The Maximum Mean Discrepancy for Training Generative Adversarial Networks

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A motivation: comparing two samples

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

Sutherland, Tung, Strathmann, De, Ramdas, Smola, G., ICLR 2017.
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.
Training generative models

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

Using MMD to train a GAN

(Binkowski, Sutherland, Arbel, G., ICLR 2018),
(Arbel, Sutherland, Binkowski, G., arXiv 2018)
Part 2: testing goodness of fit

- **Given:** A model \( P \) and samples and \( Q \).
- **Goal:** is \( P \) a good fit for \( Q \)?

Chicago crime data

Model is Gaussian mixture with **two** components.
## Part 2: testing independence

- **Given:** Samples from a distribution $P_{XY}$
- **Goal:** Are $X$ and $Y$ independent?

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Dog Image" /></td>
<td>A large animal who slings slobber, exudes a distinctive houndy odor, and wants nothing more than to follow his nose.</td>
</tr>
<tr>
<td><img src="image2.png" alt="Dog Image" /></td>
<td>Their noses guide them through life, and they're never happier than when following an interesting scent.</td>
</tr>
<tr>
<td><img src="image3.png" alt="Cat Image" /></td>
<td>A responsive, interactive pet, one that will blow in your ear and follow you everywhere.</td>
</tr>
</tbody>
</table>

Text from dogtime.com and petfinder.com
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

- Training generative adversarial networks with MMD
  - Gradient regularisation and data adaptivity
  - Evaluating GAN performance? Problems with Inception and FID.
Maximum Mean Discrepancy
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 \( \varphi(x) = x^2 \)
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 $\varphi(x) = x^2$
Feature mean difference

- Gaussian and Laplace distributions
- Same mean \textit{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

Kernels: dot products of features

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

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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

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

Features: Gaussian Processes for Machine learning, Rasmussen and Williams, Ch. 4.
Consider (truncated) Gaussian density on $\mathcal{X} \subset \mathbb{R}$,

$$p(x) \propto \exp\left(-x^2\right) \mathbb{1}_{\mathcal{X}}(x)$$

Define the eigenexpansion of $k(x, x')$ wrt this density:

$$\lambda_\ell e_\ell(x) = \int_{\mathcal{X}} k(x, x') e_\ell(x') p(x') dx'$$

$$\int_{\mathcal{X}} e_i(x) e_j(x) p(x) dx = \begin{cases} 1 & i = j \\ 0 & i \neq j. \end{cases}$$

We can write

$$k(x, x') = \sum_{\ell=1}^{\infty} \lambda_\ell e_\ell(x) e_\ell(x') = \sum_{\ell=1}^{\infty} \left(\sqrt{\lambda_\ell} e_\ell(x)\right) \left(\sqrt{\lambda_\ell} e_\ell(x')\right) \varphi_\ell(x) \varphi_\ell(x')$$

which converges in $L_2(p)$.

**Warning:** for RKHS, need absolute and uniform convregence, eg via Mercer’s theorem for compact $\mathcal{X}$. 

14/75
Feature space construction: details

Consider (truncated) Gaussian density on $\mathcal{X} \subset \mathbb{R}$,

$$p(x) \propto \exp \left( -x^2 \right) \mathbb{1}_\mathcal{X}(x)$$

Define the eigenexpansion of $k(x, x')$ wrt this density:

$$\lambda_\ell e_\ell(x) = \int_{\mathcal{X}} k(x, x') e_\ell(x') p(x') \, dx'$$

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We can write

$$k(x, x') = \sum_{\ell=1}^{\infty} \lambda_\ell e_\ell(x) e_\ell(x') = \sum_{\ell=1}^{\infty} \left( \sqrt{\lambda_\ell} e_\ell(x) \right) \left( \sqrt{\lambda_\ell} e_\ell(x') \right)$$

which converges in $L_2(p)$.

**Warning:** for RKHS, need absolute and uniform convergence, eg via Mercer’s theorem for compact $\mathcal{X}$. 

14/75
Infinitely many features of *distributions*

Given *P* a Borel *probability measure* on *X*, define *feature map of probability* *P*,

\[ \mu_P = [\ldots E_P [\varphi_i(x)] \ldots ] \]

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

\[ \langle \mu_P, \mu_Q \rangle_{\mathcal{F}} = E_{P,Q} k(x, y) \]

for *x* ~ *P* and *y* ~ *Q*.

*Fine print:* is this allowed for infinite feature spaces?
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: is this allowed for infinite feature spaces?
Does the feature space mean exist?

Does there exist an element $\mu_P \in \mathcal{F}$ such that

$$E_P f(x) = \langle f, \mu_P \rangle_{\mathcal{F}} \quad \forall f \in \mathcal{F}$$

We recall the concept of a bounded operator: a linear operator $A : \mathcal{F} \to \mathbb{R}$ is bounded when

$$|Af| \leq \lambda_A \|f\|_{\mathcal{F}} \quad \forall f \in \mathcal{F}.$$ 

Riesz representation theorem: In a Hilbert space $\mathcal{F}$, all bounded linear operators $A$ can be written $\langle \cdot, g_A \rangle_{\mathcal{F}}$, for some $g_A \in \mathcal{F}$,

$$Af = \langle f(\cdot), g_A(\cdot) \rangle_{\mathcal{F}}$$
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Does the feature space mean exist?

Existence of mean embedding: If \( E_P \sqrt{k(x, x)} = E_P \|\varphi(x)\|_F < \infty \) then \( \exists \mu_P \in \mathcal{F} \).

Proof:

The linear operator \( T_P f := E_P f(x) \) for all \( f \in \mathcal{F} \) is bounded under the assumption, since

\[
|T_P f| = |E_P f(x)|.
\]
\[
\leq E_P |f(x)|
\]
\[
= E_P |\langle f, \varphi(x) \rangle_\mathcal{F}|
\]
\[
\leq E_P \left( \sqrt{k(x, x)} \|f\|_F \right)
\]

Hence by Riesz (with \( \lambda_{T_P} = E_P \sqrt{k(x, x)} \)), \( \exists \mu_P \in \mathcal{F} \) such that

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Existence of mean embedding: If $E_P \sqrt{k(x,x)} = E_P \|\varphi(x)\|_F < \infty$ then $\exists \mu_P \in \mathcal{F}$.

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Hence by Riesz (with $\lambda_{T_P} = E_P \sqrt{k(x,x)}$, $\exists \mu_P \in \mathcal{F}$ such that

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Proof:

The linear operator $T_Pf := E_Pf(x)$ for all $f \in \mathcal{F}$ is bounded under the assumption, since

$$|T_Pf| = |E_Pf(x)|.$$

$$\leq E_P |f(x)|$$

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

$$\leq E_P \left( \sqrt{k(x, x)} \|f\|_F \right).$$

Hence by Riesz (with $\lambda_{TP} = E_P \sqrt{k(x, x)}$), $\exists \mu_P \in \mathcal{F}$ such that

$$T_Pf = \langle f, \mu_P \rangle_{\mathcal{F}}.$$
Does the feature space mean exist?

Existence of mean embedding: If $E_P \sqrt{k(x, x)} = E_P \|\varphi(x)\|_F < \infty$ then $\exists \mu_P \in \mathcal{F}$.

Proof:

The linear operator $T_P f := E_P f(x)$ for all $f \in \mathcal{F}$ is bounded under the assumption, since

$$|T_P f| = |E_P f(x)| \leq E_P |f(x)| = E_P \left|\langle f, \varphi(x) \rangle_\mathcal{F} \right| \leq E_P \left(\sqrt{k(x, x)} \|f\|_F \right)$$

Hence by Riesz (with $\lambda_{T_P} = E_P \sqrt{k(x, x)}$), $\exists \mu_P \in \mathcal{F}$ such that

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Proof:
The linear operator $T_P f := \mathbb{E}_P f(x)$ for all $f \in \mathcal{F}$ is bounded under the assumption, since

$$|T_P f| = |\mathbb{E}_P f(x)|.$$ 

$$\leq \mathbb{E}_P |f(x)|$$ 

$$= \mathbb{E}_P |\langle f, \varphi(x) \rangle_\mathcal{F}|$$ 

$$\leq \mathbb{E}_P \left( \sqrt{k(x, x)} \|f\|_\mathcal{F} \right)$$

Hence by Riesz (with $\lambda_{T_P} = \mathbb{E}_P \sqrt{k(x, x)}$), $\exists \mu_P \in \mathcal{F}$ such that

$$T_P f = \langle f, \mu_P \rangle_\mathcal{F}.$$
The maximum mean discrepancy is the distance between feature means:

\[
MMD^2(P, Q) = \|\mu_P - \mu_Q\|^2_F
\]

\[
= \langle \mu_P, \mu_P \rangle_F + \langle \mu_Q, \mu_Q \rangle_F - 2 \langle \mu_P, \mu_Q \rangle_F
\]

\[
= E_P k(X, X') + E_Q k(Y, Y') - 2E_{P,Q} k(X, Y)
\]

(a) (a) (b)
The maximum mean discrepancy

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

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\[
= \mathbb{E}_P k(X, X') + \mathbb{E}_Q k(Y, Y') - 2\mathbb{E}_{P, Q} k(X, Y)
\]

(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:

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

$$- \frac{2}{n^2} \sum_{i,j} k(\text{dog}_i, \text{fish}_j)$$
MMD as an integral probability metric

Are $P$ and $Q$ different?

![Samples from P and Q](image)
MMD as an integral probability metric

Are $P$ and $Q$ different?

Samples from $P$ and $Q$
MMD as an integral probability metric

Integral probability metric:
Find a "well behaved function" $f(x)$ to maximize

$$E_P f(X) - E_Q f(Y)$$
MMD as an integral probability metric

Integral probability metric:
Find a "well behaved function" $f(x)$ to maximize

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MMD as an integral probability metric

What if the function is not smooth?

$$E_P f(X) - E_Q f(Y)$$
MMD as an integral probability metric

What if the function is not smooth?

\[ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \]
MMD as an integral probability metric

Maximum mean discrepancy: smooth function for $P$ vs $Q$

\[
MMD(P, Q; F) := \sup_{\|f\| \leq 1} \left[ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \right]
\]  
($F = \text{unit ball in RKHS } \mathcal{F}$)
MMD as an integral probability metric

Maximum mean discrepancy: smooth function for $P$ vs $Q$

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

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

Functions are linear combinations of features:

$$f(x) = \langle f, \varphi(x) \rangle_{\mathcal{F}} = \sum_{\ell=1}^{\infty} f_\ell \varphi_\ell(x)$$

$$\|f\|^2_{\mathcal{F}} := \sum_{i=1}^{\infty} f_i^2 \leq 1$$
MMD as an integral probability metric

Maximum mean discrepancy: smooth function for \( P \) vs \( Q \)

\[
MMD(P, Q; F) := \sup_{\|f\| \leq 1} [E_P f(X) - E_Q f(Y)]
\]

\( F = \text{unit ball in RKHS } \mathcal{F} \)
MMD as an integral probability metric

Maximum mean discrepancy: smooth function for $P$ vs $Q$

$$\text{MMD}(P, Q; F) := \sup_{|f| \leq 1} [E_P f(X) - E_Q f(Y)]$$

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

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

Other choices for witness function class:

- Bounded continuous [Dudley, 2002]
- Bounded variation 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 $Q$

$$MMD(P, Q; F) := \sup_{\|f\| \leq 1} [E_P f(X) - E_Q f(Y)]$$

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

Reminder for next slide: expectations of functions are linear combinations of expected features

$$E_P(f(X)) = \langle f, \mu_P \rangle_{\mathcal{F}}$$

(always true if kernel is bounded)
Integral prob. metric vs feature difference

The MMD:

\[ \text{MMD}(P, Q; F') = \sup_{f \in F} [E_P f(X) - E_Q f(Y)] \]
The MMD:

\[ MMD(P, Q; F) = \sup_{f \in F} \mathbb{E} Pf(X) - \mathbb{E} Qf(Y) \]

\[ = \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_F \]

use

\[ \mathbb{E} Pf(X) = \langle \mu_P, f \rangle_F \]
Integral prob. metric vs feature difference

The MMD:

$$MMD(P, Q; F') = \sup_{f \in F} \left[ E_P f(X) - E_Q f(Y) \right]$$

$$= \sup_{f \in F} \left( f, \mu_P - \mu_Q \right)_F$$
Integral prob. metric vs feature difference

The MMD:

\[
\begin{align*}
\text{MMD}(P, Q; F) &= \sup_{f \in F} [E_P f(X) - E_Q f(Y)] \\
 &= \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_F
\end{align*}
\]
Integral prob. metric vs feature difference

The MMD:

\[
\text{MMD}(P, Q; F) = \sup_{f \in F} \left\{ \mathbb{E}_P f(X) - \mathbb{E}_Q f(Y) \right\} \\
= \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_F
\]

\[
f^* = \frac{\mu_P - \mu_Q}{\| \mu_P - \mu_Q \|}
\]
Integral prob. metric vs feature difference

The MMD:

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

\[
= \sup_{f \in F} \langle f, \mu_P - \mu_Q \rangle_F
\]

\[
= \| \mu_P - \mu_Q \|
\]

Function view and feature view equivalent
Construction of MMD witness

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

Observe $X = \{x_1, \ldots, x_n\} \sim P$

Observe $Y = \{y_1, \ldots, y_n\} \sim Q$
Construction of MMD witness

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

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

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

Recall the witness function expression

\[ f^* \propto \mu_P - \mu_Q \]
Derivation of empirical witness function

Recall the witness function expression

\[ f^* \propto \mu_P - \mu_Q \]

The empirical feature mean for \( P \)

\[ \hat{\mu}_P := \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i) \]
**Derivation of empirical witness function**

Recall the **witness function** expression

\[ f^* \propto \mu_P - \mu_Q \]

The empirical feature mean for \( P \)

\[ \hat{\mu}_P := \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i) \]

The empirical witness function at \( v \)

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

\[ f^*(v) = \langle f^*, \varphi(v) \rangle_F \]
\[ \propto \langle \hat{\mu}_P - \hat{\mu}_Q, \varphi(v) \rangle_F \]
Derivation of empirical witness function

Recall the witness function expression

\[ f^* \propto \mu_P - \mu_Q \]

The empirical feature mean for \( P \)

\[ \hat{\mu}_P := \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i) \]

The empirical witness function at \( v \)

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

\[ \propto \langle \hat{\mu}_P - \hat{\mu}_Q, \varphi(v) \rangle_{\mathcal{F}} \]

\[ = \frac{1}{n} \sum_{i=1}^{n} k(x_i, v) - \frac{1}{n} \sum_{i=1}^{n} k(y_i, v) \]

Don’t need explicit feature coefficients \( f^* := [f_1^* \ f_2^* \ \cdots] \)
Interlude: divergence measures
Divergences
Divergences

Integral prob. metrics

\[ D_\mathcal{H}(P, Q) = \sup_{g \in \mathcal{H}} |\mathbb{E}_{X \sim P} g(X) - \mathbb{E}_{Y \sim Q} g(Y)| \]

F-divergences

\[ D_f(P, Q) = \int_X q(x) f \left( \frac{p(x)}{q(x)} \right) dx \]
Divergences

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

\[ D_f(P, Q) = \int_X q(x) f \left( \frac{p(x)}{q(x)} \right) dx \]
Divergences

**Integral prob. metrics**

- Wasserstein
  \[ D_{\mathcal{H}}(P, Q) = \sup_{g \in \mathcal{H}} |E_{X \sim P} g(X) - E_{Y \sim Q} g(Y)| \]

- MMD

**F-divergences**

- Hellinger
  \[ D_f(P, Q) = \int_X q(x) f \left( \frac{p(x)}{q(x)} \right) dx \]

- KL

- Pearson chi^2
Divergences

\[ D_{\mathcal{H}}(P, Q) = \sup_{g \in \mathcal{H}} |E_{X \sim P} g(X) - E_{Y \sim Q} g(Y)| \]

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

Sriperumbudur, Fukumizu, G, Schoelkopf, Lanckriet (EJS, 2012, Theorem A.1)
Two-Sample Testing with MMD
A statistical test using MMD

The empirical MMD:

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

\[- \frac{2}{n^2} \sum_{i, j} k(x_i, y_j)\]

How does this help decide whether \( P = Q \)?
A statistical test using MMD

The empirical MMD:

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

Perspective from statistical hypothesis testing:

- **Null hypothesis** $\mathcal{H}_0$ when $P = Q$
  - should see $\hat{\text{MMD}}^2$ “close to zero”.
- **Alternative hypothesis** $\mathcal{H}_1$ when $P \neq Q$
  - should see $\hat{\text{MMD}}^2$ “far from zero”
A statistical test using MMD

The empirical MMD:

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

Perspective from statistical hypothesis testing:

- **Null hypothesis** \( \mathcal{H}_0 \) when \( P = Q \)
  - should see \( \hat{\text{MMD}}^2 \) “close to zero”.
- **Alternative hypothesis** \( \mathcal{H}_1 \) when \( P \neq Q \)
  - should see \( \hat{\text{MMD}}^2 \) “far from zero”

Want Threshold \( c_\alpha \) for \( \hat{\text{MMD}}^2 \) to get false positive rate \( \alpha \)
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.
- $\sqrt{n} \times \widehat{MMD}^2 = 1.2$
Behaviour of $\hat{MMD}^2$ when $P \neq Q$

Draw $n = 200$ i.i.d samples from $P$ and $Q$ Laplace with different y-variance.

- $\sqrt{n} \times \hat{MMD}^2 = 1.2$
Behaviour of $\widehat{MMD}^2$ when $P \neq Q$

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

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

Number of MMDs: 2
Behaviour of $\hat{MMD}^2$ when $P \neq Q$

Repeat this 150 times ...
Behaviour of $\overbrace{\text{MMD}^2}^{2}$ when $P \neq Q$

Repeat this 300 times …

Number of MMDs: 300
Behaviour of $\sqrt{n} \times \text{MMD}^2$ when $P \neq Q$

Repeat this 3000 times …

Number of MMDs: 3000
Asymptotics of $\hat{\text{MMD}}^2$ when $P \neq Q$

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

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

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

MMD density under $\mathcal{H}_1$
Behaviour of $\hat{MMD}^2$ when $P = Q$

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

Number of MMDs: 10
Behaviour of $\hat{MMD}^2$ when $P = Q$

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

Number of MMDs: 20
Behaviour of $\hat{MMD}^2$ when $P = Q$

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

Number of MMDs: 50
Behaviour of $\overline{\text{MMD}}^2$ when $P = Q$

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

Number of MMDs: 100
Behaviour of $\hat{MMD}^2$ when $P = Q$

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

Number of MMDs: 1000
Asymptotics of $\widehat{MMD}^2$ when $P = Q$

Where $P = Q$, statistic has asymptotic distribution

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

where

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

and

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

A summary of the asymptotics:

\begin{figure}
\centering
\includegraphics[width=\textwidth]{graph.png}
\caption{A graph showing the probability of \( n \times \hat{MMD}^2 \) for \( P = Q \) and \( P \neq Q \).}
\end{figure}
A statistical test

Test construction: (G., Borgwardt, Rasch, Schoelkopf, and Smola, JMLR 2012)
How do we get test threshold $c_\alpha$?

Original empirical MMD for dogs and fish:

\[ X = \begin{bmatrix} \text{dogs} & \text{dogs} & \text{dogs} & \ldots \end{bmatrix} \]

\[ Y = \begin{bmatrix} \text{fish} & \text{fish} & \text{fish} & \ldots \end{bmatrix} \]

\[
\widehat{\text{MMD}}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} k(x_i, x_j) \\
+ \frac{1}{n(n-1)} \sum_{i \neq j} k(y_i, y_j) \\
- \frac{2}{n^2} \sum_{i,j} k(x_i, y_j)
\]
How do we get test threshold $c_\alpha$?

Permuted dog and fish samples (merdogs):

$$\tilde{X} = \begin{bmatrix} \text{fish} & \text{dog} & \ldots \end{bmatrix}$$

$$\tilde{Y} = \begin{bmatrix} \text{dog} & \text{fish} & \ldots \end{bmatrix}$$
How do we get test threshold $c_\alpha$?

Permuted dog and fish samples (merdogs):

$$\tilde{X} = [\text{dog, fish, [...] }]$$
$$\tilde{Y} = [\text{dog, fish, [...] }]$$

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

Permutation simulates $P = Q$
How to choose the best kernel: optimising the kernel parameters
**Graphical illustration**

- Maximising **test power** same as minimizing **false negatives**

![Graph](image)
The power of our test \( (\Pr_1 \text{ denotes probability under } P \neq Q) \):

\[
\Pr_1 \left( n \hat{\text{MMD}}^2 > \hat{c}_\alpha \right)
\]
Optimizing kernel for test power

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

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

$$\rightarrow \Phi \left( \frac{\text{MMD}^2(P, Q)}{\sqrt{V_n(P, Q)}} - \frac{c_\alpha}{n \sqrt{V_n(P, Q)}} \right)$$

where

- $\Phi$ is the CDF of the standard normal distribution.
- $\hat{c}_\alpha$ is an estimate of $c_\alpha$ test threshold.
Optimizing kernel for test power

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

$$\Pr_1 \left( nMMD^2 > \hat{c}_\alpha \right)$$

$$\to \Phi \left( \frac{MMD^2(P, Q)}{\sqrt{V_n(P, Q)}} \right) - \frac{c_\alpha}{n \sqrt{V_n(P, Q)}}$$

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 ($\Pr_1$ denotes probability under $P \neq Q$):

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

$$\rightarrow \Phi \left( \frac{\text{MMD}^2(P, Q)}{\sqrt{V_n(P, Q)}} - \frac{c_\alpha}{n \sqrt{V_n(P, Q)}} \right)$$

To maximize test power, maximize

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

(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
Troubleshooting for generative adversarial networks

MNIST samples

Samples from a GAN

- Power for **optimized ARD kernel**: 1.00 at $\alpha = 0.01$
- Power for optimized RBF kernel: 0.57 at $\alpha = 0.01$
Troubleshooting generative adversarial networks
Training GANs with MMD
What is a Generative Adversarial Network (GAN)?

- **Generator** *(student)*

  - Task: critic must teach generator to draw images (here dogs)

- **Critic** *(teacher)*
What is a Generative Adversarial Network (GAN)?
What is a Generative Adversarial Network (GAN)?
What is a Generative Adversarial Network (GAN)?
Why is classification not enough?

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

(otherwise student can just produce the same dog over and over)
MMD for GAN critic

Can you use MMD as a critic to train GANs?

From ICML 2015:

Generative Moment Matching Networks

Yujia Li¹
Kevin Swersky¹
Richard Zemel¹,²

¹Department of Computer Science, University of Toronto, Toronto, ON, CANADA
²Canadian 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

Can you use MMD as a critic to train GANs?

Need better image features.
How to improve the critic witness

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

**MMD GAN** Li et al., [NIPS 2017]
**Coulomb GAN** Unterthiner et al., [ICLR 2018]
WGAN-GP

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

Gradient close to 1 here
**WGAN-GP**

**Wasserstein GAN** Arjovsky et al. [ICML 2017]

**WGAN-GP** Gukrajani et al. [NeurIPS 2017]

- Given a generator $G_\theta$ with parameters $\theta$ to be trained. Samples $Y \sim G_\theta(Z)$ where $Z \sim R$

- Given critic features $h_\psi$ with parameters $\psi$ to be trained. $f_\psi$ a **linear function** of $h_\psi$. 


**WGANGP**

**Wasserstein GAN** Arjovsky et al. [ICML 2017]

**WGANGP** Gukrajani et al. [NeurIPS 2017]

- Given a generator $G_\theta$ with parameters $\theta$ to be trained.
  
  Samples $Y \sim G_\theta(Z)$ where $Z \sim \mathbb{R}$

- Given critic features $h_\psi$ with parameters $\psi$ to be trained. $f_\psi$ a linear function of $h_\psi$.

**WGANGP** gradient penalty:

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

where

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

$\gamma \sim \mathcal{U}([0, 1])$  $x_i \in \{x_l\}_{l=1}^m$  $z_j \in \{z_l\}_{l=1}^n$
The (W)MMD

Train MMD critic features with the witness function gradient penalty
Binkowski, Sutherland, Arbel, G. [ICLR 2018], Bellemare et al. [2017] for energy distance:

$$\max_{\psi} \text{MMD}^2(h_{\psi}(X), h_{\psi}(G_{\theta}(Z))) + \lambda \mathbb{E}_{\tilde{X}} \left(\|\nabla_{\tilde{X}} f_{\psi}(\tilde{X})\| - 1\right)^2$$

where

$$f_{\psi}(\cdot) = \frac{1}{m} \sum_{i=1}^{m} k(h_{\psi}(x_i), \cdot) - \frac{1}{n} \sum_{j=1}^{n} k(h_{\psi}(G_{\theta}(z_j)), \cdot)$$

New

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

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

Remark by Bottou et al. (2017): gradient penalty modifies the function class. So critic is not an MMD in RKHS $\mathcal{F}$. 
MMD for GAN critic: revisited

Samples are better!
MMD for GAN critic: revisited

Samples are better!

Can we do better still?
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]

The Dirac-GAN

\[ P = \delta_0 \quad Q = \delta_\theta \quad f_\psi(x) = \psi \cdot x \]
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]

The Dirac-GAN

\[ P = \delta_0 \quad Q = \delta_\theta \quad f_\psi(x) = \psi \cdot x \]

Figure from Mescheder et al. [ICML 2018]
A better gradient penalty

- New MMD GAN witness regulariser (NeurIPS 2018)
  Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
- Based on semi-supervised learning regulariser Bousquet et al. [NeurIPS 2004]
- Related to Sobolev GAN Mroueh et al. [ICLR 2018]
A better gradient penalty

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A better gradient penalty

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- **Based on semi-supervised learning regulariser** Bousquet et al. [NeurIPS 2004]
- **Related to Sobolev GAN** Mroueh et al. [ICLR 2018]

Modified witness function:

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

where

\[
\|f\|_S^2 = \|f\|_{L_2(P)}^2 + \|\nabla f\|_{L_2(P)}^2 + \lambda \|f\|_k^2
\]

- L₂ norm control
- Gradient control
- RKHS smoothness
A better gradient penalty

- **New MMD GAN witness regulariser (NeurIPS 2018)**
  - Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
- **Based on semi-supervised learning regulariser** Bousquet et al. [NeurIPS 2004]
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\]

where

\[
\|f\|_S^2 = \|f\|_{L_2(P)}^2 + \|\nabla f\|_{L_2(P)}^2 + \lambda \|f\|_{k}^2
\]

**Problem:** not computationally feasible: \(O(n^3)\) per iteration.
A better gradient penalty

- **New MMD GAN witness regulariser** (NeurIPS 2018)
  Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
- Based on **semi-supervised learning regulariser** Bousquet et al. [NeurIPS 2004]
- Related to **Sobolev GAN** Mroueh et al. [ICLR 2018]

The scaled MMD:

\[ \text{SMMD} = \sigma_{k, \mathcal{P}, \lambda} \ MMD \]

where

\[
\sigma_{k, \mathcal{P}, \lambda} = \left( \lambda + \int k(x, x) \ d\mathcal{P}(x) + \sum_{i=1}^{d} \int \partial_i \partial_{i+d} k(x, x) \ d\mathcal{P}(x) \right)^{-1/2}
\]

Replace expensive constraint with **cheap upper bound**:

\[
\|f\|_{S}^2 \leq \sigma_{k, \mathcal{P}, \lambda}^{-1} \|f\|_{k}^2
\]
A better gradient penalty

- New MMD GAN witness regulariser (NeurIPS 2018)
  Arbel, Sutherland, Binkowski, G. [NeurIPS 2018]
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The scaled MMD:

$$SMMD = \sigma_{k, P, \lambda} MMD$$

where

$$\sigma_{k, P, \lambda} = \left( \lambda + \int k(x, x) dP(x) + \sum_{i=1}^{d} \int \partial_i \partial_i + d k(x, x) dP(x) \right)^{-1/2}$$

Replace expensive constraint with cheap upper bound:

$$\|f\|_{S}^2 \leq \sigma_{k, P, \lambda}^{-1} \|f\|_{k}^2$$

Idea: rather than regularise the critic or witness function, regularise features directly
Evaluation and experiments
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).
Evaluation of GANs

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

High when:

- predictive label distribution $P(y|x)$ has low entropy (good quality images)
- label entropy $P(y)$ is high (good variety).

**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 \(\mu_P\) and \(\Sigma_P\) are the feature mean and covariance of \(P\)
Evaluation of GANs

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Heusel et al. [NeurIPS 2017]

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\]

where \( \mu_P \) and \( \Sigma_P \) 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 practice.

Let $d = 2048$, and define

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

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

For a random draw of $C$:

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

With $m = 50,000$ samples,

$$\text{FID}(\widehat{P}_1, Q) \approx 1133.7 < 1136.2 \approx \text{FID}(\widehat{P}_2, Q)$$

At $m = 100,000$ samples, the ordering of the estimates is correct. This behavior is similar for other random draws of $C$. 
Evaluation of GANs

The FID can give the wrong answer in practice.
Let \( d = 2048 \), and define

\[
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For a random draw of \( C \):

\[
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\]

With \( m = 50000 \) samples,

\[
FID(\hat{P}_1, Q) \approx 1133.7 < 1136.2 \approx FID(\hat{P}_2, Q)
\]

At \( m = 100000 \) samples, the ordering of the estimates is correct. This behavior is similar for other random draws of \( C \).
Evaluation of GANs

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Evaluation of GANs

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

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At $m = 100000$ samples, the ordering of the estimates is correct.

This behavior is similar for other random draws of $C$. 

---

67/75
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
The kernel inception distance (KID)

The Kernel inception distance  Binkowski, Sutherland, Arbel, G.  [ICLR 2018]
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...“but isn’t KID is computationally costly?”
The kernel inception distance (KID)

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

...“but isn’t KID is computationally costly?”

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

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

[Bounliphone et al. ICLR 2016]
Benchmarks for comparison (all from ICLR 2018)

Spectral Normalization for Generative Adversarial Networks
Takeru Miyato¹, Toshiki Kataoka¹, Masanori Koyama², Yuichi Yoshida³
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²koyama.masanori1@gmail.com
³yoshida@三菱电机ac.jp

Sobolev GAN
Youssef Mroueh¹, Chun-Liang Li²⁺*, Tom Sercu¹⁺*, Anant Raj³⁺ & Yu Cheng¹
¹IBM Research AI
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³Max Planck Institute for Intelligent Systems
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tom.sercul@ibm.com, anant.raj@tuebingen.mpg.de

Demystifying MMD GANs
Mikołaj Bifikowski¹
Department of Mathematics
Imperial College London
mikbinkowski@gmail.com

Boundary-Seeking Generative Adversarial Networks
R Devon Hjelm¹
MILA, University of Montréal, IVADO
eroneus@gmail.com

We combine with scaled MMD

Our ICLR 2018 paper
Results: what does MMD buy you?

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

MMD GAN samples, $f = 64$, KID=3

WGAN samples, $f = 64$, KID=4
Results: what does MMD buy you?

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

MMD GAN samples, $f = 16$, KID=9

WGAN samples, $f = 16$, $f = 64$, KID=37 70/75
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. Around 20 000 classes.
Results: unconditional imagenet $64 \times 64$

KID scores:

- **BGAN:**
  - 47

- **SN-GAN:**
  - 44

- **SMMD GAN:**
  - 35

ILSVRC2012 (ImageNet) dataset, 1,281,167 images, resized to $64 \times 64$. Around 20,000 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. Around 20 000 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 \( h_\psi \) features possible.
  - Better gradient/feature regulariser gives better critic

“Generative Models and Model Criticism via Optimized Maximum Mean Discrepancy,” ICLR 2017 [https://github.com/dougalsutherland/opt-mmd](https://github.com/dougalsutherland/opt-mmd)

“Demystifying MMD GANs,” including KID score, ICLR 2018: [https://github.com/mbinkowski/MMD-GAN](https://github.com/mbinkowski/MMD-GAN)

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Questions?