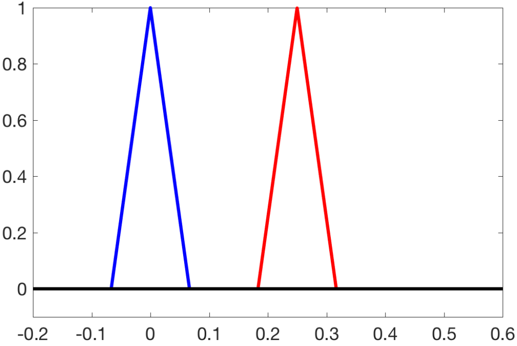

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What is done in practice?

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What is done in practice?

- Use a variational approximation to the critic, alternate generator and critic training Goodfellow et al. [NeurIPS 2014], Nowozin et al. [NeurIPS 2016]

F-divergence as critic

An unhelpful critic? Jensen-Shannon,

Goodfellow et al. (NeurIPS 2014), Arjovsky and Bottou [ICLR 2017]

$$D_{JS}(P, Q) = \frac{1}{2} D_{KL}\left(p, \frac{p+q}{2}\right) + \frac{1}{2} D_{KL}\left(q, \frac{p+q}{2}\right)$$

What is done in practice?

- Use a variational approximation to the critic, alternate generator and critic training Goodfellow et al. [NeurIPS 2014], Nowozin et al. [NeurIPS 2016]
- Add "instance noise" to the reference and generator observations Sonderby et al. [arXiv 2016], Arjovsky and Bottou [ICLR 2017]

F-divergence as critic

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- Add "instance noise" to the reference and generator observations Sonderby et al. [arXiv 2016], Arjovsky and Bottou [ICLR 2017]
  - ...or (approx. equivalently) a data-dependent gradient penalty for the variational critic Roth et al [NeurIPS 2017], Nagarajan and Kolter [NeurIPS 2017], Mescheder et al. [ICML 2018]

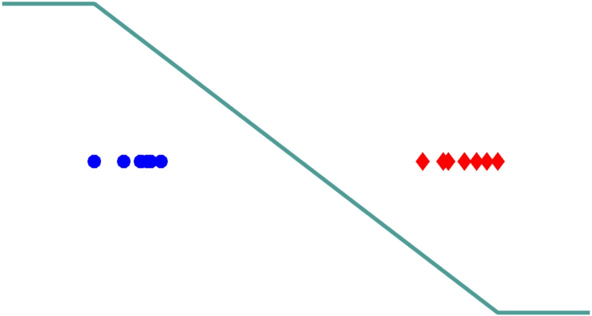
Wasserstein distance as critic

A helpful critic witness:

$$W_1(P, Q) = \sup_{\|f\|_L \le 1} E_P f(X) - E_Q f(Y).$$

$\|f\|_L := \sup_{x \neq y} |f(x) - f(y)| / \|x - y\|$

W_1=0.88



Santambrogio, Optimal Transport for Applied Mathematicians (2015, Section 5.4)

G Peyré, M Cuturi, Computational Optimal Transport (2019)

M. Cuturi, J. Solomon, NeurIPS tutorial (2017)

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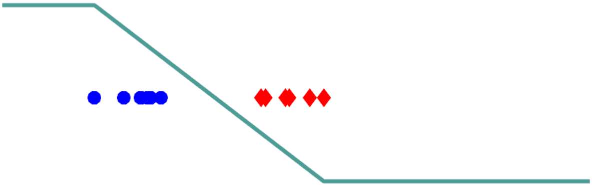

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MMD as critic

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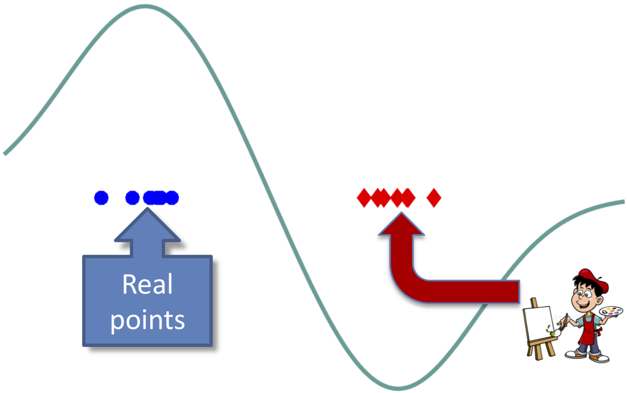
MMD=1.8

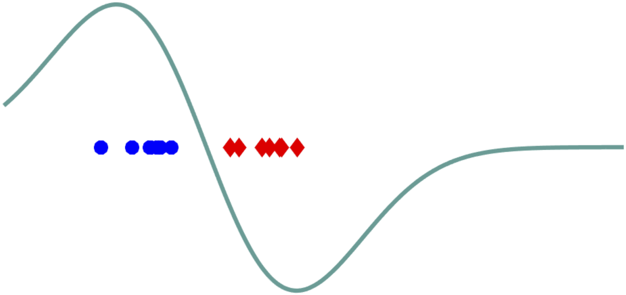


MMD as critic

A helpful critic witness:

$$MMD(P, Q) = \sup_{\|f\|_{\mathcal{F}} \leq 1} E_P f(X) - E_Q f(Y)$$

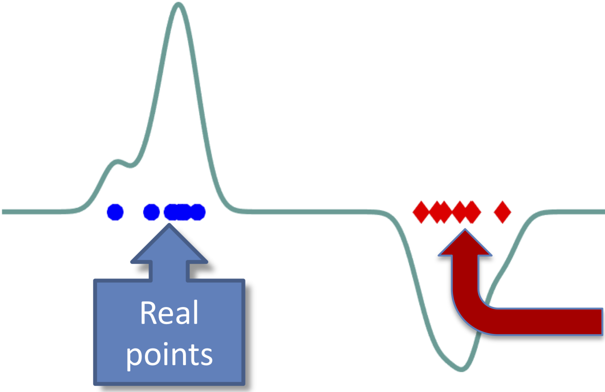
MMD=1.1



MMD as critic

An unhelpful critic witness:
$MMD(P, Q)$ with a narrow kernel.

MMD=0.64



Real points

MMD as critic

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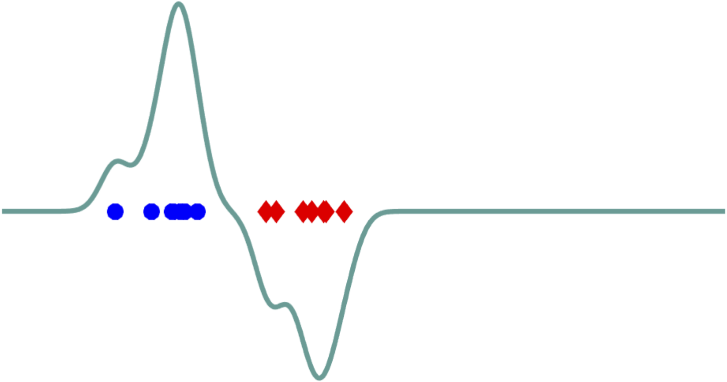
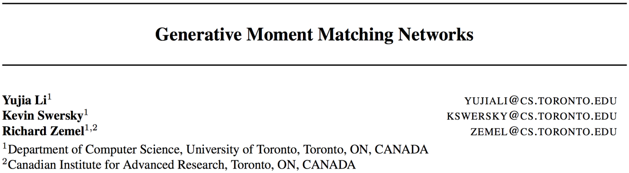


Gradient penalty: the regularisation viewpoint

MMD for GAN critic

Can you use MMD as a critic to train GANs?

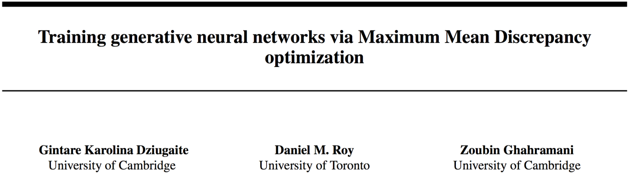
From ICML 2015:



Generative Moment Matching Networks

Yujia Li[1] YUJIALI@CS.TORONTO.EDU
Kevin Swersky[1] KSWERSKY@CS.TORONTO.EDU
Richard Zemel[1,2] ZEMEL@CS.TORONTO.EDU
[1]Department of Computer Science, University of Toronto, Toronto, ON, CANADA
[2]Canadian Institute for Advanced Research, Toronto, ON, CANADA

From UAI 2015:



Training generative neural networks via Maximum Mean Discrepancy optimization

Gintare Karolina Dziugaite
University of Cambridge

Daniel M. Roy
University of Toronto

Zoubin Ghahramani
University of Cambridge

MMD for GAN critic

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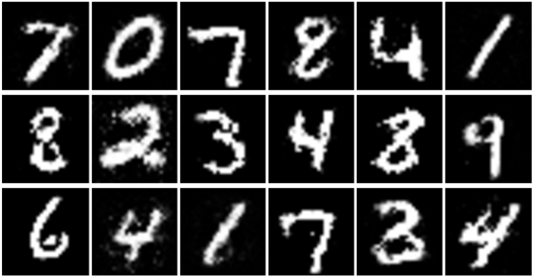
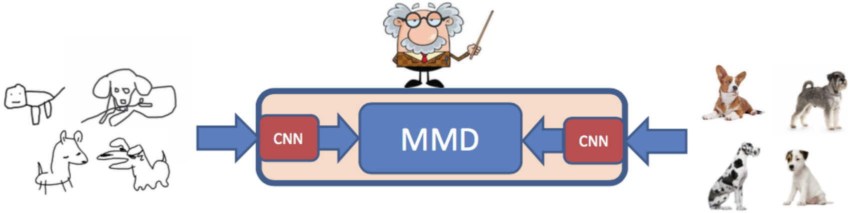


Need better image features.

CNN features for IPM witness functions

- Add convolutional features!
- The critic (teacher) also needs to be trained.



$\mathfrak{K}(x, y) = {h_\psi}^\top(x) h_\psi(y)$
where $h_\psi(x)$ is a CNN map:

- Wasserstein GAN Arjovsky et al. [ICML 2017]
- WGAN-GP Gulrajani et al. [NeurIPS 2017]

$\mathfrak{K}(x, y) = k(h_\psi(x), h_\psi(y))$
where $h_\psi(x)$ is a CNN map,
k is e.g. an exponentiated quadratic kernel

MMD Li et al., [NeurIPS 2017]
Cramer Bellemare et al. [2017]
Coulomb Unterthiner et al., [ICLR 2018]
Demystifying MMD GANs Binkowski, Sutherland, Arbel, G., [ICLR 2018]

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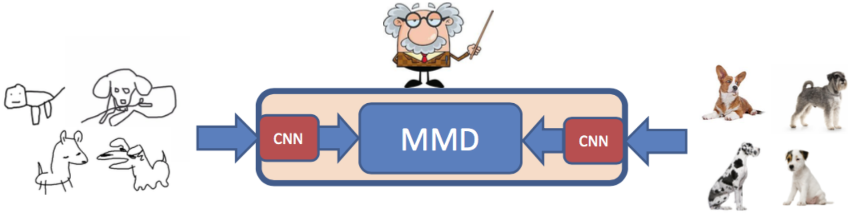

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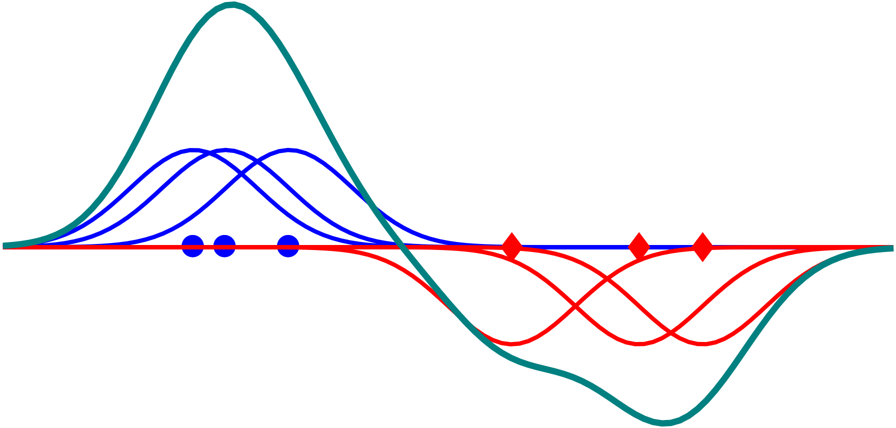
Witness function, kernels on deep features

Reminder: witness function,

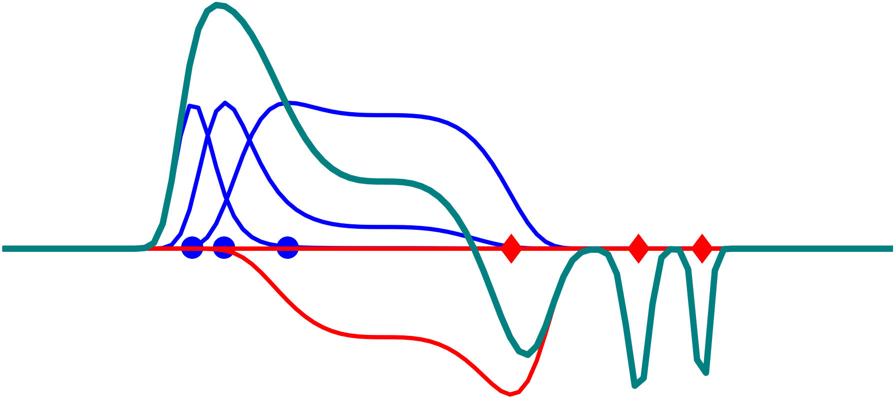
$k(x,y)$ is exponentiated quadratic



Witness function, kernels on deep features

Reminder: witness function,

$k(h_\psi(x), h_\psi(y))$ with nonlinear h_ψ and exp. quadratic k



Challenges for learned critic features

Learned critic features:

MMD with kernel $k(h_\psi(x), h_\psi(y))$ must give useful gradient to generator.

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If the MMD with kernel $k(h_\psi(x), h_\psi(y))$ gives a powerful test, will it be a good critic?

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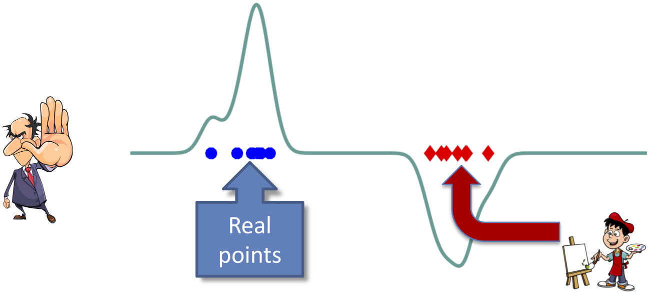
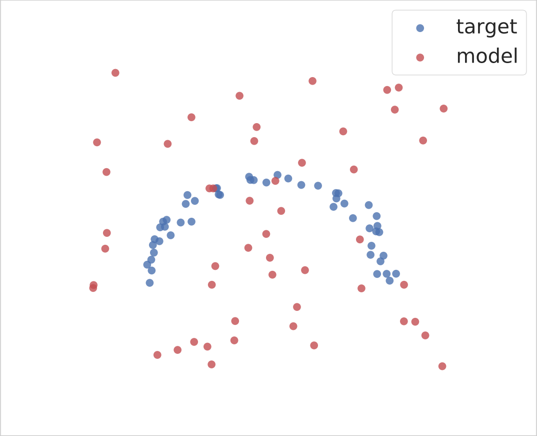


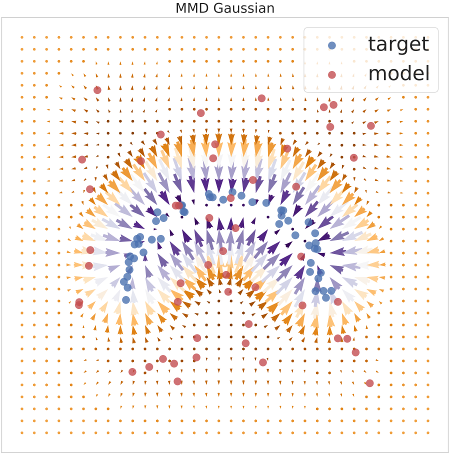
A simple 2-D example

Samples from target P and model Q



A simple 2-D example

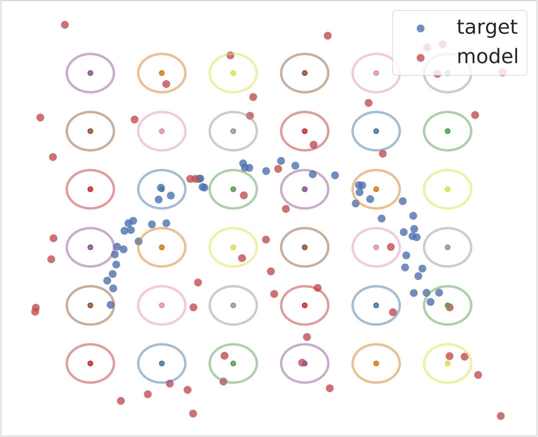
Witness gradient, MMD with exp. quad. kernel $k(x, y)$



A simple 2-D example

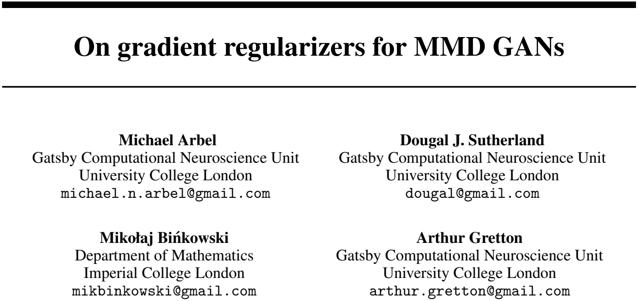
What the kernels $k(x, y)$ look like

MMD Gaussian



A data-adaptive gradient penalty: NeurIPS 2018

- New gradient regulariser Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
- Also related to Sobolev GAN Mroueh et al. [ICLR 2018]



On gradient regularizers for MMD GANs

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Dougal J. Sutherland
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Mikołaj Bińkowski
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Arthur Gretton
Gatsby Computational Neuroscience Unit
University College London
arthur.gretton@gmail.com

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- New gradient regulariser Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
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Maximise scaled MMD over critic features:

$$SMMD(P, \lambda) = \sigma_{P,\lambda} \; MMD$$

where

$$\sigma^2_{P,\lambda} = \lambda + \int k(h_\psi(x), h_\psi(x)) dP(x) + \sum_{i=1}^{d} \int \partial_i \partial_{i+d} k(h_\psi(x), h_\psi(x)) \; dP(x)$$

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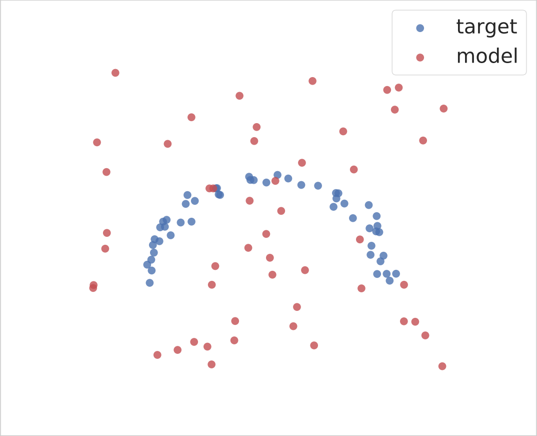
Idea: rather than regularise the critic or witness function, regularise features directly

Simple 2-D example revisited

Samples from target P and model Q



Simple 2-D example revisited

Use kernels $k(h_\psi(x), h_\psi(y))$ with features

$$h_\psi(x) = L_3\left(\begin{bmatrix} x \\ L_2(L_1(x)) \end{bmatrix}\right)$$

where L_1, L_2, L_3 are fully connected with quadratic nonlinearity.

Simple 2-D example revisited

Witness gradient, maximise $SMMD(P, \lambda)$
to learn $h_\psi(x)$ for $k(h_\psi(x), h_\psi(y))$

vector field movie, use Acrobat Reader to play

Simple 2-D example revisited

What the kenels $k(h_\psi(x), h_\psi(y))$ look like

isolines movie, use Acrobat Reader to play

Our empirical observations

Data-adaptive critic loss:

- Witness function class for $SMMD(P, \lambda)$ depends on P.
  - Without data-dependent regularisation, maximising MMD over features h_ψ of kernel $k(h_\psi(x), h_\psi(y))$ can be unhelpful.
  - WGAN-GP is a pretty good data-dependent regularisation strategy
- Similar regularisation strategies apply to variational form in f-GANs

  Roth et al [NeurIPS 2017, eq. 19 and 20]

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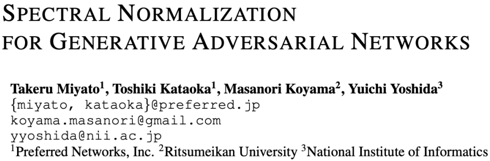
Roth et al [NeurIPS 2017, eq. 19 and 20]

Alternate critic and generator training:

- Weaker critics can give better signals to poor (early stage) generators.
- Incomplete training of the critic is also a regularisation strategy

Don’t *just* use gradient regularizers!

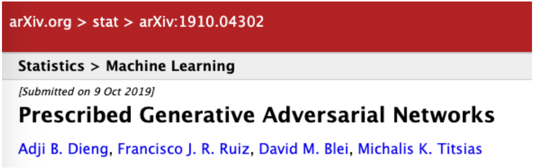
Spectral norm regularizer (effectively smooths critic class; ICLR 2018):



SPECTRAL NORMALIZATION
FOR GENERATIVE ADVERSARIAL NETWORKS

Takeru Miyato[1], Toshiki Kataoka[1], Masanori Koyama[2], Yuichi Yoshida[3]
{miyato, kataoka}@preferred.jp
koyama.masanori@gmail.com
yyoshida@nii.ac.jp
[1]Preferred Networks, Inc. [2]Ritsumeikan University [3]National Institute of Informatics

Entropic regularizer (avoid mode collapse):



arXiv.org > stat > arXiv:1910.04302

Statistics > Machine Learning

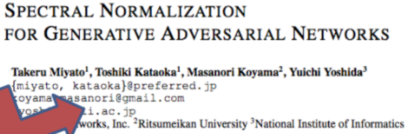
[Submitted on 9 Oct 2019]

Prescribed Generative Adversarial Networks

Adji B. Dieng, Francisco J. R. Ruiz, David M. Blei, Michalis K. Titsias

Evaluation and experiments

Benchmarks for comparison (all from ICLR 2018)



SPECTRAL NORMALIZATION FOR GENERATIVE ADVERSARIAL NETWORKS

Takeru Miyato[1], **Toshiki Kataoka**[1], **Masanori Koyama**[2], **Yuichi Yoshida**[3]
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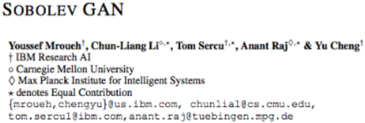
oyama masanori@gmail.com
yos i.ac.jp
works, Inc. [2]Ritsumeikan University [3]National Institute of Informatics

We combine with scaled MMD



SOBOLEV GAN

Youssef Mroueh†, **Chun-Liang Li**◦,⋆, **Tom Sercu**†,⋆, **Anant Raj**◊,⋆ **& Yu Cheng**†
† IBM Research AI
◦ Carnegie Mellon University
◊ Max Planck Institute for Intelligent Systems
⋆ denotes Equal Contribution
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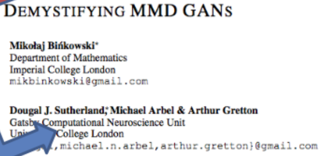
tom.sercu1@ibm.com,anant.raj@tuebingen.mpg.de



DEMYSTIFYING MMD GANS

Mikołaj Bińkowski*
Department of Mathematics
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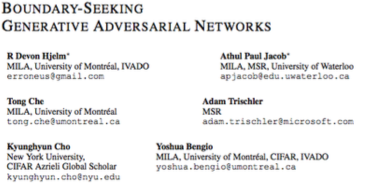
Dougal J. Sutherland,* Michael Arbel & Arthur Gretton
Gatsb Computational Neuroscience Unit
Uni College London
,michael.n.arbel,arthur.gretton}@gmail.com

Our ICLR 2018 paper



BOUNDARY-SEEKING GENERATIVE ADVERSARIAL NETWORKS

R Devon Hjelm*
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Tong Che
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Adam Trischler
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Yoshua Bengio
MILA, University of Montréal, CIFAR, IVADO
yoshua.bengio@umontreal.ca

Results: unconditional imagenet 64×64

KID scores:

- BGAN: 47
- SN-GAN: 44
- SMMD GAN: 35

ILSVRC2012 (ImageNet) dataset, 1 281 167 images, resized to 64 × 64. 1000 classes.

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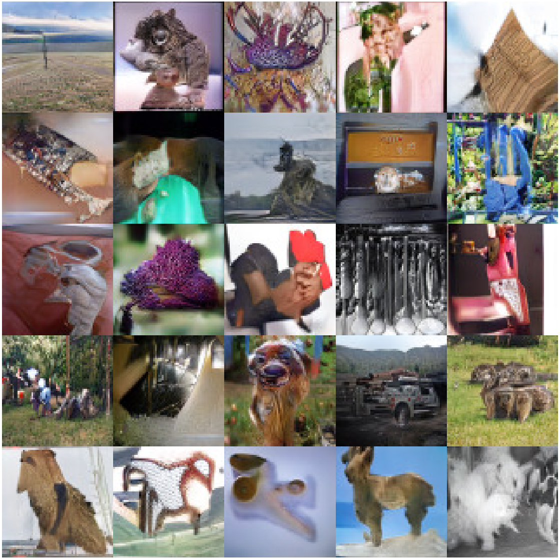

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Summary

- GAN critics rely on two sources of regularisation
  - Regularisation by incomplete training
  - Data-dependent gradient regulariser
- Some advantages of hybrid kernel/neural features:
  - MMD loss still a valid critic when features not optimal (unlike WGAN-GP)
  - Kernel features do some of the "work", so simpler h_ψ features possible.

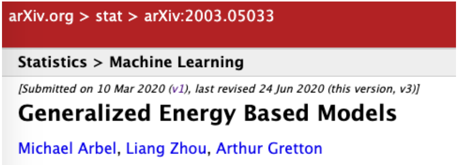
"Demystifying MMD GANs," including KID score, ICLR 2018:

https://github.com/mbinkowski/MMD-GAN

Gradient regularised MMD, NeurIPS 2018:

https://github.com/MichaelArbel/Scaled-MMD-GAN

Post-credit scene: Generalised Energy-Based Models



arXiv.org > stat > arXiv:2003.05033

Statistics > Machine Learning

[Submitted on 10 Mar 2020 (v1), last revised 24 Jun 2020 (this version, v3)]

Generalized Energy Based Models

Michael Arbel, Liang Zhou, Arthur Gretton

https://github.com/MichaelArbel/GeneralizedEBM

Linear vs nonlinear kenels

- Critic features from DCGAN: an f-filter critic has f, $2f$, $4f$ and $8f$ convolutional filters in layers 1-4. LSUN 64 × 64.

$k(h_\psi(x), h_\psi(y))$, $f = 64$, KID=3

${h_\psi}^\top(x)h_\psi(y)$, $f = 64$, KID=4

Linear vs nonlinear kenels

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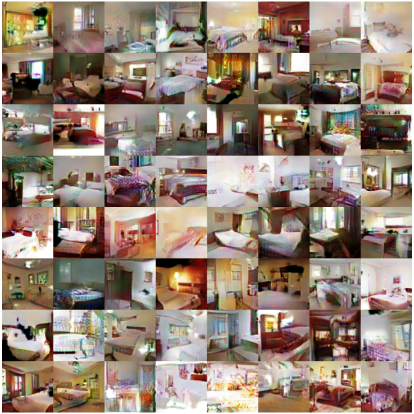
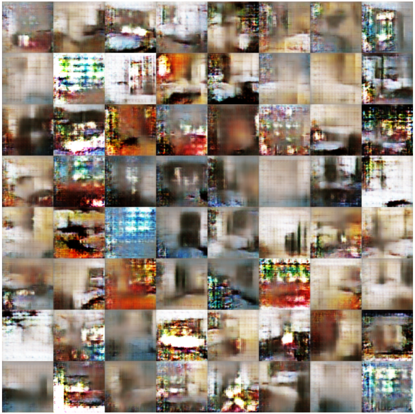


$k(h_\psi(x), h_\psi(y))$, $f = 16$, KID=9



${h_\psi}^\top(x) h_\psi(y)$, $f = 16$, KID=37

Evaluation of GANs

The inception score? Salimans et al. [NeurIPS 2016]

Based on the classification output $p(y|x)$ of the inception model Szegedy et al. [ICLR 2014],

$$E_X \exp KL(P(y|X)\|P(y)).$$

High when:

- predictive label distribution $P(y|x)$ has low entropy (good quality images)
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Problem: relies on a trained classifier! Can't be used on new categories (celeb, bedroom...)

Evaluation of GANs

The Frechet inception distance? Heusel et al. [NeurIPS 2017]

Fits Gaussians to features in the inception architecture (pool3 layer):

$$FID(P, Q) = \|\mu_P - \mu_Q\|^2 + \text{tr}(\Sigma_P) + \text{tr}(\Sigma_Q) - 2\text{tr}\left((\Sigma_P \Sigma_Q)^{\frac{1}{2}}\right)$$

where μ_P and Σ_P are the feature mean and covariance of P

Evaluation of GANs

The Frechet inception distance? Heusel et al. [NeurIPS 2017]

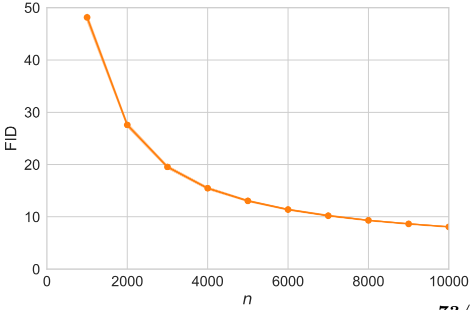
Fits Gaussians to features in the inception architecture (pool3 layer):

$$FID(P, Q) = \|\mu_P - \mu_Q\|^2 + \mathrm{tr}(\Sigma_P) + \mathrm{tr}(\Sigma_Q) - 2\mathrm{tr}\left((\Sigma_P \Sigma_Q)^{\frac{1}{2}}\right)$$

where μ_P and Σ_P are the feature mean and covariance of P

Problem: **bias**. For finite samples can consistently give incorrect answer.

- Bias demo, CIFAR-10 train vs test



Evaluation of GANs

The FID can give the wrong answer in theory.

Assume m samples from P and $n \to \infty$ samples from Q.

Given two alternatives:

$$P_1 \sim \mathcal{N}(0, (1 - m^{-1})^2) \qquad P_2 \sim \mathcal{N}(0, 1) \qquad Q \sim \mathcal{N}(0, 1).$$

Clearly,

$$FID(P_1, Q) = \frac{1}{m^2} > FID(P_2, Q) = 0$$

Given m samples from P_1 and P_2,

$$FID(\widehat{P_1}, Q) < FID(\widehat{P_2}, Q).$$

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Evaluation of GANs

The FID can give the wrong answer in practice.

Let $d = 2048$, and define

$$P_1 = \text{relu}(\mathcal{N}(\mathbf{0}, I_d)) \quad P_2 = \text{relu}(\mathcal{N}(\mathbf{1}, .8\Sigma + .2I_d)) \qquad Q = \text{relu}(\mathcal{N}(\mathbf{1}, I_d))$$

where $\Sigma = \frac{4}{d}CC^T$, with C a $d \times d$ matrix with iid standard normal entries.

For a random draw of C:

$$FID(P_1, Q) \approx 1123.0 > 1114.8 \approx FID(P_2, Q)$$

With $m = 50\,000$ samples,

$$FID(\widehat{P_1}, Q) \approx 1133.7 < 1136.2 \approx FID(\widehat{P_2}, Q)$$

At $m = 100\,000$ samples, the ordering of the estimates is correct.

This behavior is similar for other random draws of C.

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The kernel inception distance (KID)

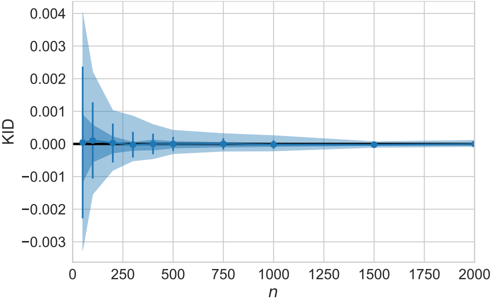
The Kernel inception distance Binkowski, Sutherland, Arbel, G. [ICLR 2018]

Measures similarity of the samples' representations in the inception architecture (pool3 layer)

MMD with kernel

$$k(x, y) = \left(\frac{1}{d} x^\top y + 1\right)^3 .$$

- Checks match for feature means, variances, skewness
- Unbiased : eg CIFAR-10 train/test



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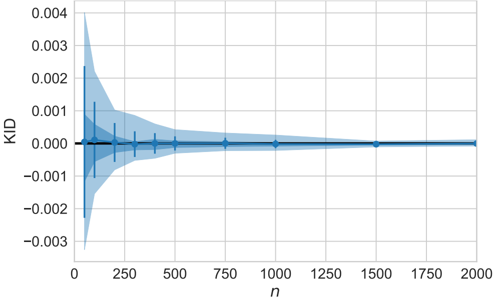

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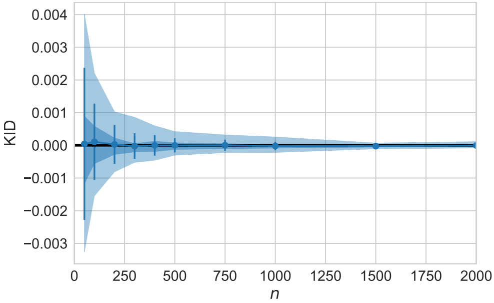

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"Block" KID implementation is cheaper than FID: see paper (or use Tensorflow implementation)!

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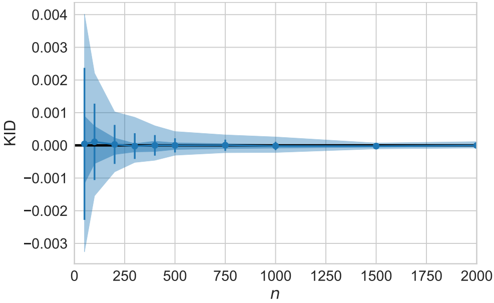

Also used for automatic learning rate adjustment: if $KID(\widehat{P}_{t+1}, Q)$ not significantly better than $KID(\widehat{P}_t, Q)$ then reduce learning rate.

[Bounliphone et al. ICLR 2016]

Related: "An empirical study on evaluation metrics of generative adversarial networks", Xu et al. [arxiv, June 2018]