The maximum mean discrepancy and Generative Adversarial Networks

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MLSS Moscow, 2019

A motivation: comparing two samples

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

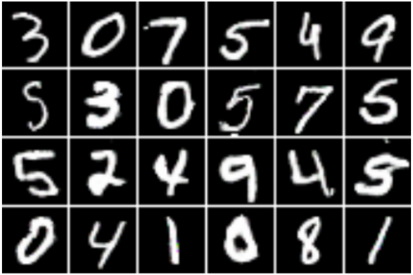
$$\sim P$$

$$\sim Q$$

A real-life example: two-sample tests

- **Have:** Two collections of samples X, Y from unknown distributions P and Q.
- **Goal:** do P and Q differ?

MNIST samples



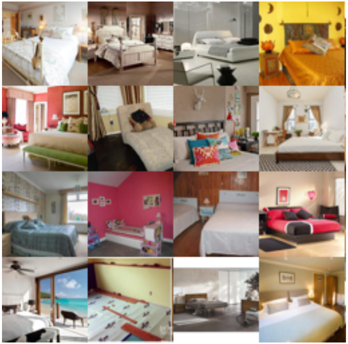
Samples from a GAN

Significant difference in GAN and MNIST?

T. Salimans, I. Goodfellow, W. Zaremba, V. Cheung, A. Radford, Xi Chen, NeurIPS 2016
Sutherland, Tung, Strathmann, De, Ramdas, Smola, G., ICLR 2017.

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)

Training generative models

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The Guardian

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A portrait created by AI just sold for $432,000. But is it really art?

An image of Edmond de Belamy, created by a computer, has just been sold at Christie's. But no algorithm can capture our complex human consciousness

1,085 455

▲ Portrait of Edmond Bellamy at Christie's in New York. Photograph: Timothy A Clary/AFP/Getty Images

Outline

- Measures of distance between distributions...
  - Difference in feature means
  - Integral probability metrics (not just a technicality!)

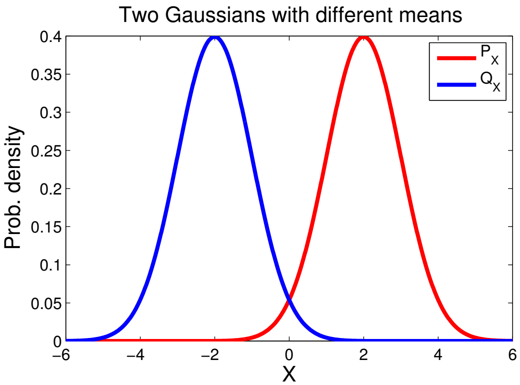
- Statistical testing for evaluating GAN quality

- GAN critic design
  - Gradient regularisation and data adaptivity
  - Evaluating GAN performance? Problems with Inception and FID.

Differences in distributions

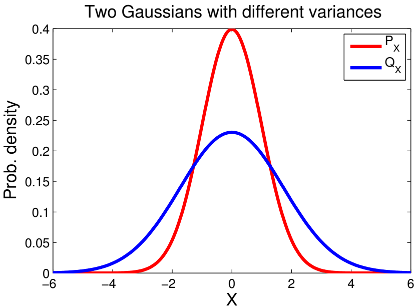
Feature mean difference

- 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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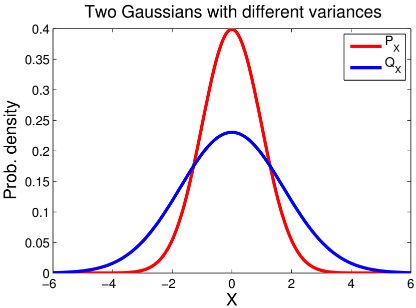
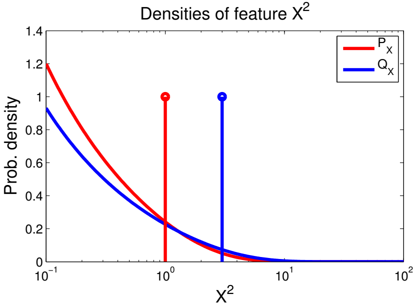
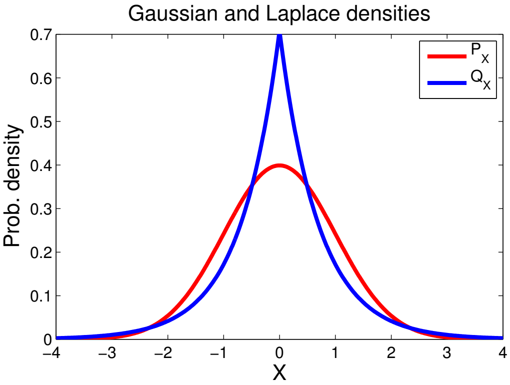




Feature mean difference

- 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!

Infinitely many features using kernels

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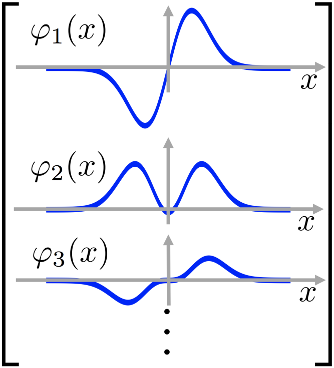
Exponentiated quadratic kernel

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

$$\varphi(x) =$$



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

The maximum mean discrepancy

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

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

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

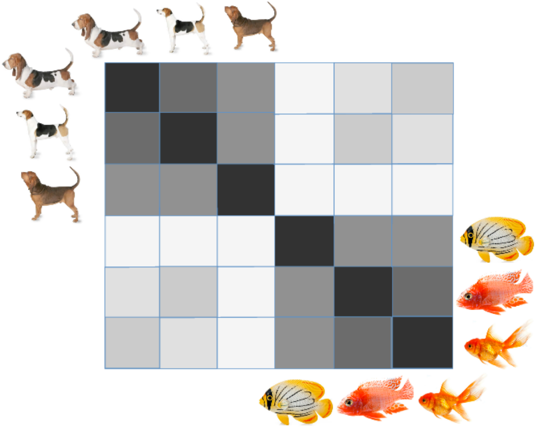
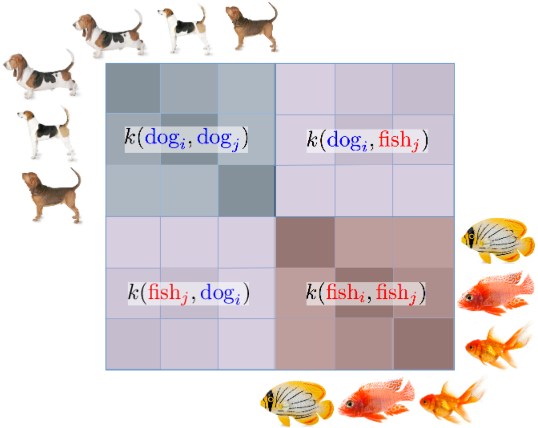


Illustration of MMD

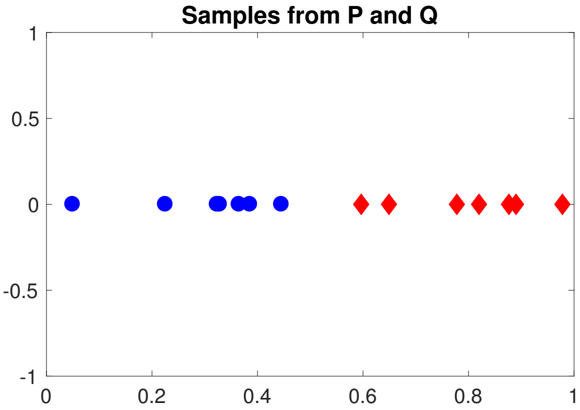
The maximum mean discrepancy:

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



Integral probability metrics

Are P and Q different?



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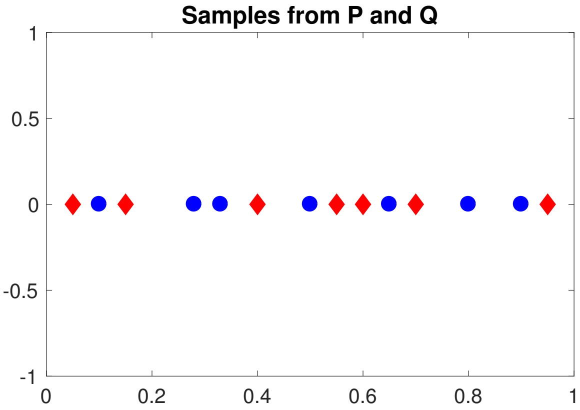
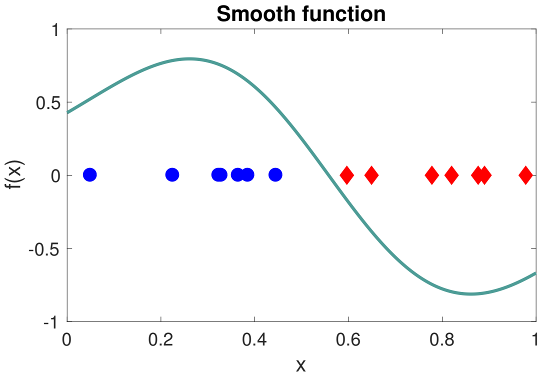


Integral probability metrics

Integral probability metric:

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

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



MMD as an integral probability metric

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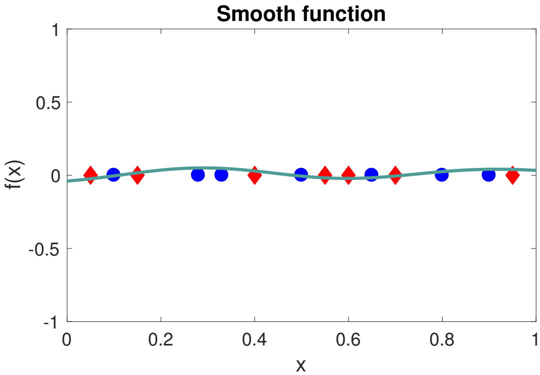
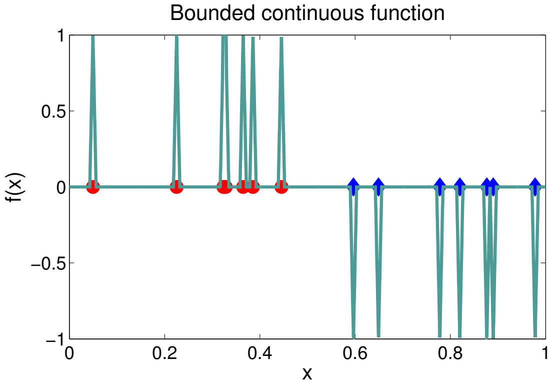


MMD as an integral probability metric

What if the function is not well behaved?

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



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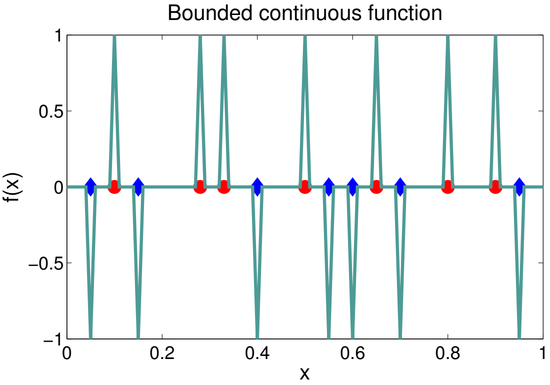

MMD as an integral probability metric

Maximum mean discrepancy: smooth function for P vs Q

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

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

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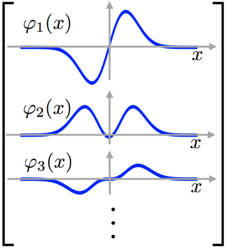
(F = unit ball in RKHS $\mathcal{F}$)

Functions are linear combinations of features:

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



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

MMD as an integral probability metric

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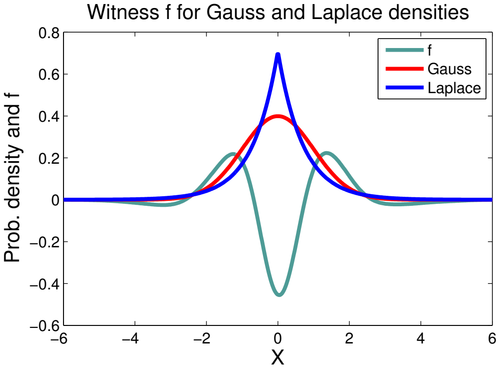

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$$(F = \text{unit ball in RKHS } \mathcal{F})$$

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]
- 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

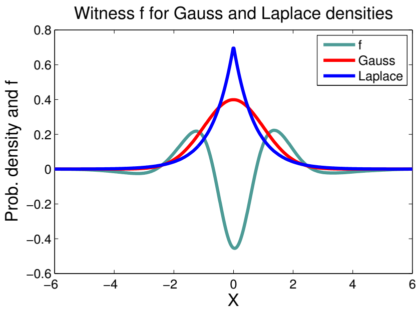
$$\mathbf{E}_P(f(X)) = \langle f, \mathbf{E}_P \varphi(X) \rangle_{\mathcal{F}} = \langle f, \mu_P \rangle_{\mathcal{F}}$$

(always true if kernel is bounded)

Integral prob. metric vs feature difference

The MMD:

$$MMD(P, Q; F) = \sup_{f \in F} \left[\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y) \right]$$



Integral prob. metric vs feature difference

The MMD:

use

$$MMD(P, Q; F)$$

$$= \sup_{f \in F} \left[\mathbf{E}_P f(X) - \mathbf{E}_Q f(Y)\right]$$

$$= \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}}$$

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

Integral prob. metric vs feature difference

The MMD:

$$MMD(P, Q; F)$$
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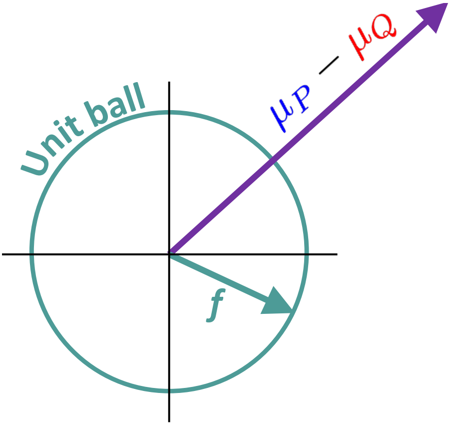

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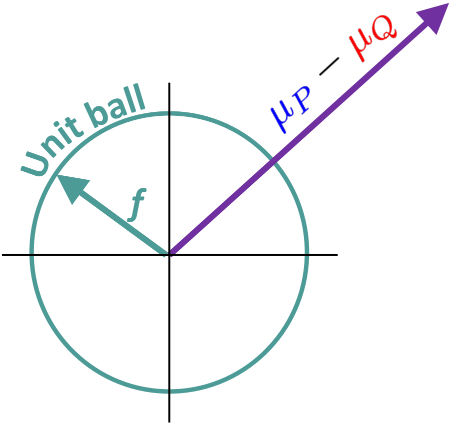

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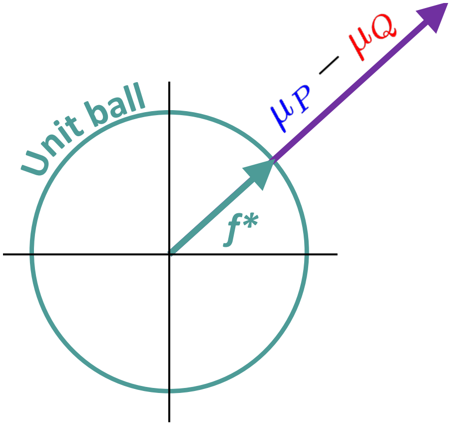

$$f^* = \frac{\mu_P - \mu_Q}{\|\mu_P - \mu_Q\|}$$

Integral prob. metric vs feature difference

The MMD:

$$
\begin{aligned}
& MMD(P, Q; F) \\
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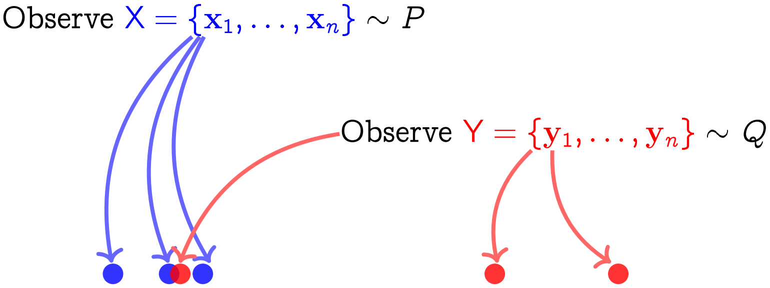
&= \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_{\mathcal{F}} \\
&= \| \mu_P - \mu_Q \|
\end{aligned}
$$

Function view and feature view equivalent
(kernel case only)

Construction of MMD witness

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



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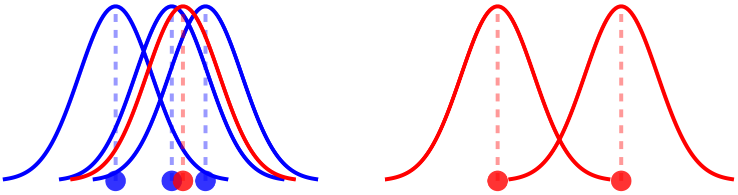

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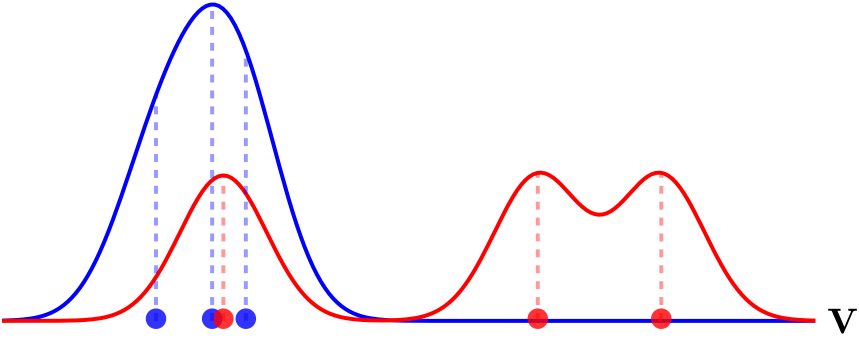

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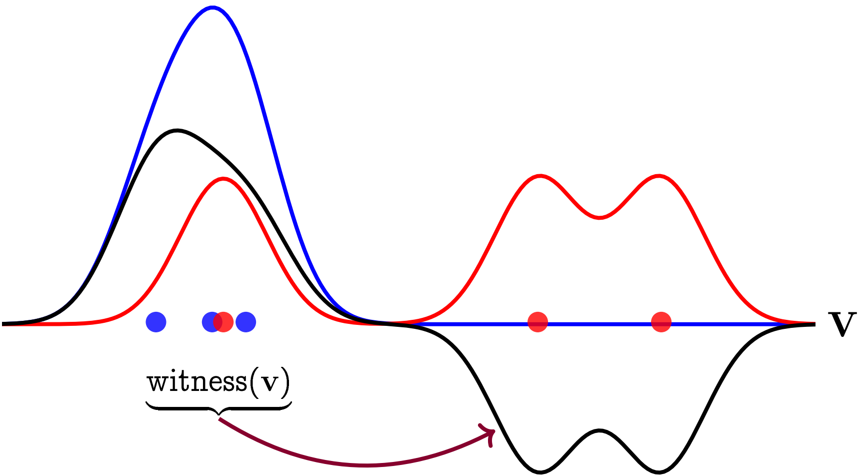

Derivation of empirical witness function

Recall the witness function expression

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

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The empirical feature mean for P

$$\widehat{\mu}_P := \frac{1}{n}\sum_{i=1}^{n} \varphi(x_i)$$

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

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Derivation of empirical witness function

Recall the witness function expression

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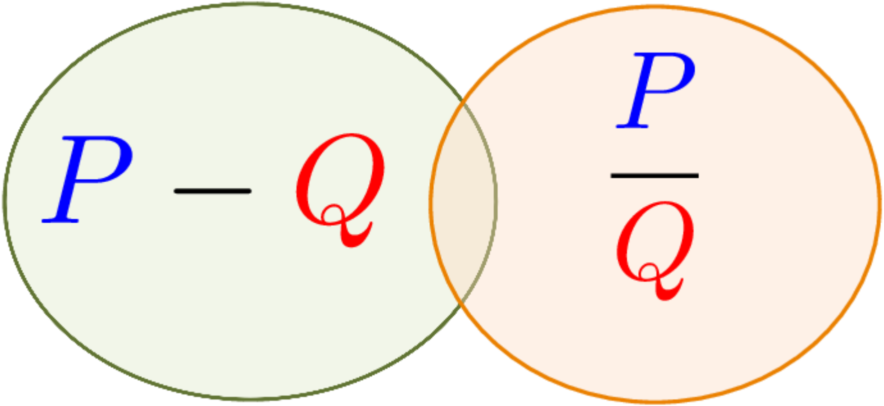
The empirical witness function at v

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

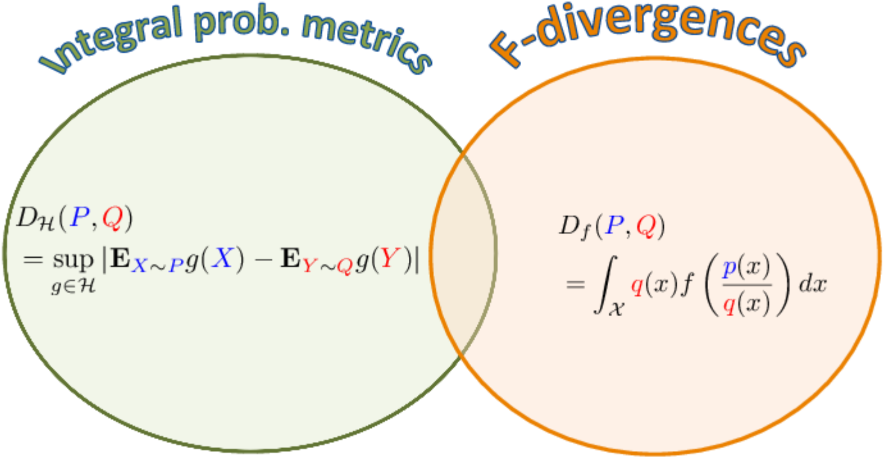
Don't need explicit feature coefficients $f^* := \begin{bmatrix} f_1^* & f_2^* & \dots \end{bmatrix}$

Interlude: divergence measures

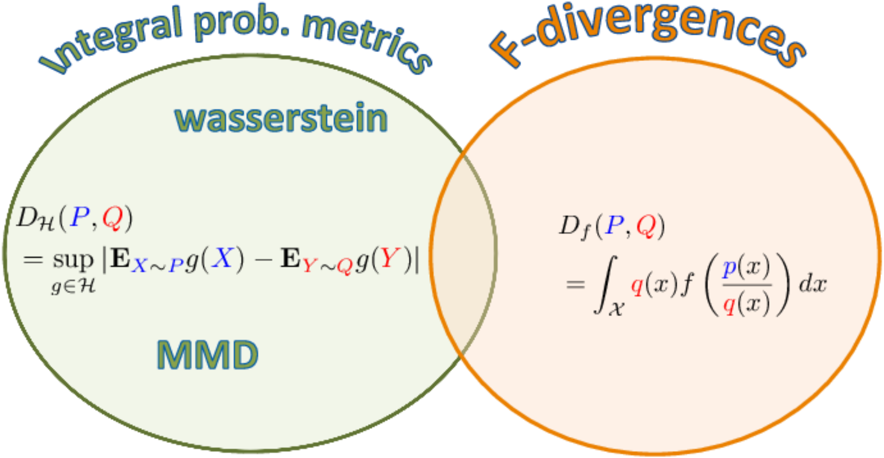
Divergences



Divergences



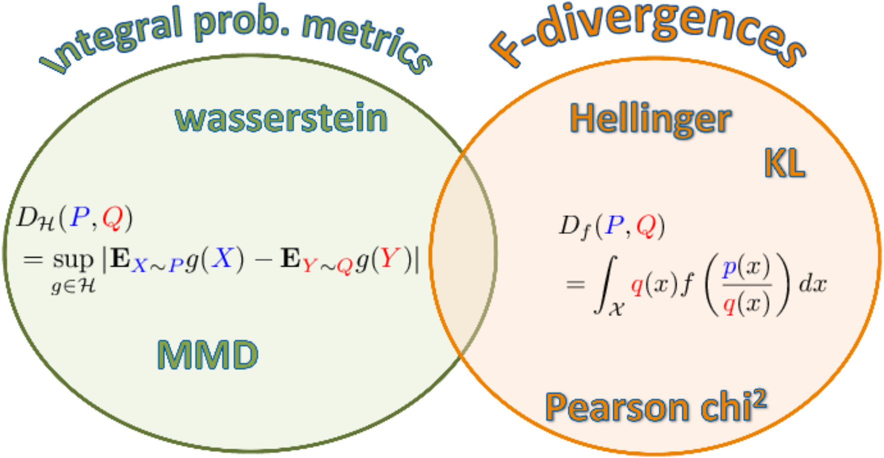
Divergences



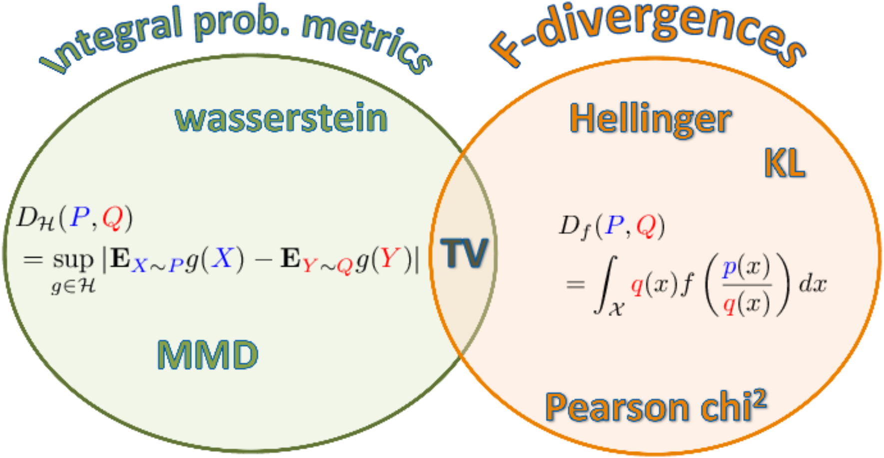
$$D_{\mathcal{H}}(P, Q) = \sup_{g \in \mathcal{H}} \left| \mathbf{E}_{X \sim P}\, g(X) - \mathbf{E}_{Y \sim Q}\, g(Y) \right|$$

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

Divergences



Divergences



Sriperumbudur, Fukumizu, G, Schoelkopf, Lanckriet (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

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

A statistical test using MMD

The empirical MMD:

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

Perspective from statistical hypothesis testing:

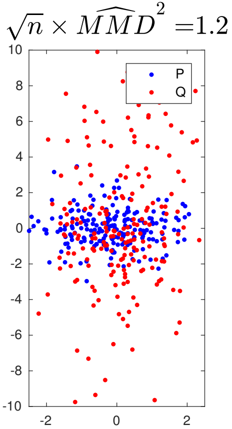
- **Null hypothesis $\mathcal{H}_0$ when $P = Q$**
  - should see $\widehat{MMD}^2$ "close to zero".
- **Alternative hypothesis $\mathcal{H}_1$ when $P \neq Q$**
  - should see $\widehat{MMD}^2$ "far from zero"

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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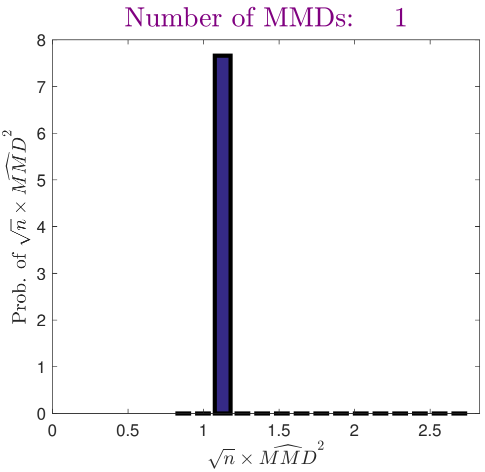
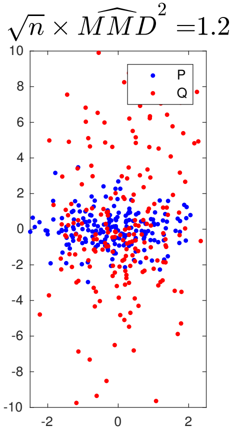
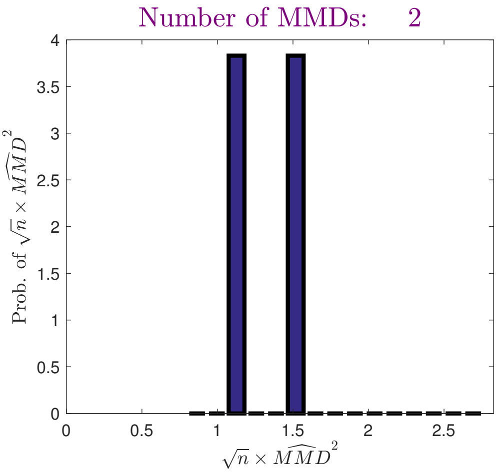


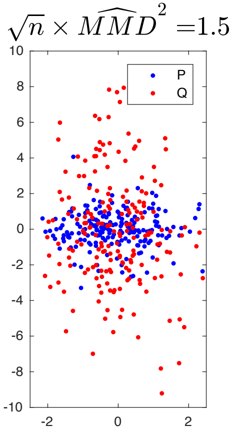


Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

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

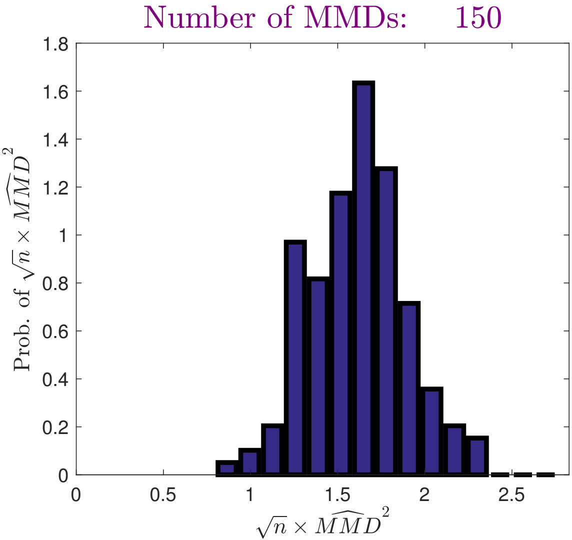
- Laplace with different y-variance.
- $\sqrt{n} \times \widehat{MMD}^2 = 1.5$





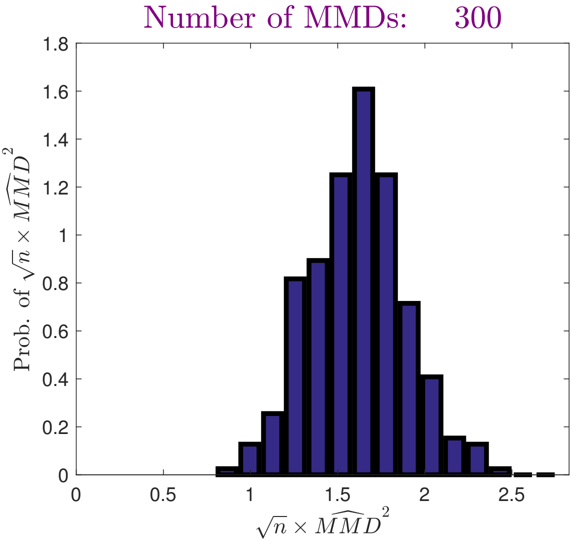
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 150 times . . .



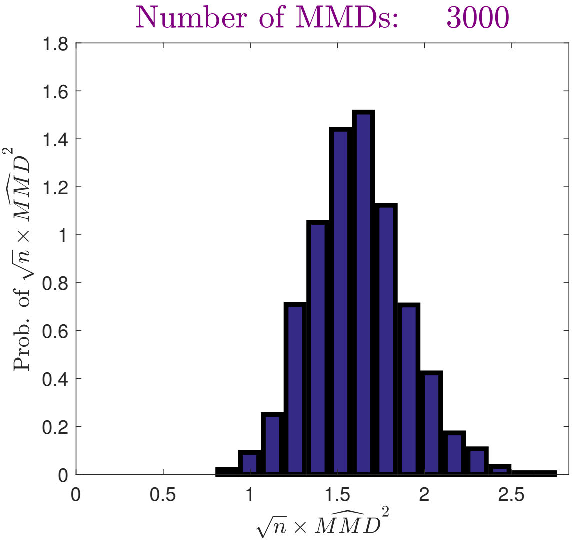
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

Repeat this 300 times . . .



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

Repeat this 3000 times ...

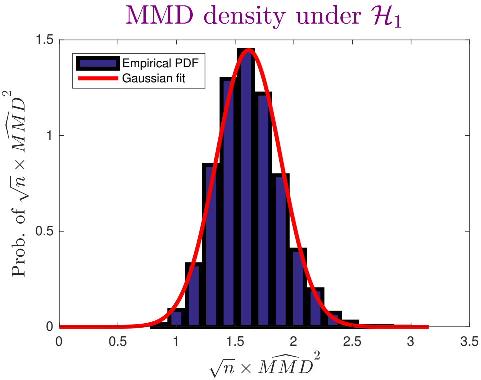


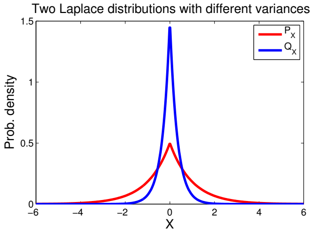
Asymptotics of $\widehat{MMD}^2$ when $P \neq Q$

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

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

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



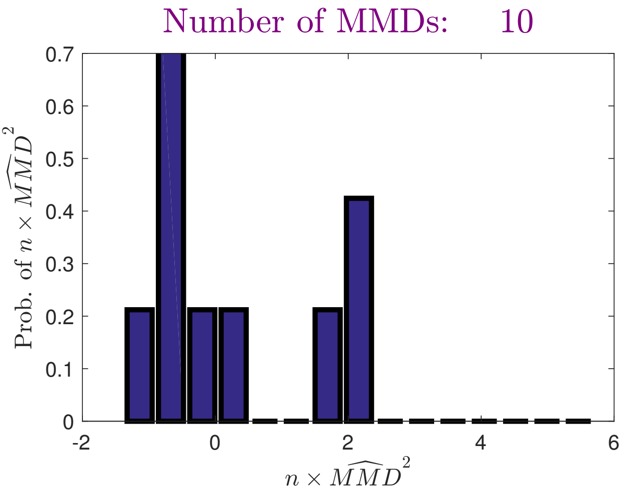


Behaviour of $\widehat{MMD}^2$ when $P = Q$

What happens when P and Q are the same?

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

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



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

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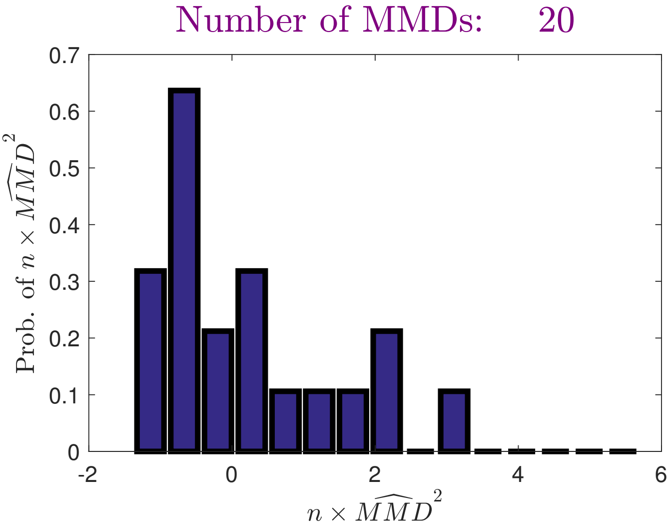

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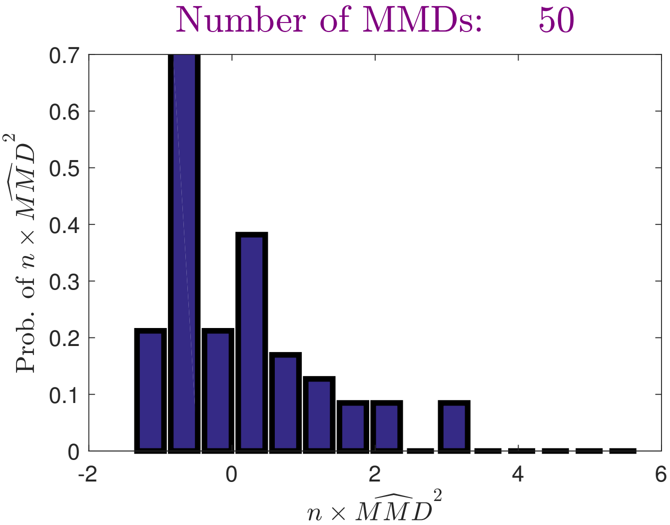

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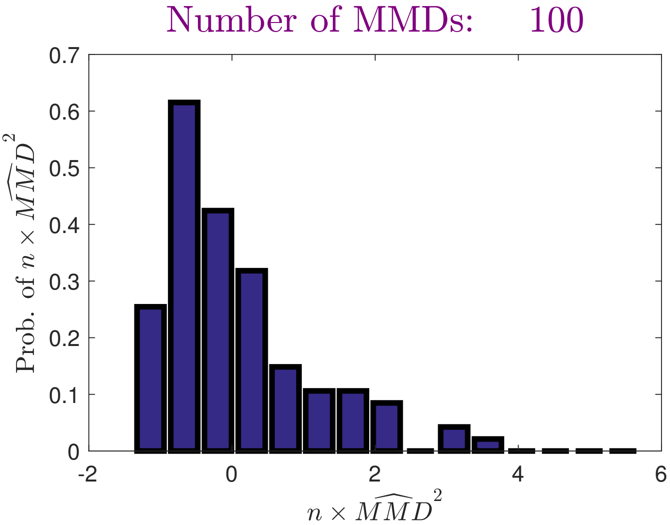

Behaviour of $\widehat{MMD}^2$ when $P = Q$

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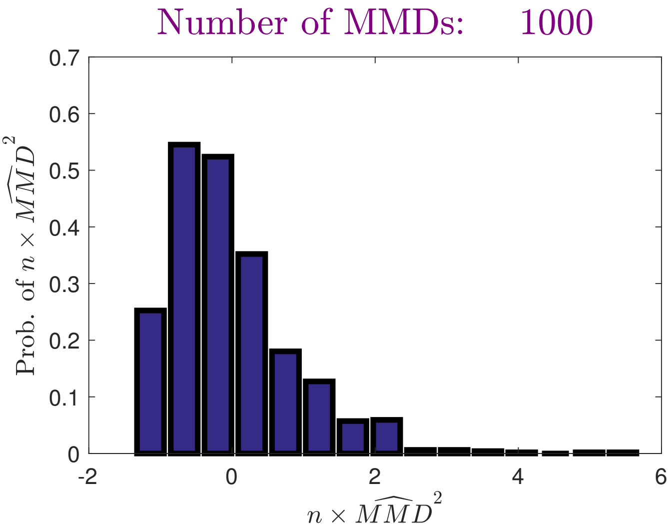
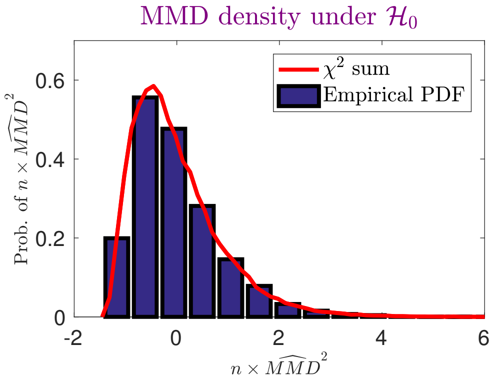


Asymptotics of $\widehat{MMD}^2$ when $P = Q$

Where $P = Q$, statistic has asymptotic distribution

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



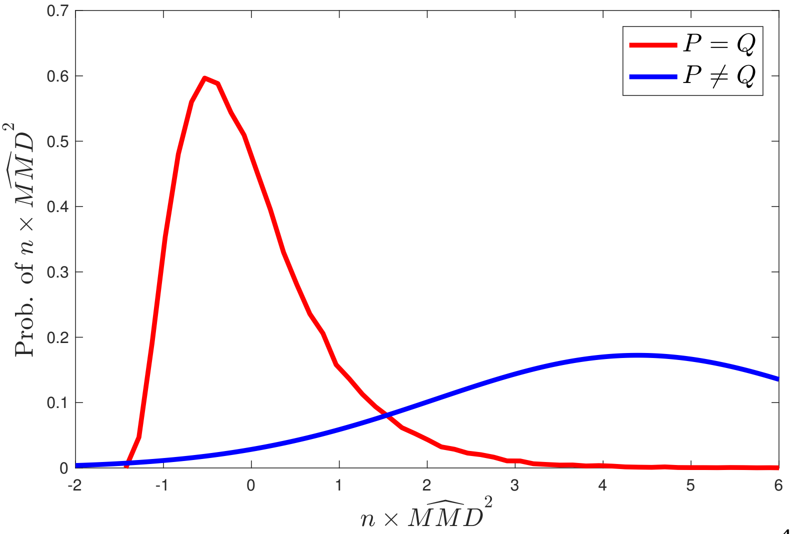
where

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

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

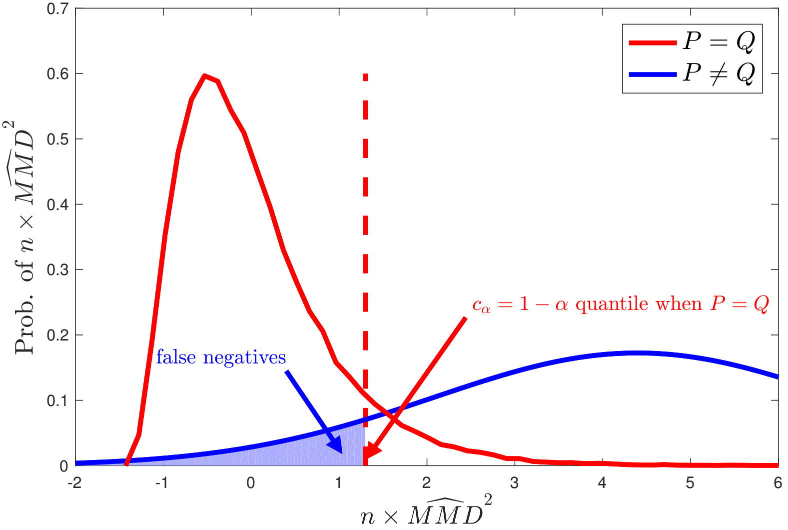
A statistical test

A summary of the asymptotics:



A statistical test

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



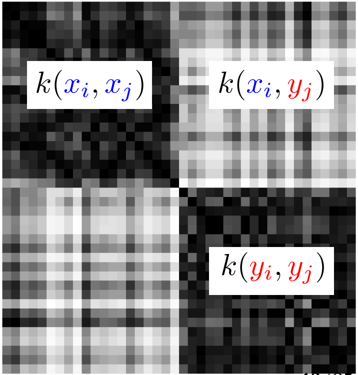
How do we get test threshold c_α?

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**):

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

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

How do we get test threshold c_α?

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

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

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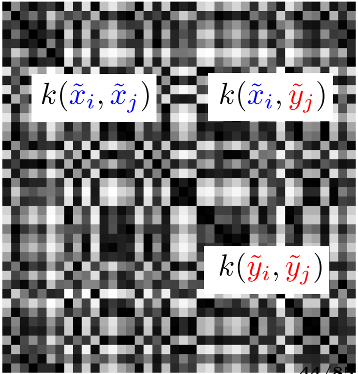


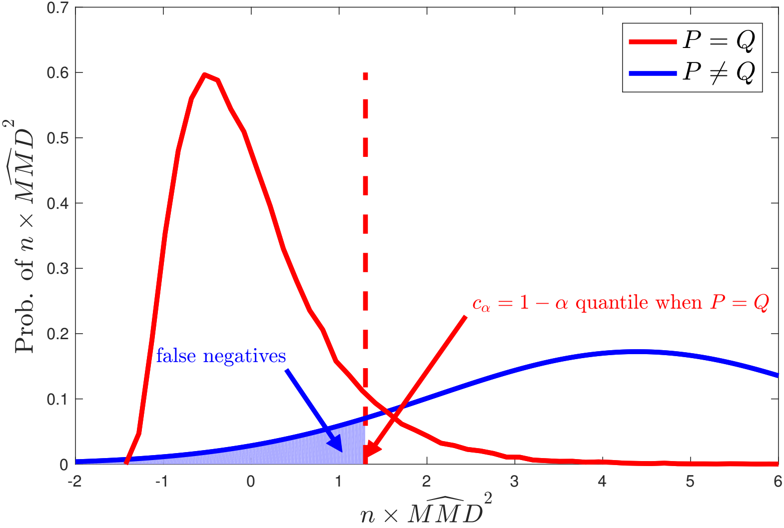
Permutation simulates

$P = Q$

How to choose the best kernel: optimising the kernel parameters

Graphical illustration

- Maximising test power same as minimizing false negatives



Optimizing kernel for test power

The power of our test:

$$\Pr_{P \neq Q}\left(n\widehat{\mathrm{MMD}}^2 > \hat{c}_\alpha\right)$$

Optimizing kernel for test power

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

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:

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

Variance under $\mathcal{H}_1$ decreases as $\sqrt{V_n(P,Q)} \sim O(n^{-1/2})$

For large n, second term negligible!

Optimizing kernel for test power

The power of our test:

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

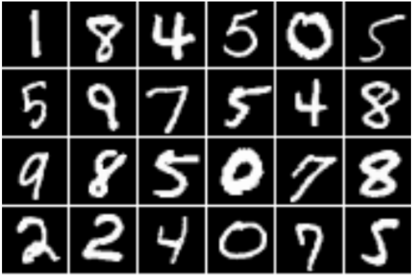
To maximize test power, maximize

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

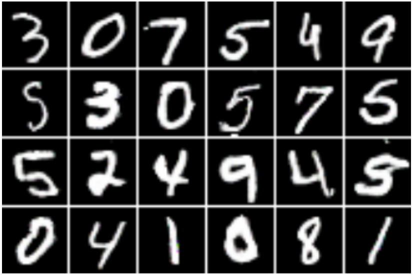
(Sutherland, Tung, Strathmann, De, Ramdas, Smola, G., ICLR 2017)

Code: github.com/dougalsutherland/opt-mmd

Troubleshooting for generative adversarial networks

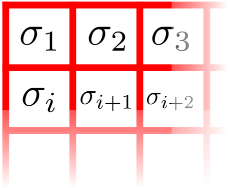


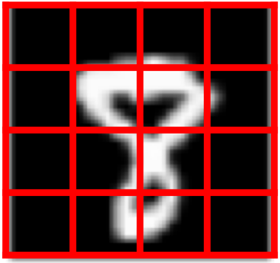
MNIST samples



Samples from a GAN

The ARD kernel

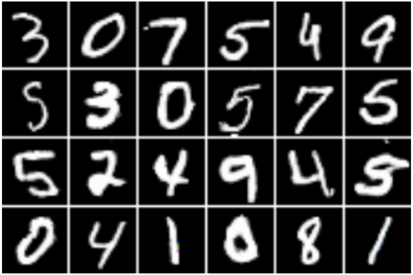




$$k(4, 2) = \prod_{i=1}^{D} \exp\left(\frac{-(4[i] - 2[i])^2}{\sigma_i^2}\right)$$

Troubleshooting for generative adversarial networks

MNIST samples



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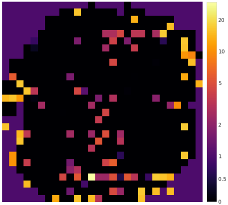
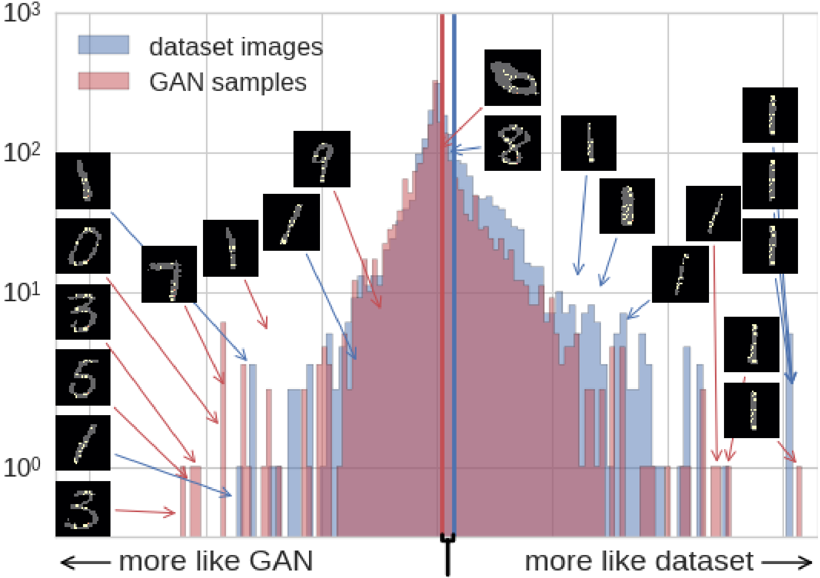


ARD map

- Power for **optimzed ARD kernel**: 1.00 at $\alpha = 0.01$
- Power for optimized RBF kernel: 0.57 at $\alpha = 0.01$

Troubleshooting generative adversarial networks

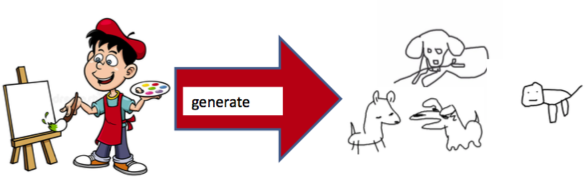


$\mathrm{MMD}^2 = 0.0001$

Training Generative Adversarial Networks with MMD Critic

Training Generative Adversarial Networks: Myths and Conjectures

Reminder: GAN setting



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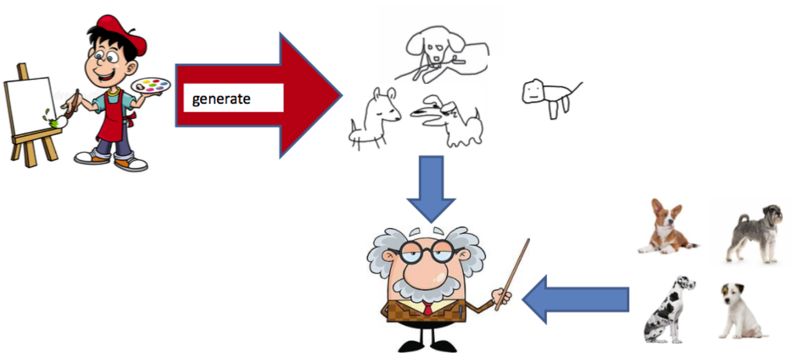

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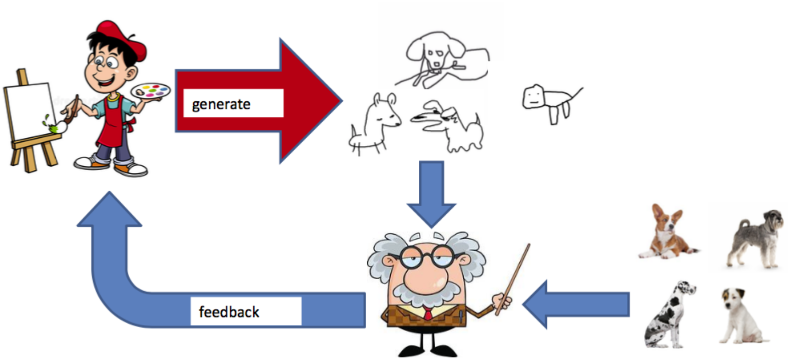
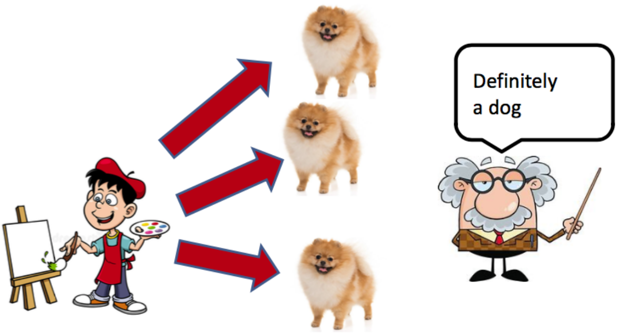


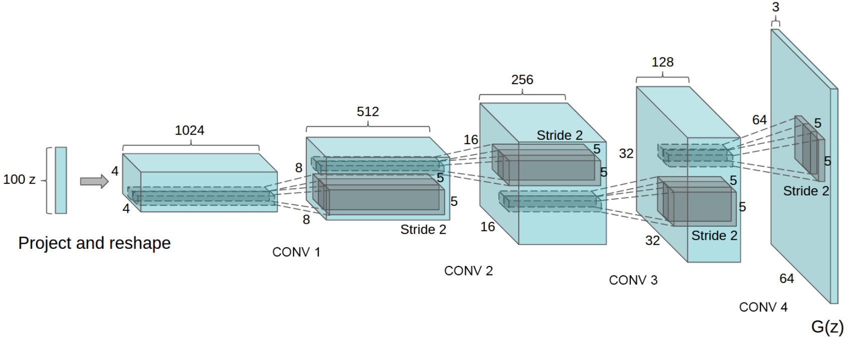
Why is classification not enough?



Classification **not** enough!
Need to compare **sets**

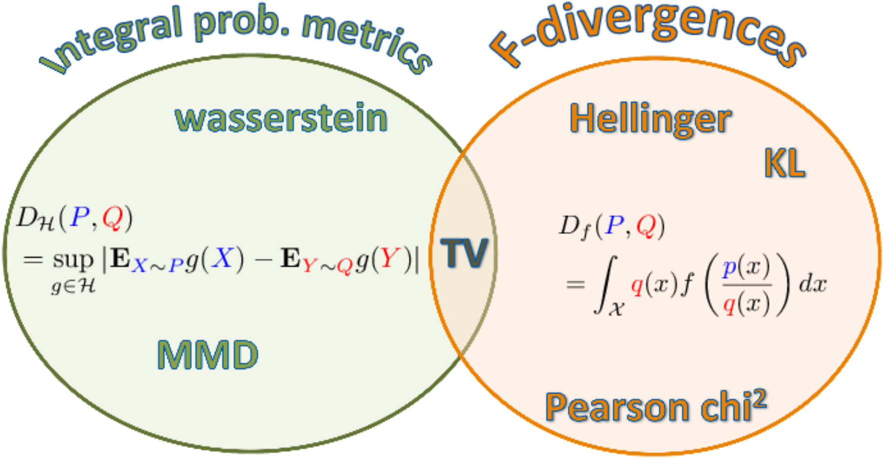
(otherwise student can just produce the same dog over and over)

What I *won't* cover: the generator



Radford, Metz, Chintala, ICLR 2016

Choices of critic



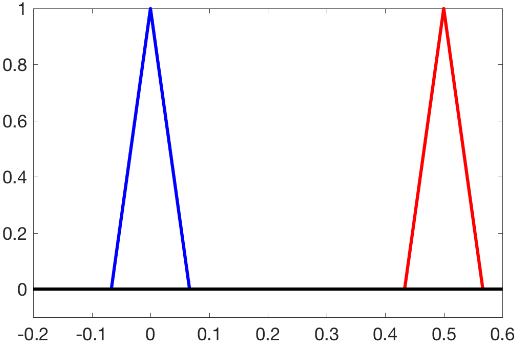
Sriperumbudur, Fukumizu, G, Schoelkopf, Lanckriet (2012)

F-divergence as critic

An unhelpful critic: Jensen-Shannon, 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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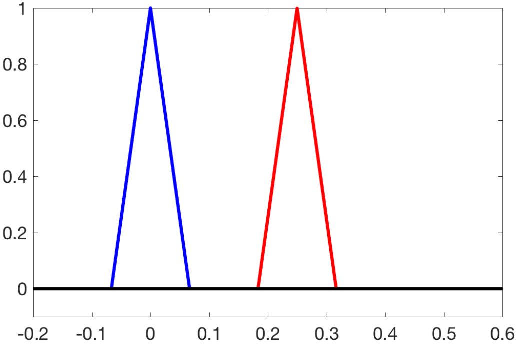

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- Use a variational approximation to the critic, alternate generator and critic training (we will return to this!) Goodfellow et al. [NeurIPS 2014], Nowozin et al. [NeurIPS 2016]

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

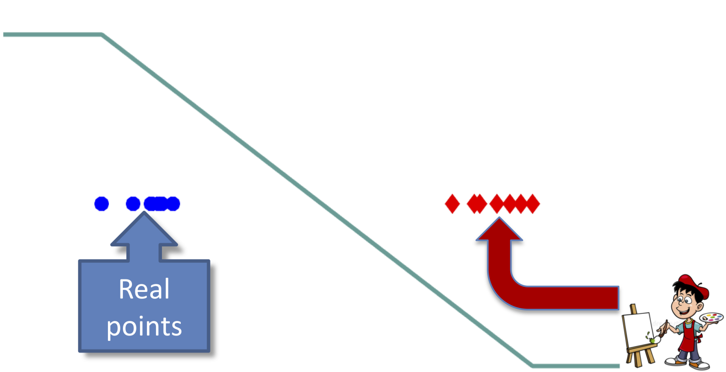
Wasserstein distance as critic

A helpful critic witness:

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

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

W_1=0.88



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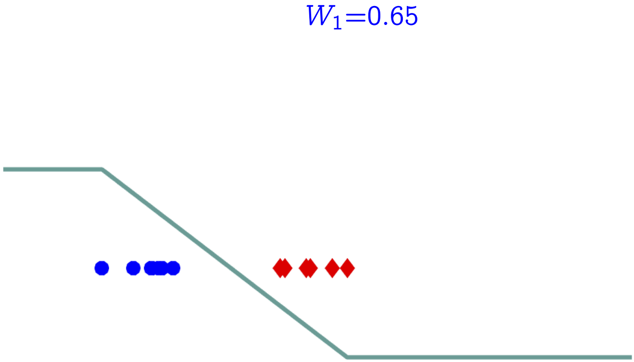
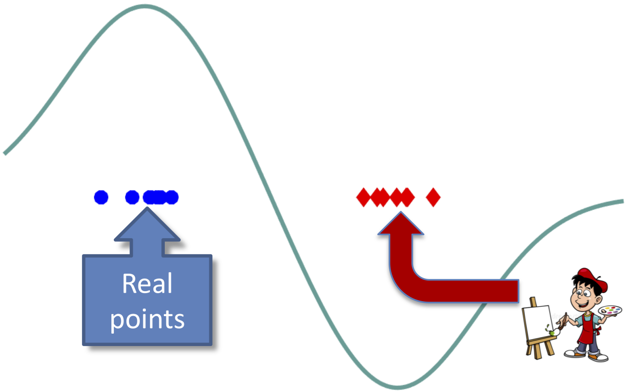


MMD as critic

A helpful critic witness:

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

MMD=1.8

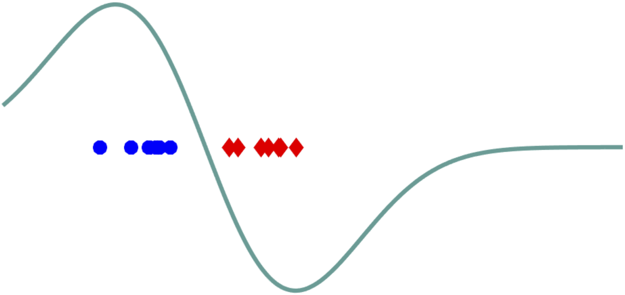


MMD as critic

A helpful critic witness:

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

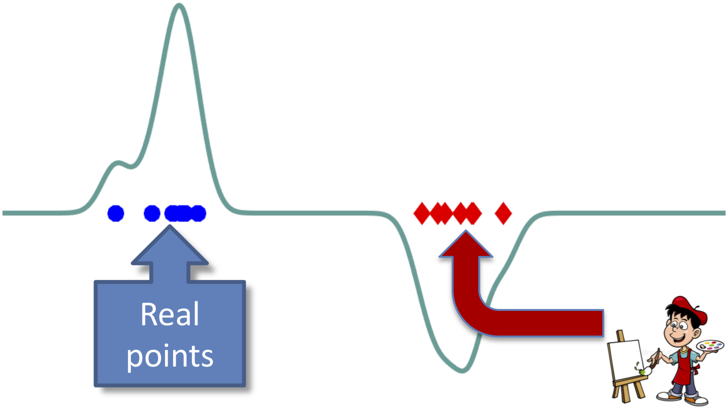
MMD=1.1



MMD as critic

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

MMD=0.64



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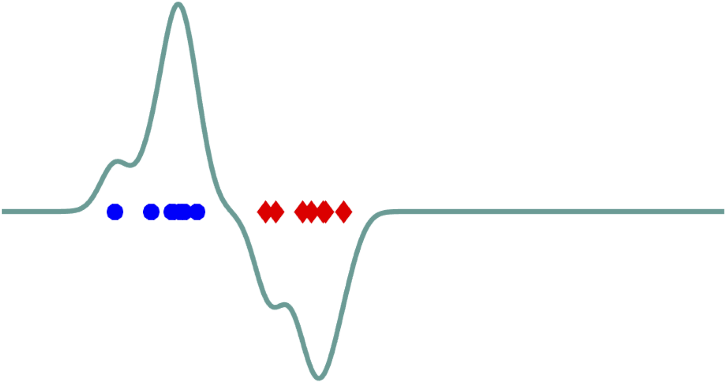

MMD for GAN critic

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

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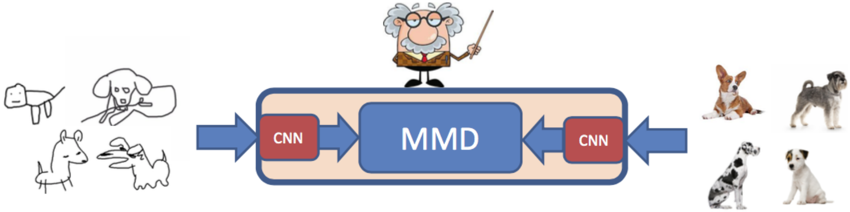
MMD for GAN critic

Can you use MMD as a critic to train GANs?

Need better image features.

CNN features for an MMD witness

- 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]

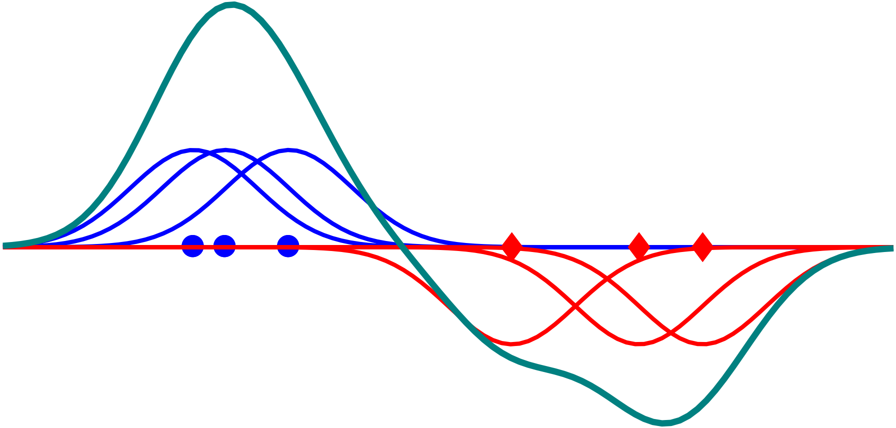
$\mathfrak{K}(x, y) = k(h_\psi(x), h_\psi(y))$
where $h_\psi(x)$ is a CNN map,
k is e.g. an exponentiated quadratic kernel

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]

Witness function, kernels on deep features

Reminder: witness function,

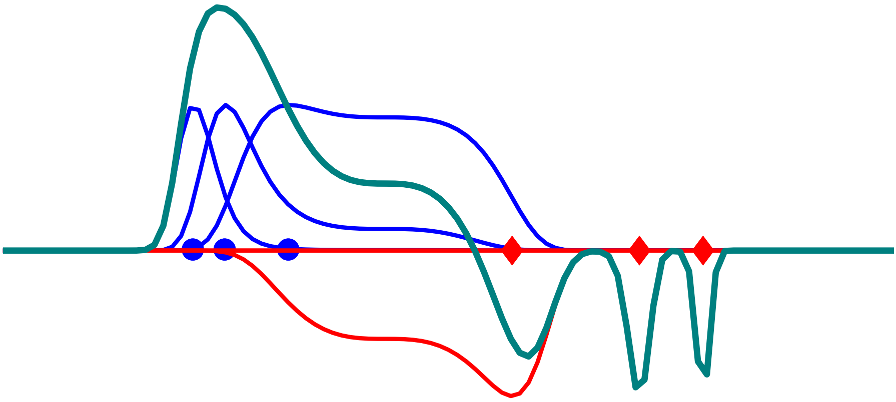
$k(x, y)$ is exponentiated quadratic



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.

Challenges for learned critic features

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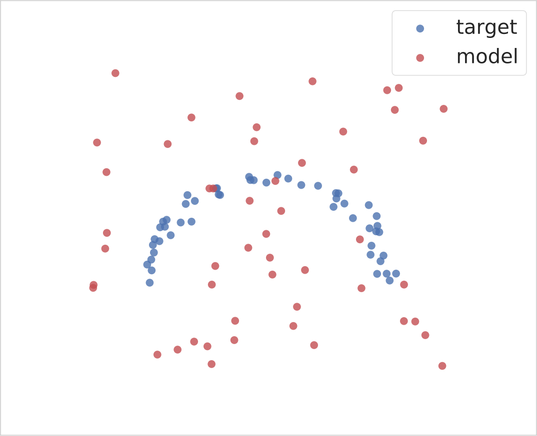
Relation with test power?

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

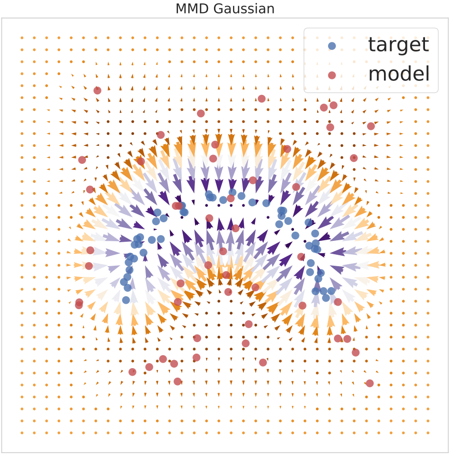
A simple 2-D example

Samples from target P and model Q



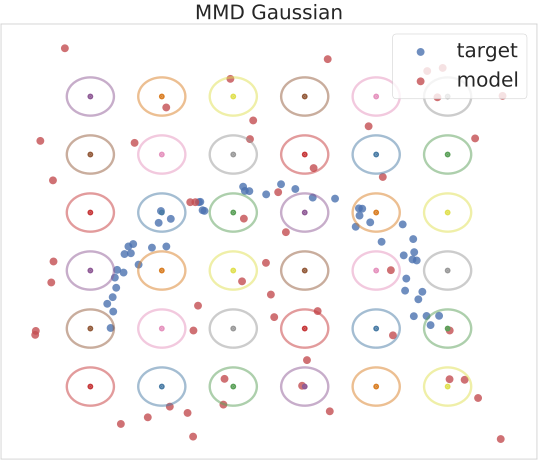
A simple 2-D example

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



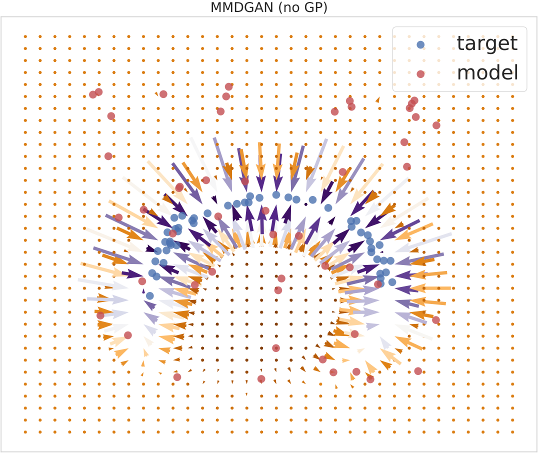
A simple 2-D example

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



A simple 2-D example

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



(4 layer, fully connected, RELU, skipthrough 1-4, early stage)

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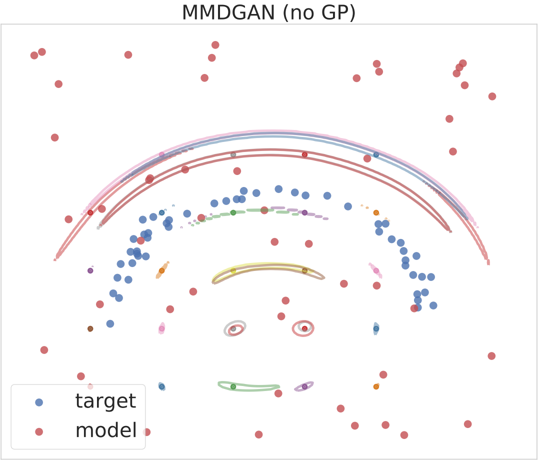
What the kenels $k(h_\psi(x), h_\psi(y))$ look like



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A simple 2-D example

A data-adaptive gradient penalty

- 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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Modified witness constraint:

$$\widetilde{MMD} := \sup_{\boxed{\|f\|_S \leq 1}} \left[\mathbb{E}_P f(X) - \mathbb{E}_Q f(Y)\right]$$

where

$$\|f\|_S^2 = \underbrace{\|f\|_{L_2(P)}^2}_{\text{L}_2\text{ norm control}} + \underbrace{\|\nabla f\|_{L_2(P)}^2}_{\text{Gradient control}} + \underbrace{\lambda \|f\|_k^2}_{\text{RKHS smoothness}}$$

Maximise $\widetilde{MMD}$ wrt critic features

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Problem: not computationally feasible: $O(n^3)$ per iteration.

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Maximise scaled MMD over critic features:

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

where

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

Replace expensive constraint with cheap upper bound:

$$\|f\|_S^2 \leq \sigma^{-1}_{P,\lambda}\ \|f\|_k^2$$

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

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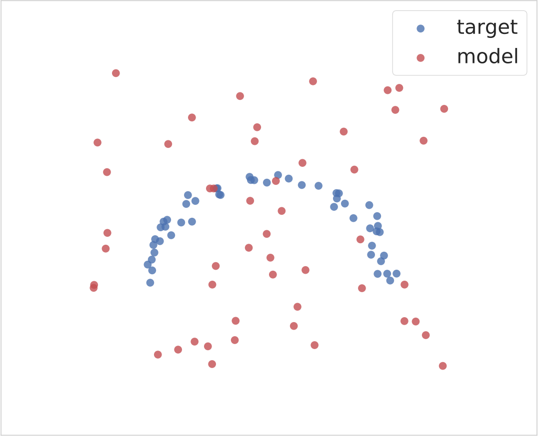

Simple 2-D example revisited

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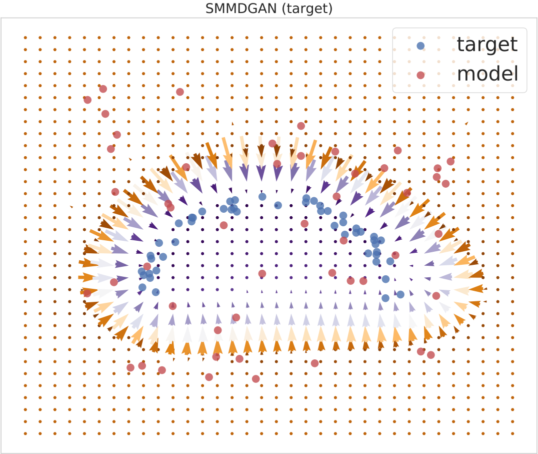
to learn $h_\psi(x)$ for $k(h_\psi(x), h_\psi(y))$



(early stage of critic optimisation)

Simple 2-D example revisited

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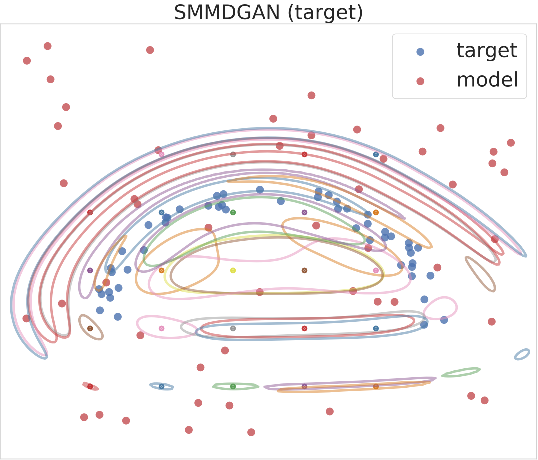

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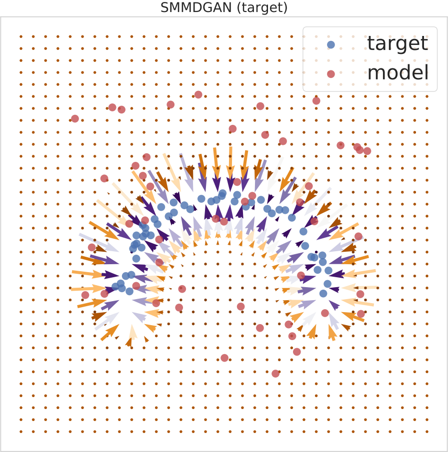

(late stage of critic optimisation)

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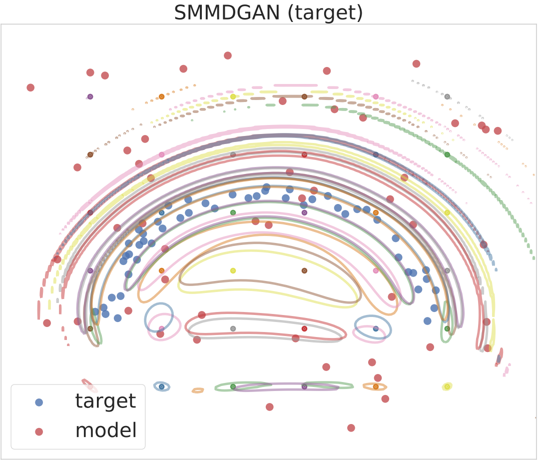
What the kenels $k(h_\psi(x), h_\psi(y))$ look like



(late stage of critic optimisation)

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 $k(h_\psi(x), h_\psi(y))$ is unhelpful.
- Data-dependent regularisation also applies to variational form in f-GANs Roth et al [NeurIPS 2017, eq. 19 and 20]

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Alternate critic and generator training:

- Weaker critics can give better signals to poor (early stage) generators.

WGAN-GP

Wasserstein GAN Arjovsky et al. [ICML 2017]
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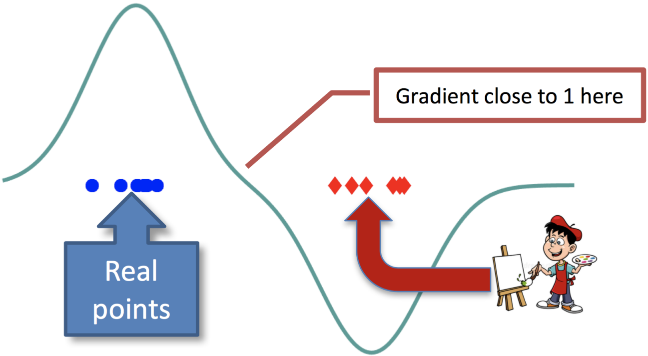

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-  Given a generator G_θ with parameters θ to be trained. Samples $Y \sim G_\theta(Z)$ where $Z \sim R$
-  Given critic features h_ψ with parameters ψ to be trained. f_ψ a linear function, $\mathfrak{K}(x, y) = h_\psi{}^\top(x) h_\psi(y)$.

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WGAN-GP gradient penalty:

$$\max_{\psi} \mathbf{E}_{X \sim P} f_\psi(X) - \mathbf{E}_{Z \sim R} f_\psi(G_\theta(Z)) + \lambda \mathbf{E}_{\widetilde{X}} \left(\left\| \nabla_{\widetilde{X}} f_\psi(\widetilde{X}) \right\| - 1 \right)^2$$

where

$$\widetilde{X} = \gamma x_i + (1-\gamma) G_\theta(z_j)$$

$$\gamma \sim \mathcal{U}([0,1]) \quad x_i \in \{x_\ell\}_{\ell=1}^m \quad z_j \in \{z_\ell\}_{\ell=1}^n$$

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Again: data-dependent gradient regularisation on witness class

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

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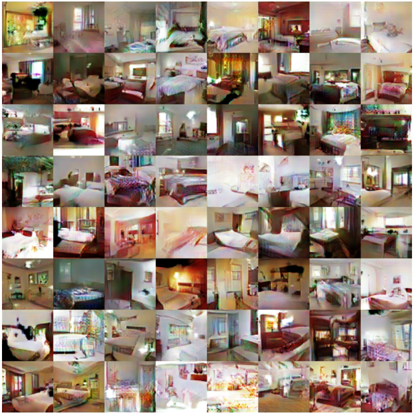
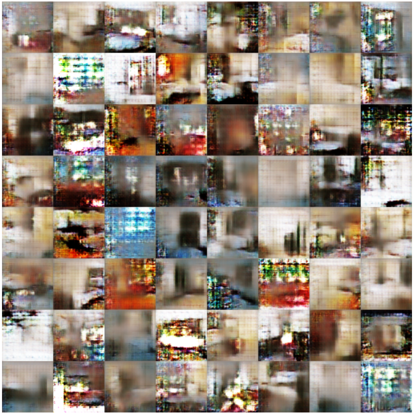


$k(h_\psi(x), h_\psi(y))$, $f = 16$, KID=9



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

Evaluation and experiments

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)
- label entropy $P(y)$ is high (good variety).

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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):

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

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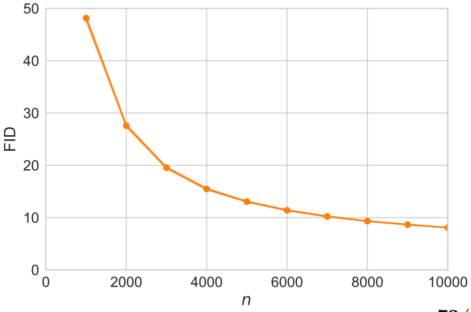
Problem: **bias**. For finite samples can consistently give incorrect answer.

- 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

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

where $\Sigma = \frac{4}{d} C C^T$, 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,

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

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The kernel inception distance (KID)

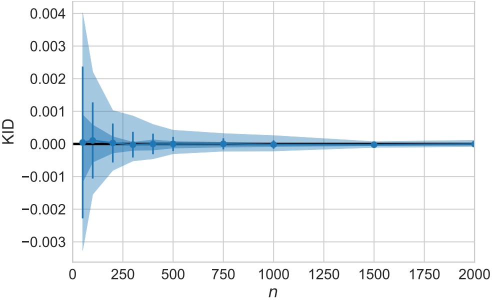
The Kernel inception distance Binkowski, Sutherland, Arbel, G. [ICLR 2018]

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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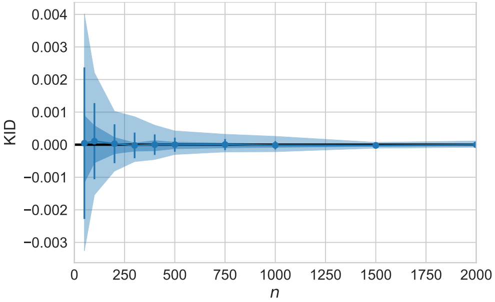

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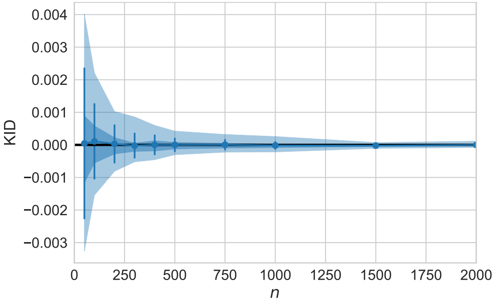

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"Block" KID implementation is cheaper than FID: see paper (or use Tensorflow implementation)!

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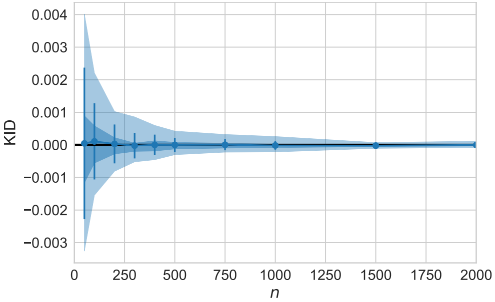

- Checks match for feature means, variances, skewness
- Unbiased : eg CIFAR-10 train/test

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]

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]
{miyato, kataoka}@preferred.jp
koyama 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
{mroueh,chengyu}@us.ibm.com, chunlial@cs.cmu.edu,
tom.sercu1@ibm.com,anant.raj@tuebingen.mpg.de

Demystifying MMD GANs

Mikołaj Bińkowski*
Department of Mathematics
Imperial College London
mikbinkowski@gmail.com

Dougal J. Sutherland*, Michael Arbel & Arthur Gretton
Gatsby 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
MSR
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Kyunghyun Cho
New York University,
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kyunghyun.cho@nyu.edu

Yoshua Bengio
MILA, University of Montréal, CIFAR, IVADO
yoshua.bengio@umontreal.ca

Results: celebrity faces 160×160

KID scores:

- Sobolev GAN: 14
- SN-GAN: 18
- Old MMD GAN: 13
- SMMD GAN: 6

202 599 face images, resized and cropped to 160 × 160

Results: unconditional imagenet 64×64

KID scores:

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

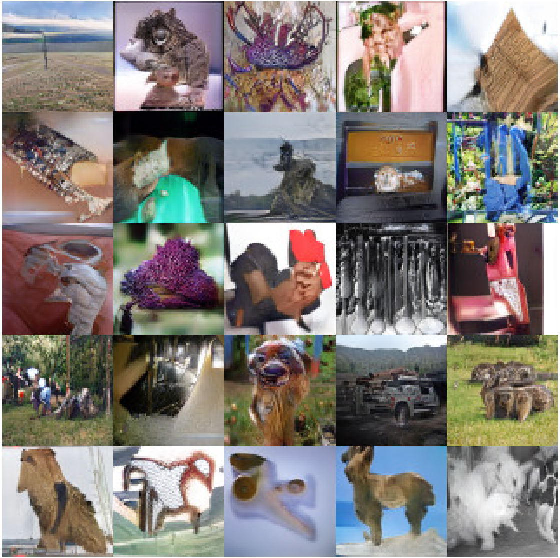
ILSVRC2012 (ImageNet) dataset, 1 281 167 images, resized to 64 × 64. 1000 classes.

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.



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.

Summary

- MMD critic gives state-of-the-art performance for GAN training (FID and KID)
  - use convolutional input features
  - train with new gradient regulariser
- Faster training, simpler critic network
- Reasons for good performance:
  - Unlike WGAN-GP, MMD loss still a valid critic when features not optimal
  - Kernel features do some of the "work", so simpler h_ψ features possible.
  - Better gradient/feature regulariser gives better critic

"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

Co-authors

From Gatsby:

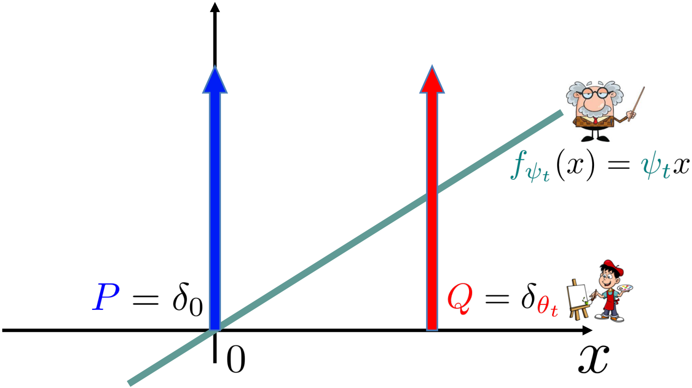
- Michael Arbel
- Mikolaj Binkowski
- Heiko Strathmann
- Dougal Sutherland

External collaborators:

- Soumyajit De
- Aaditya Ramdas
- Bernhard Schoelkopf
- Alex Smola
- Hsiao-Yu Tung

Questions?


THE KERNEL
BREWERY
LONDON
BALTIC PORTER
THE KERNEL
EXPORT STOUT

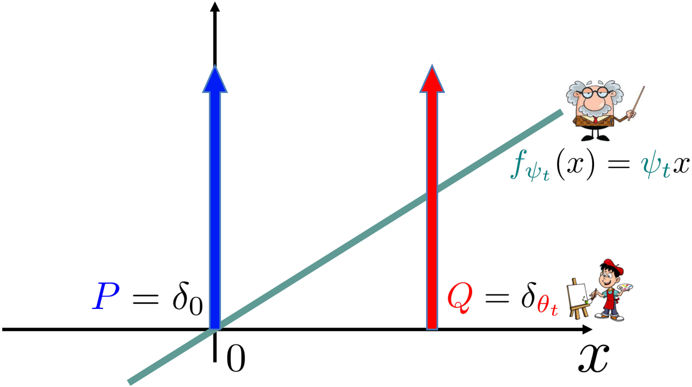


$$D(P, Q; \psi_t) = \mathbf{E}_Q f_{\psi_t}(Y) - \mathbf{E}_P f_{\psi_t}(X)$$
$$= \psi_t \theta_t$$

Mescheder et al. [ICML 2018]

Optimization: simple example

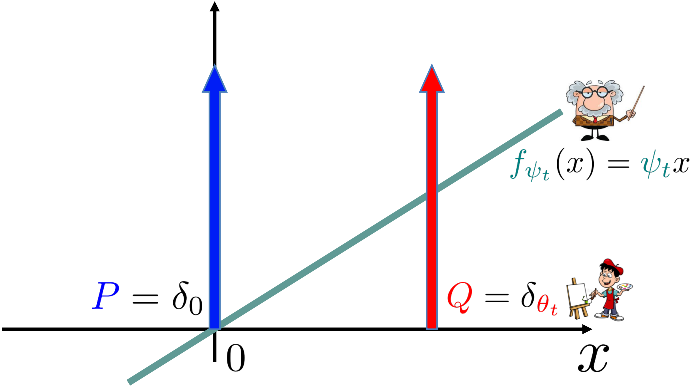
Gradient descent on generator:



$$\frac{\partial}{\partial \theta} D(P, Q; \psi_t) = \frac{\partial}{\partial \theta} \psi_t \theta_t = \psi_t$$

Optimization: simple example

Gradient descent on generator:

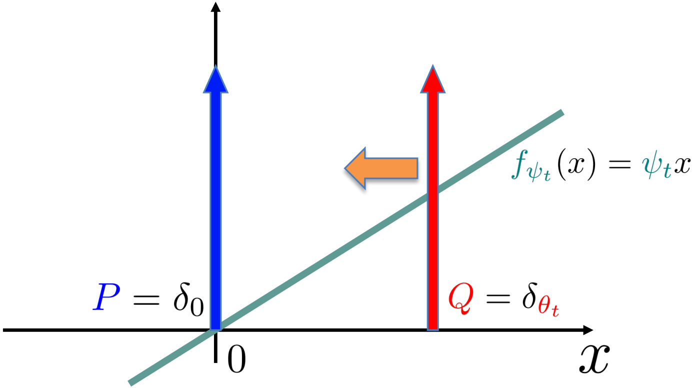


$$\frac{\partial}{\partial \theta} D(P, Q; \psi_t) = \frac{\partial}{\partial \theta} \psi_t \theta_t = \psi_t$$

$$\theta_{t+1} = \theta_t - \gamma \frac{\partial}{\partial \theta} D(P, Q; \psi_t) = \theta_t - \gamma \psi_t$$

Optimization: simple example

Gradient descent on generator:



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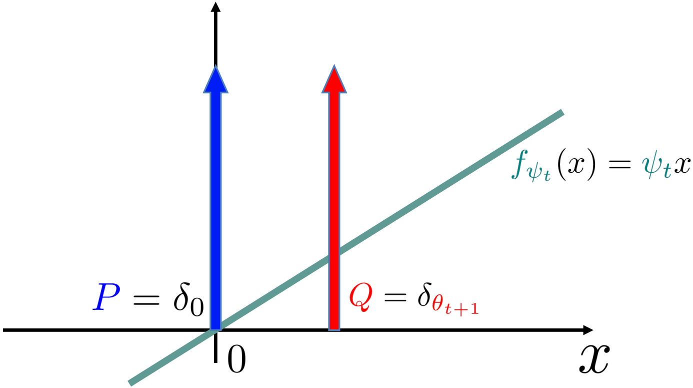

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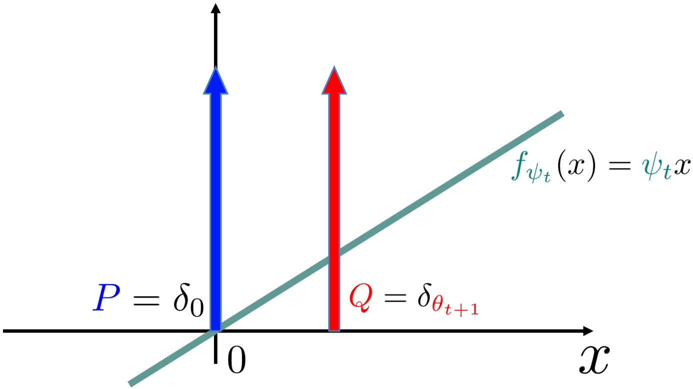
Optimization: simple example

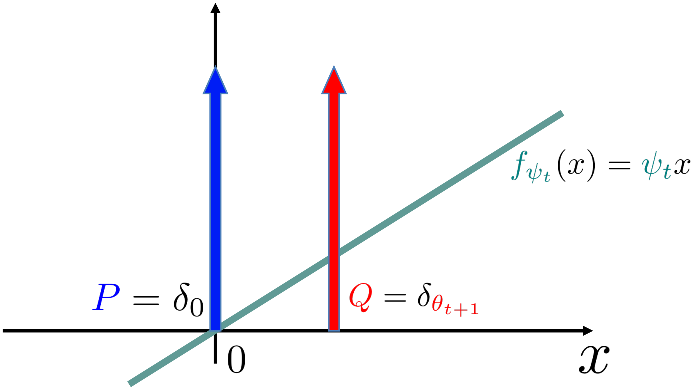
Gradient ascent on critic:



$$\frac{\partial}{\partial \psi} D(P, Q; \psi_t) = \theta_{t+1}$$

Optimization: simple example

Gradient ascent on critic:

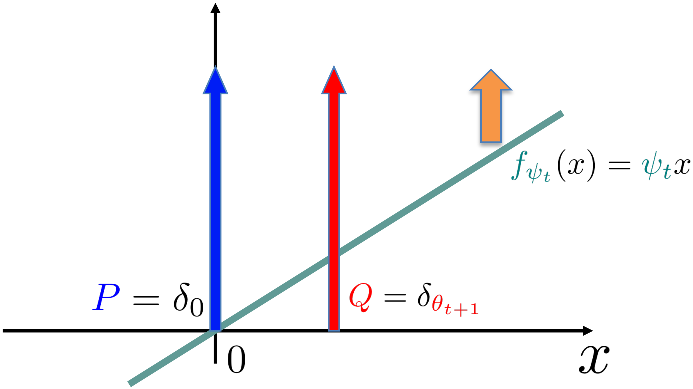


$$\frac{\partial}{\partial \psi} D(P, Q; \psi_t) = \theta_{t+1}$$

$$\psi_{t+1} = \psi_t + \lambda \frac{\partial}{\partial \psi} D(P, Q; \psi_t) = \psi_t + \lambda \theta_{t+1}$$

Optimization: simple example

Gradient ascent on critic:



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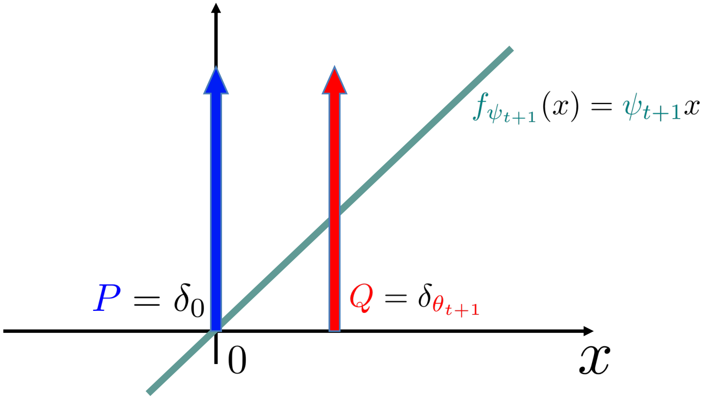
Optimization: simple example

Gradient ascent on critic:



$$\frac{\partial}{\partial \psi} D(P, Q; \psi_t) = \theta_{t+1}$$

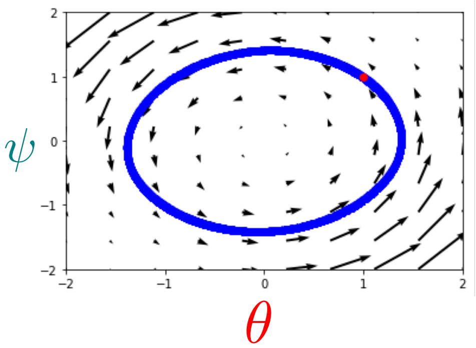
$$\psi_{t+1} = \psi_t + \lambda \frac{\partial}{\partial \psi} D(P, Q; \psi_t) = \psi_t + \lambda \theta_{t+1}$$

Optimization: simple example

Idealised continuous system (infinitely small learning rate)

$$\begin{bmatrix} \dot{\theta} \\ \dot{\psi} \end{bmatrix} = \begin{bmatrix} -\nabla_{\psi} D(P, Q; \psi) \\ \nabla_{\theta} D(P, Q; \psi) \end{bmatrix}$$

Every integral curve $(\psi(t), \theta(t))$ of the gradient vector field satisfies $\psi^2(t) + \theta^2(t) = c$ for all $t \in [0, \infty)$.



Mescheder et al. [ICML 2018, Lemma 2.3]

Optimization: simple example

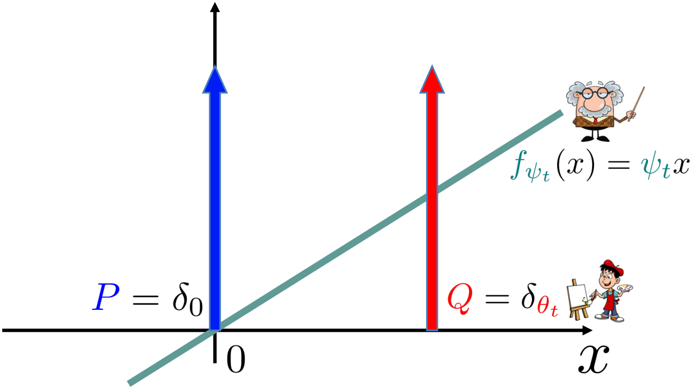
Idealised continuous system (infinitely small learning rate)

$$\left[\begin{array}{c}\dot{\theta}\\ \dot{\psi}\end{array}\right]=\left[\begin{array}{c}-\nabla_{\psi}D(P,Q;\psi)\\ \nabla_{\theta}D(P,Q;\psi)\end{array}\right]$$

Every integral curve $(\psi(t),\theta(t))$ of the gradient vector field satisfies $\psi^2(t)+\theta^2(t)=c$ for all $t\in[0,\infty)$.

A solution: control witness gradient

Mescheder et al. [ICML 2018, Lemma 2.3]



$$
\begin{aligned}
D(P, Q; \psi_t) &= \mathbf{E}_Q f_{\psi_t}(Y) - \mathbf{E}_P f_{\psi_t}(X) \\
&= \psi_t \theta_t
\end{aligned}
$$

Mescheder et al. [ICML 2018]

Convergence issues for WGAN-GP penalty

WGAN-GP style gradient penalty may not converge near solution

Nagarajan and Kolter [NeurIPS 2017], Mescheder et al. [ICML 2018], Balduzzi et al. [ICML 2018]

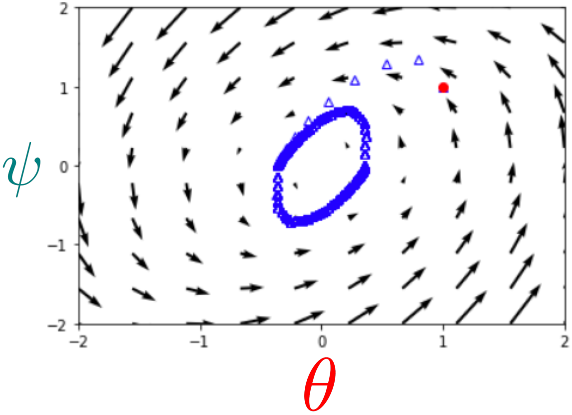


Figure from Mescheder et al. [ICML 2018]