Representing and comparing probabilities with kernels: Part 3

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MLSS Madrid, 2018
Training GANs with MMD
What is a Generative Adversarial Network (GAN)?

- **Generator (student)**
- **Critic (teacher)**

- Task: critic must teach generator to draw images (here dogs)
What is a Generative Adversarial Network (GAN)?
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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 Li
Kevin Swersky
Richard Zemel

1Department of Computer Science, University of Toronto, Toronto, ON, CANADA
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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. [NIPS 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 $h_\psi$. 
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 $h_\psi$.

**WGAN-GP** gradient penalty:

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

where

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

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

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

\[
\tilde{X} = \gamma x_i + (1 - \gamma) G_\psi(z_j)
\]

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

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

From ICLR 2018:

DEMYSTIFYING MMD GANs

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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 [NIPS 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
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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 (just accepted, NIPS 2018)
  Arbel, Sutherland, Binkowski, G. [NIPS 2018]
- Based on semi-supervised learning regulariser Bousquet et al. [NIPS 2004]
- Related to Sobolev GAN Mroueh et al. [ICLR 2018]
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Modified witness function:

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

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**

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Modified witness function:

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where

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\]

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

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The scaled MMD:

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

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:

$$\|f\|_S^2 \leq \sigma_{k,P,\lambda}^{-1} \|f\|_k^2$$
A better gradient penalty

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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
Evaluation of GANs

The inception score? Salimans et al. [NIPS 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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**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. [NIPS 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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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 theory.

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

Given two alternatives:

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

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

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

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

For a random draw of $C$:

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

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 $C$. 
Evaluation of GANs

The FID can give the **wrong answer in practice**.

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

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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 \( KID(\hat{P}_{t+1}, Q) \) not significantly better than \( KID(\hat{P}_t, Q) \) 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]
Benchmark for comparison (all from ICLR 2018)

SPECTRAL NORMALIZATION FOR GENERATIVE ADVERSARIAL NETWORKS

Takeru Miyato, Toshiki Kataoka, Masanori Koyama, Yuichi Yoshida

Sobolev GAN

Youssef Mroueh¹, Chun-Liang Li², Tom Sercu¹, Anant Raj² & Yu Cheng¹

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Demystifying MMD GANs

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Boundary-Seeking Generative Adversarial Networks

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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 $64 \times 64$.

MMD GAN samples, $f = 64$, FID=32, KID=3

WGAN samples, $f = 64$, FID=41, 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 $64 \times 64$.

MMD GAN samples, $f = 16$, FID=86, KID=9

WGAN samples, $f = 16$, $f = 64$, FID=293, KID=37
The kernel inception distance (KID)

Faster training: performance scores vs generator iterations on MNIST
Results: celebrity faces $160 \times 160$

KID (FID) scores:

- Sobolev GAN: 14 (20)
- SN-GAN: 18 (28)
- Old MMD GAN: 13 (21)
- SMMD GAN: 6 (12)

202,599 face images, resized and cropped to $160 \times 160$
Results: imagenet $64 \times 64$

KID (FID) scores:

- **BGAN:** 47 (44)
- **SN-GAN:** 44 (48)
- **SMMD GAN:** 35 (37)

ILSVRC2012 (ImageNet) dataset, 1,281,167 images, resized to $64 \times 64$. Around 20,000 classes.
Results: imagenet 64×64

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ILSVRC2012 (ImageNet) dataset, 1 281 167 images, resized to 64 × 64. Around 20 000 classes.
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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


Code for new SMMD:
https://github.com/MichaelArbel/Scaled-MMD-GAN
Testing against a probabilistic model
Statistical model criticism

\[ MMD(P, Q) = \|f^*\|^2 = \sup_{\|f\|_{\mathcal{F}} \leq 1} [E_Q f - E_P f] \]

\( f^*(x) \) is the witness function

Can we compute MMD with samples from \( Q \) and a model \( P \)?

**Problem:** usually can’t compute \( E_P f \) in closed form.
Stein idea

To get rid of $E_p f$ in

$$\sup_{\|f\|_{\mathcal{F}} \leq 1} [E_q f - E_p f]$$

we define the Stein operator

$$[T_p f](x) = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x))$$

Then

$$E_P T_P f = 0$$

subject to appropriate boundary conditions. (Oates, Girolami, Chopin, 2016)
Stein idea: proof

\[ E_p \left[ T_p f \right] = \int \left[ \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \right] p(x) dx \]

\[ = \int \left[ \frac{d}{dx} (f(x)p(x)) \right] dx \]

\[ = [f(x)p(x)]_{-\infty}^{\infty} \]

\[ = 0 \]
Stein idea: proof

$$E_p [T_p f] = \int \left[ \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \right] p(x) dx$$

$$\int \left[ \frac{d}{dx} (f(x)p(x)) \right] dx$$

$$= [f(x)p(x)]_{-\infty}^{\infty}$$

$$= 0$$
Stein idea: proof

\[ E_p [T_p f] = \int \left[ \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \right] p(x) \, dx \]
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\[ = 0 \]
Kernel Stein Discrepancy

Stein operator

\[ T_p f = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \]

Kernel Stein Discrepancy (KSD)

\[ KSD(p, q, \mathcal{F}) = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g - E_p T_p g \]
Kernel Stein Discrepancy

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\[ T_p f = \frac{1}{p(x)} \frac{d}{dx} (f(x)p(x)) \]

Kernel Stein Discrepancy (KSD)

\[
KSD(p, q, F) = \sup_{\|g\|_{F} \leq 1} E_q T_p g - \underbrace{E_p T_p g}_{= 0} = \sup_{\|g\|_{F} \leq 1} E_q T_p g
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Kernel Stein Discrepancy (KSD)

\[ KSD(p, q, \mathcal{F}) = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g - E_p T_p g = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g \]

\[ p(x) \quad q(x) \quad g^*(x) \]
**Kernel Stein Discrepancy**

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**Kernel Stein Discrepancy (KSD)**

\[
KSD(p, q, \mathcal{F}) = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g - E_p T_p g = \sup_{\|g\|_{\mathcal{F}} \leq 1} E_q T_p g
\]
Kernel stein discrepancy

Closed-form expression for KSD: given \( Z, Z' \sim q \), then

(Chwialkowski, Strathmann, G., ICML 2016) (Liu, Lee, Jordan ICML 2016)

\[
\text{KSD}(p, q, \mathcal{F}) = E_q h_p(Z, Z')
\]

where

\[
h_p(x, y) := \partial_x \log p(x) \partial_x \log p(y) k(x, y)
+ \partial_y \log p(y) \partial_x k(x, y)
+ \partial_x \log p(x) \partial_y k(x, y)
+ \partial_x \partial_y k(x, y)
\]

and \( k \) is RKHS kernel for \( \mathcal{F} \)

Only depends on kernel and \( \partial_x \log p(x) \). Do not need to normalize \( p \), or sample from it.
Statistical model criticism

Chicago crime data
Statistical model criticism

Chicago crime data
Model is Gaussian mixture with two components.
Statistical model criticism

Chicago crime data

Model is Gaussian mixture with two components

Stein witness function
Chicago crime data

Model is Gaussian mixture with ten components.
Statistical model criticism

Chicago crime data

Model is Gaussian mixture with ten components

Stein witness function

Code: https://github.com/karlnapf/kernel_goodness_of_fit
Kernel stein discrepancy

Further applications:

- Evaluation of approximate MCMC methods.
  (Chwialkowski, Strathmann, G., ICML 2016; Gorham, Mackey, ICML 2017)

What kernel to use?

- The inverse multiquadric kernel,

\[ k(x, y) = \left( c + \|x - y\|_2^2 \right)^\beta \]

for \( \beta \in (-1, 0) \).
Testing statistical dependence
## Dependence testing

- **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="dog.png" alt="Dog" /></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="beagle.png" alt="Beagle" /></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="cat.png" alt="Cat" /></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](http://dogtime.com) and [petfinder.com](http://petfinder.com)
MMD as a dependence measure?

Could we use MMD?

\[ MMD(P_{XY}, P_X P_Y, \mathcal{H}_\kappa) \]

- We don’t have samples from \( Q := P_X P_Y \), only pairs \( \{(x_i, y_i)\}_{i=1}^n \text{i.i.d. } P_{XY} \)
  - Solution: simulate \( Q \) with pairs \((x_i, y_j)\) for \( j \neq i \).

- What kernel \( \kappa \) to use for the RKHS \( \mathcal{H}_\kappa \)?
MMD as a dependence measure?

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MMD as a dependence measure

Kernel $k$ on images with feature space $\mathcal{F}$,

$$k(\text{dog}, \text{cat})$$

Kernel $l$ on captions with feature space $\mathcal{G}$,

$$l(\text{A large animal who slings slobber, ...}, \text{A responsive, interactive pet ...})$$
MMD as a dependence measure

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Kernel $l$ on captions with feature space $\mathcal{G}$,

$$l(\text{A large animal who slings slobber, ...}, \text{A responsive, interactive pet, ...})$$

Kernel $\kappa$ on image-text pairs: are images and captions similar?

$$\kappa(\text{A large animal who slings slobber, ...}, \text{A responsive, interactive pet, ...}) = k(\text{dog, cat}) \times l(\text{A large animal who slings slobber, ...}, \text{A responsive, interactive pet, ...})$$
MMD as a dependence measure

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

\[
MMD^2(\hat{P}_{XY}, \hat{P}_X \hat{P}_Y, \mathcal{H}_\kappa) := \frac{1}{n^2} \text{trace}(KL)
\]

($K, L$ column centered)
MMD as a dependence measure

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

$$MMD^2(\hat{P}_{XY}, \hat{P}_X \hat{P}_Y, \mathcal{H}_\kappa) := \frac{1}{n^2} \text{trace}(KL)$$

Text from dogtime.com and petfinder.com
MMD as a dependence measure

Two questions:

- **Why the product kernel?** Many ways to combine kernels - why not e.g. a sum?
- Is there a more interpretable way of defining this dependence measure?
Illustration: dependence $\neq$ correlation

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

### Correlation: 0.88

![Scatter plot with correlation 0.88](image-url)
Illustration: dependence $\neq$ correlation

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

![Scatter plot with correlation 0.07](image)

Correlation: 0.07
Illustration: dependence ≠ correlation

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

![Correlation: 0.00](image)
Finding covariance with smooth transformations

Illustration: two variables with no correlation but strong dependence.
Finding covariance with smooth transformations

Illustration: two variables with no correlation but strong dependence.
Finding covariance with smooth transformations

Illustration: two variables with no correlation but strong dependence.
Define two spaces, one for each witness

**Function in** $\mathcal{F}$

\[
f(x) = \sum_{j=1}^{\infty} f_j \varphi_j(x)
\]

**Feature map**

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

**Kernel for RKHS $\mathcal{F}$ on $\mathcal{X}$:**

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

**Function in** $\mathcal{G}$

\[
g(y) = \sum_{j=1}^{\infty} g_j \phi_j(y)
\]

**Feature map**

\[
\phi(y) = \begin{bmatrix}
\phi_1(y) \\
\phi_2(y) \\
\phi_3(y) \\
\vdots
\end{bmatrix}
\]

**Kernel for RKHS $\mathcal{G}$ on $\mathcal{Y}$:**

\[
l(x, x') = \langle \phi(y), \phi(y') \rangle_{\mathcal{G}}
\]
The constrained covariance is

\[
\text{COCO}(P_{XY}) = \sup \text{cov}[f(x)g(y)]
\]

\[
\|f\|_F \leq 1
\]

\[
\|g\|_g \leq 1
\]
The constrained covariance

The constrained covariance is

$$\text{COCO}(P_{XY}) = \sup_{\|f\|_F \leq 1, \|g\|_g \leq 1} \text{cov} \left[ \left( \sum_{j=1}^{\infty} f_j \varphi_j(x) \right) \left( \sum_{j=1}^{\infty} g_j \varphi_j(y) \right) \right]$$
The constrained covariance

The constrained covariance is

\[
\text{COCO}(P_{XY}) = \sup_{\|f\|_{\mathcal{F}} \leq 1, \|g\|_{\mathcal{G}} \leq 1} E_{xy} \left[ \left( \sum_{j=1}^{\infty} f_j \varphi_j(x) \right) \left( \sum_{j=1}^{\infty} g_j \phi_j(y) \right) \right]
\]

Fine print: feature mappings \(\varphi(x)\) and \(\phi(y)\) assumed to have zero mean.
The constrained covariance

The constrained covariance is

\[
\text{COCO}(P_{XY}) = \sup \quad E_{xy} \left[ \left( \sum_{j=1}^{\infty} f_j \varphi_j(x) \right) \left( \sum_{j=1}^{\infty} g_j \phi_j(y) \right) \right]
\]

\[
\|f\|_F \leq 1 \\
\|g\|_g \leq 1
\]

Fine print: feature mappings \( \varphi(x) \) and \( \phi(y) \) assumed to have zero mean.

Rewriting:

\[
E_{xy}[f(x)g(y)]
\]

\[
= \begin{bmatrix} f_1 \\ f_2 \\ \vdots \end{bmatrix}^\top \quad E_{xy} \left( \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \vdots \end{bmatrix} \right) \left( \begin{bmatrix} \phi_1(y) & \phi_2(y) & \ldots \end{bmatrix} \right) \begin{bmatrix} g_1 \\ g_2 \\ \vdots \end{bmatrix}
\]

\[
C_{\varphi(x)\phi(y)}
\]
The constrained covariance

The constrained covariance is

$$\text{COCO}(P_{XY}) = \sup_{\|f\|_{\mathcal{F}} \leq 1, \|g\|_{\mathcal{G}} \leq 1} E_{xy} \left[ \left( \sum_{j=1}^{\infty} f_j \varphi_j(x) \right) \left( \sum_{j=1}^{\infty} g_j \phi_j(y) \right) \right]$$

Fine print: feature mappings $\varphi(x)$ and $\phi(y)$ assumed to have zero mean.

Rewriting:

$$E_{xy}[f(x)g(y)] = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \end{bmatrix}^\top \underbrace{E_{xy} \begin{bmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \vdots \end{bmatrix} \begin{bmatrix} \phi_1(y) & \phi_2(y) & \ldots \end{bmatrix}}_{C_{\varphi(x)\phi(y)}} \begin{bmatrix} g_1 \\ g_2 \\ \vdots \end{bmatrix}$$

COCO: max singular value of feature covariance $C_{\varphi(x)\phi(y)}$
Given sample \( \{(x_i, y_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} P_{XY} \), what is empirical \( \widehat{COCO} \)?
Computing COCO in practice

Given sample \( \{(x_i, y_i)\}_{i=1}^{n} \overset{\text{i.i.d.}}{\sim} P_{XY} \), what is empirical \( \widehat{\text{COCO}} \)?

\( \widehat{\text{COCO}} \) is largest eigenvalue \( \gamma_{\text{max}} \) of

\[
\begin{bmatrix}
0 & \frac{1}{n} KL \\
\frac{1}{n} LK & 0
\end{bmatrix}
\begin{bmatrix}
\alpha \\
\beta
\end{bmatrix}
= \gamma
\begin{bmatrix}
K & 0 \\
0 & L
\end{bmatrix}
\begin{bmatrix}
\alpha \\
\beta
\end{bmatrix}.
\]

\( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(y_i, y_j) \).

**Fine print:** kernels are computed with empirically centered features \( \varphi(x) - \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i) \) and \( \phi(y) - \frac{1}{n} \sum_{i=1}^{n} \phi(y_i) \).

G., Smola., Bousquet, Herbrich, Belitski, Augath, Murayama, Pauls, Schoelkopf, and Logothetis, AISTATS’05
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Given sample \( \{(x_i, y_i)\}_{i=1}^{n} \overset{\text{i.i.d.}}{\sim} P_{XY} \), what is empirical \( \widehat{\text{COCO}} \)?

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\beta
\end{bmatrix}.
\]

\( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(y_i, y_j) \).

Witness functions (singular vectors):

\[
f(x) \propto \sum_{i=1}^{n} \alpha_i k(x_i, x) \quad g(y) \propto \sum_{i=1}^{n} \beta_i l(y_i, y)
\]

Fine print: kernels are computed with empirically centered features \( \varphi(x) - \frac{1}{n} \sum_{i=1}^{n} \varphi(x_i) \) and \( \phi(y) - \frac{1}{n} \sum_{i=1}^{n} \phi(y_i) \).

G., Smola., Bousquet, Herbrich, Belitski, Augath, Murayama, Pauls, Schoelkopf, and Logothetis, AISTATS’05
Empirical COCO: proof (1)

The Lagrangian is

$$\mathcal{L}(f, g, \lambda, \gamma) = \frac{1}{n} \sum_{i=1}^{n} [f(x_i)g(y_i)] - \frac{\lambda}{2} \left( \|f\|_{\mathcal{F}}^2 - 1 \right) - \frac{\gamma}{2} \left( \|g\|_{\mathcal{G}}^2 - 1 \right).$$

\[\text{covariance}\]

\[\text{smoothness constraints}\]

Fine print: $f(x_i)g(y_i)$ centered to have zero empirical mean.
The Lagrangian is

\[
\mathcal{L}(f, g, \lambda, \gamma) = \frac{1}{n} \sum_{i=1}^{n} [f(x_i)g(y_i)] - \frac{\lambda}{2} \left( \|f\|_{\mathcal{F}}^2 - 1 \right) - \frac{\gamma}{2} \left( \|g\|_{\mathcal{G}}^2 - 1 \right).
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**covariance**

**smoothness constraints**

**Fine print:** \(f(x_i)g(y_i)\) centered to have zero empirical mean.

**Assume** (cf representer theorem):

\[
f = \sum_{i=1}^{n} \alpha_i \varphi(x_i) \quad g = \sum_{i=1}^{n} \beta_i \psi(y_i)
\]

for centered \(\varphi(x_i), \phi(y_i)\).
Empirical COCO: proof (1)

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for centered $\varphi(x_i), \phi(y_i)$.

First step is smoothness constraint:

$$\|f\|_F^2 - 1 = \langle f, f \rangle_F - 1$$
The Lagrangian is

$$\mathcal{L}(f, g, \lambda, \gamma) = \frac{1}{n} \sum_{i=1}^{n} [f(x_i)g(y_i)] - \frac{\lambda}{2} \left( \| f \|_{\mathcal{F}}^2 - 1 \right) - \frac{\gamma}{2} \left( \| g \|_{\mathcal{G}}^2 - 1 \right).$$

Fine print: $f(x_i)g(y_i)$ centered to have zero empirical mean.

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First step is smoothness constraint:

$$\| f \|_{\mathcal{F}}^2 - 1 = \langle f, f \rangle_{\mathcal{F}} - 1$$

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Empirical COCO: proof (1)

The Lagrangian is

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\mathcal{L}(f, g, \lambda, \gamma) = \frac{1}{n} \sum_{i=1}^{n} [f(x_i) g(y_i)] - \frac{\lambda}{2} \left\| f \right\|_{\mathcal{F}}^2 - 1 - \frac{\gamma}{2} \left\| g \right\|_{\mathcal{G}}^2 - 1.
\]

\[
\mathcal{L}(f, g, \lambda, \gamma) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} [f(x_i) g(y_i)]}_{\text{covariance}} - \underbrace{\frac{\lambda}{2} \left\| f \right\|_{\mathcal{F}}^2 - 1}_{\text{smoothness constraints}} - \underbrace{\frac{\gamma}{2} \left\| g \right\|_{\mathcal{G}}^2 - 1}_{\text{smoothness constraints}}.
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for centered \(\varphi(x_i), \phi(y_i)\).

First step is smoothness constraint:

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\left\| f \right\|_{\mathcal{F}}^2 - 1 = \langle f, f \rangle_{\mathcal{F}} - 1
\]

\[
= \left\langle \sum_{i=1}^{n} \alpha_i \varphi(x_i), \sum_{i=1}^{n} \alpha_i \varphi(x_i) \right\rangle_{\mathcal{F}} - 1
\]

\[
= \alpha^\top K \alpha - 1
\]
Proof sketch (2)

Second step is covariance:

\[
\frac{1}{n} \sum_{i=1}^{n} [f(x_i)g(y_i)] = \frac{1}{n} \sum_{i=1}^{n} \langle f, \varphi(x_i) \rangle_{\mathcal{F}} \langle g, \varphi(y_i) \rangle_{\mathcal{G}}
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\langle \sum_{\ell=1}^{n} \alpha_{\ell} \varphi(x_{\ell}), \varphi(x_i) \right\rangle_{\mathcal{F}} \langle g, \varphi(y_i) \rangle_{\mathcal{G}}
\]

\[
= \frac{1}{n} \alpha^{\top} K L \beta
\]
Proof sketch (2)

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\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \left\langle \sum_{\ell=1}^{n} \alpha_{\ell} \varphi(x_{\ell}), \varphi(x_i) \right\rangle \mathcal{F} \langle g, \varphi(y_i) \rangle_g
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= \frac{1}{n} \alpha^\top KL \beta
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where \( K_{ij} = k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle_{\mathcal{F}} \) \( L_{ij} = l(y_i, y_j) \).
Proof sketch (2)

Second step is covariance:

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\frac{1}{n} \sum_{i=1}^{n} [f(x_i)g(y_i)] = \frac{1}{n} \sum_{i=1}^{n} \langle f, \varphi(x_i) \rangle_F \langle g, \varphi(y_i) \rangle_G \\
= \frac{1}{n} \sum_{i=1}^{n} \left( \sum_{\ell=1}^{n} \alpha_\ell \varphi(x_\ell), \varphi(x_i) \right) \langle g, \varphi(y_i) \rangle_G \\
= \frac{1}{n} \alpha^T KL \beta
\]

where \( K_{ij} = k(x_i, x_j) = \langle \varphi(x_i), \varphi(x_j) \rangle_F \quad L_{ij} = l(y_i, y_j) \).

The Lagrangian is now:

\[
\mathcal{L}(f, g, \lambda, \gamma) = \frac{1}{n} \alpha^T KL \beta - \frac{\lambda}{2} (\alpha^T K \alpha - 1) - \frac{\gamma}{2} (\beta^T L \beta - 1)
\]
What is a large dependence with COCO?

Density takes the form:

\[ P_{XY} \propto 1 + \sin(\omega x) \sin(\omega y) \]

Which of these is the more “dependent”? 
Finding covariance with smooth transformations

Case of $\omega = 1$:

- Correlation: 0.31
- COCO: 0.09

- Correlation: 0.50
- COCO: 0.09
Finding covariance with smooth transformations

Case of $\omega = 2$:

Correlation: 0.02

Correlation: 0.54  COCO: 0.07
Finding covariance with smooth transformations

Case of $\omega = 3$:
Finding covariance with smooth transformations

Case of $\omega = 4$:
Finding covariance with smooth transformations

Case of $\omega = ??$:

- Correlation: 0.01
- Correlation: 0.14
- COCO: 0.02
Finding covariance with smooth transformations

Case of $\omega = 0$: uniform noise! (shows bias)

---

Correlation: 0.01

Correlation: 0.14  COCO: 0.02

---

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Dependence largest when at “low” frequencies

- As dependence is encoded at higher frequencies, the smooth mappings $f, g$ achieve lower linear dependence.
- Even for independent variables, COCO will not be zero at finite sample sizes, since some mild linear dependence will be found by $f, g$ (bias).
- This bias will decrease with increasing sample size.
Can we do better than COCO?

A second example with zero correlation.

First singular value of feature covariance $C_{\varphi(x)\varphi(y)}$:

\[
\begin{array}{c|c|c|c|c|}
-1 & -0.5 & 0 & 0.5 & 1 \\
\hline
-0.8 & -0.6 & -0.4 & -0.2 & 0 \\
\end{array}
\]

Correlation: 0.80     COCO 1 : 0.11
Can we do better than COCO?

A second example with zero correlation.

Second singular value of feature covariance $C_{\varphi(x)\phi(y)}$:
Can we do better than COCO?

A second example with zero correlation.

Second singular value of feature covariance $\mathcal{C}_\varphi(x)\phi(y)$:
The Hilbert-Schmidt Independence Criterion

Writing the $i$th singular value of the feature covariance $C_{\varphi(x)\varphi(y)}$ as

$$\gamma_i := COCO_i(P_{XY}; \mathcal{F}, \mathcal{G}),$$

define Hilbert-Schmidt Independence Criterion (HSIC)

$$HSIC^2(P_{XY}; \mathcal{F}, \mathcal{G}) = \sum_{i=1}^{\infty} \gamma_i^2.$$
The Hilbert-Schmidt Independence Criterion

Writing the $i$th singular value of the feature covariance $C_{\varphi(x)\phi(y)}$ as

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$$HSIC^2(P_{XY}; \mathcal{F}, \mathcal{G}) = \sum_{i=1}^{\infty} \gamma_i^2.$$ 

G., Bousquet, Smola., and Schoelkopf, ALT05; G.,, Fukumizu, Teo., Song., Schoelkopf., and Smola, NIPS 2007.,

HSIC is MMD with product kernel!

$$HSIC^2(P_{XY}; \mathcal{F}, \mathcal{G}) = MMD^2(P_{XY}, P_X P_Y; \mathcal{H}_\kappa)$$

where $\kappa((x, y), (x', y')) = k(x, x')l(y, y').$
Asymptotics of HSIC under independence

- **Given sample** \( \{(x_i, y_i)\}_{i=1}^n \overset{i.i.d.}{\sim} P_{XY} \), what is empirical \( \widehat{HSIC} \)?

- **Empirical HSIC** (biased)

  \[
  \widehat{HSIC} = \frac{1}{n^2} \text{trace}(KL)
  \]

  \( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(y_i y_j) \) \((K \text{ and } L \text{ computed with empirically centered features}) \)

- **Statistical testing:** given \( P_{XY} = P_X P_Y \), what is the threshold \( c_\alpha \) such that \( P(\widehat{HSIC} > c_\alpha) < \alpha \) for small \( \alpha \)?

- **Asymptotics of \( \widehat{HSIC} \) when \( P_{XY} = P_X P_Y \):

  \[
  n\widehat{HSIC} \xrightarrow{D} \sum_{l=1}^{\infty} \lambda_l z_l^2, \quad z_l \sim \mathcal{N}(0, 1) \text{i.i.d.}
  \]

  where \( \lambda_l \psi_l(z_j) = \int h_{ijqr} \psi_l(z_i) dF_{i,q,r} \), \( h_{ijqr} = \frac{1}{4!} \sum_{(i,j,q,r)} k_{tu} l_{tu} + k_{tu} l_{vw} - 2k_{tu} l_{tv} \)
Asymptotics of HSIC under independence

- Given sample \( \{(x_i, y_i)\}_{i=1}^n \overset{i.i.d.}{\sim} P_{XY} \), what is empirical \( \hat{HSIC} \)?
- Empirical HSIC (biased)

\[
\hat{HSIC} = \frac{1}{n^2} \text{trace}(KL)
\]

\( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(y_i y_j) \) (K and L computed with empirically centered features)

- Statistical testing: given \( P_{XY} = P_X P_Y \), what is the threshold \( c_\alpha \) such that \( P(\hat{HSIC} > c_\alpha) < \alpha \) for small \( \alpha \)?
- Asymptotics of \( \hat{HSIC} \) when \( P_{XY} = P_X P_Y \):

\[
n \hat{HSIC} \overset{D}{\to} \sum_{l=1}^{\infty} \lambda_l z_l^2, \quad z_l \sim N(0, 1) \text{i.i.d.}
\]

where \( \lambda_l \psi_l(z_j) = \int h_{ijqr} \psi_l(z_i) dF_{i,q,r}, \quad h_{ijqr} = \frac{1}{4!} \sum_{(i,j,q,r)} k_{tu} l_{tu} + k_{tu} l_{vw} - 2k_{tu} l_{tv} \)
Asymptotics of HSIC under independence

- Given sample \( \{(x_i, y_i)\}_{i=1}^{n} \overset{\text{i.i.d.}}{\sim} P_{XY} \), what is empirical \( \hat{HSIC} \)?

- **Empirical HSIC** (biased)

\[
\hat{HSIC} = \frac{1}{n^2} \text{trace}(KL)
\]

where \( K_{ij} = k(x_i, x_j) \) and \( L_{ij} = l(y_i y_j) \) (\( K \) and \( L \) computed with empirically centered features)

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A statistical test

- Given $P_{XY} = P_X P_Y$, what is the threshold $c_\alpha$ such that $P(\text{HSIC} > c_\alpha) < \alpha$ for small $\alpha$ (prob. of false positive)?

- Original time series:

  $X_1 \ X_2 \ X_3 \ X_4 \ X_5 \ X_6 \ X_7 \ X_8 \ X_9 \ X_{10}$
  $Y_1 \ Y_2 \ Y_3 \ Y_4 \ Y_5 \ Y_6 \ Y_7 \ Y_8 \ Y_9 \ Y_{10}$

- Permutation:

  $X_1 \ X_2 \ X_3 \ X_4 \ X_5 \ X_6 \ X_7 \ X_8 \ X_9 \ X_{10}$
  $Y_7 \ Y_3 \ Y_9 \ Y_2 \ Y_4 \ Y_8 \ Y_5 \ Y_1 \ Y_6 \ Y_{10}$

- Null distribution via permutation

  - Compute HSIC for $\{x_i, y_{\pi(i)}\}_{i=1}^n$ for random permutation $\pi$ of indices $\{1, \ldots, n\}$. This gives HSIC for independent variables.
  - Repeat for many different permutations, get empirical CDF
  - Threshold $c_\alpha$ is $1 - \alpha$ quantile of empirical CDF
A statistical test

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  \[
  \begin{array}{ccccccccccc}
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  Y_1 & Y_2 & Y_3 & Y_4 & Y_5 & Y_6 & Y_7 & Y_8 & Y_9 & Y_{10}
  \end{array}
  \]

- Permutation:

  \[
  \begin{array}{ccccccccccc}
  X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 & X_8 & X_9 & X_{10} \\
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  \end{array}
  \]

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### Application: dependence detection across languages

#### Testing task: detect dependence between English and French text

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>Honourable senators, I have a question for the Leader of the</td>
<td>Honorables sénateurs, ma question s’adresse au leader du</td>
</tr>
<tr>
<td>Government in the Senate</td>
<td>gouvernement au Sénat</td>
</tr>
<tr>
<td>No doubt there is great pressure on provincial and municipal</td>
<td>Les ordres de gouvernements provinciaux et municipaux subissent</td>
</tr>
<tr>
<td>governments</td>
<td>de fortes pressions</td>
</tr>
<tr>
<td>In fact, we have increased federal investments for early</td>
<td>Au contraire, nous avons augmenté le financement fédéral pour le</td>
</tr>
<tr>
<td>childhood development.</td>
<td>développement des jeunes</td>
</tr>
</tbody>
</table>

Text from the aligned hansards of the 36th parliament of Canada, https://www.isi.edu/natural-language/download/hansard/
**Application: dependence detection across languages**

**Testing task:** detect dependence between English and French text

$k$-spectrum kernel, $k = 10$, sample size $n = 10$

$$\hat{HSIC} = \frac{1}{n^2} \text{trace}(KL)$$

($K$ and $L$ column centered)
Results (for $\alpha = 0.05$)

- k-spectrum kernel: average Type II error 0
- Bag of words kernel: average Type II error 0.18

Settings: Five line extracts, averaged over 300 repetitions, for “Agriculture” transcripts. Similar results for Fisheries and Immigration transcripts.
Testing higher order interactions
Detecting higher order interaction

How to detect V-structures with pairwise weak individual dependence?
Detecting higher order interaction

How to detect V-structures with pairwise weak individual dependence?
Detecting higher order interaction

How to detect V-structures with pairwise weak individual dependence?

\( X \perp Y, \ Y \perp Z, \ X \perp Z \)

\[ \begin{align*}
X_{1} & \text{ vs } Y_{1} \\
Y_{1} & \text{ vs } Z_{1} \\
X_{1} & \text{ vs } Z_{1} \\
X_{1}^*Y_{1} & \text{ vs } Z_{1}
\end{align*} \]

\( X, \ Y \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \)

\( Z | X, Y \sim \text{sign}(XY)Exp(\frac{1}{\sqrt{2}}) \)

Fine print: Faithfulness violated here!
**V-structure discovery**

Assume $X \perp Y$ has been established.

V-structure can then be detected by:

- **Consistent CI test:** $H_0 : X \perp Y \mid Z$ [Fukumizu et al. 2008, Zhang et al. 2011]
- **Factorisation test:** $H_0 : (X, Y) \perp Z \lor (X, Z) \perp Y \lor (Y, Z) \perp X$
  (multiple standard two-variable tests)

How well do these work?
Detecting higher order interaction

Generalise earlier example to $p$ dimensions

$X \perp Y, Y \perp Z, X \perp Z$

$X_1 \text{ vs } Y_1$
$Y_1 \text{ vs } Z_1$
$X_1 \text{ vs } Z_1$
$X_1^*Y_1 \text{ vs } Z_1$

$X, Y \overset{i.i.d.}{\sim} \mathcal{N}(0, 1)$

$Z | X, Y \sim \text{sign}(X Y) \text{Exp}(\frac{1}{\sqrt{2}})$

$X_{2:p}, Y_{2:p}, Z_{2:p} \overset{i.i.d.}{\sim} \mathcal{N}(0, I_{p-1})$

Fine print: Faithfulness violated here!
CI test for $X \perp Y | Z$ from Zhang et al. (2011), and a factorisation test, $n = 500$
Lancaster interaction measure

Lancaster interaction measure of \((X_1, \ldots, X_D) \sim P\) is a signed measure \(\Delta P\) that vanishes whenever \(P\) can be factorised non-trivially.

\[
D = 2 : \quad \Delta_L P = P_{XY} - P_X P_Y
\]
Lancaster interaction measure

Lancaster interaction measure of \((X_1, \ldots, X_D) \sim P\) is a signed measure \(\Delta P\) that vanishes whenever \(P\) can be factorised non-trivially.

\[
D = 2 : \quad \Delta_L P = P_{XY} - P_X P_Y \\
D = 3 : \quad \Delta_L P = P_{XYZ} - P_X P_{YZ} - P_Y P_{XZ} - P_Z P_{XY} + 2 P_X P_Y P_Z
\]
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\(D = 2:\) \hspace{1cm} \Delta_L P = P_{XY} - P_X P_Y
\(D = 3:\) \hspace{1cm} \Delta_L P = P_{XYZ} - P_X P_{YZ} - P_Y P_{XZ} - P_Z P_{XY} + 2P_X P_Y P_Z

\[\Delta_L P =
\begin{align*}
P_{XYZ} & -P_X P_{YZ} \\
X & \quad \quad Y & \quad \quad Z
\end{align*}\]

\[\begin{align*}
P_{XYZ} & -P_Y P_{XZ} \\
X & \quad \quad Y & \quad \quad Z
\end{align*}\]

\[\begin{align*}
P_{XYZ} & -P_Z P_{XY} \\
X & \quad \quad Y & \quad \quad Z
\end{align*}\]

\[\begin{align*}
+2P_X P_Y P_Z \\
X & \quad \quad Y & \quad \quad Z
\end{align*}\]
Lancaster interaction measure

Lancaster interaction measure of \((X_1, \ldots, X_D) \sim P\) is a signed measure \(\Delta P\) that **vanishes** whenever \(P\) can be factorised non-trivially.

\[ D = 2 : \quad \Delta_L P = P_{XY} - P_X P_Y \]
\[ D = 3 : \quad \Delta_L P = P_{XYZ} - P_X P_{YZ} - P_Y P_{XZ} - P_Z P_{XY} + 2P_X P_Y P_Z \]

\(\Delta_L P = 0\)

\[ P_{XYZ} \quad \overline{P_X P_{YZ}} \]

\(\neg P_{XZ} P_Y \quad \neg P_{XY} P_Z \quad +2P_X P_Y P_Z \)

Case of \(P_X \perp \!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\!\![65/71]
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\]

\[
D = 3 : \quad \Delta_L P = P_{XYZ} - P_X P_{YZ} - P_Y P_{XZ} - P_Z P_{XY} + 2 P_X P_Y P_Z
\]

\[(X, Y) \perp\!
\!
\!\perp Z \lor (X, Z) \perp\!
\!
\!\perp Y \lor (Y, Z) \perp\!
\!
\!\perp X \implies \Delta_L P = 0.
\]

...so what might be missed?
Lancaster interaction measure

Lancaster interaction measure of \((X_1, \ldots, X_D) \sim P\) is a signed measure \(\Delta P\) that vanishes whenever \(P\) can be factorised non-trivially.

\[
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\end{align*}
\]

\[\Delta_L P = 0 \not\Rightarrow (X, Y) \perp \!
\!
\!
\perp Z \lor (X, Z) \perp \!
\!
\!
\perp Y \lor (Y, Z) \perp \!
\!
\!
\perp X\]

Example:

<table>
<thead>
<tr>
<th>((0, 0, 0))</th>
<th>((0, 0, 1))</th>
<th>((1, 0, 0))</th>
<th>((1, 0, 1))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>((0, 1, 0))</td>
<td>((0, 1, 1))</td>
<td>((1, 1, 0))</td>
<td>((1, 1, 1))</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.2</td>
</tr>
</tbody>
</table>
A kernel test statistic using Lancaster Measure

Construct a test by estimating $\|\mu_\kappa (\Delta_L P)\|_{\mathcal{H}_\kappa}^2$, where $\kappa = k \otimes l \otimes m$:

$$\|\mu_\kappa (P_{XYZ} - P_{XY} P_Z - \cdots)\|_{\mathcal{H}_\kappa}^2 =$$

$$\langle \mu_\kappa P_{XYZ}, \mu_\kappa P_{XYZ} \rangle_{\mathcal{H}_\kappa} - 2 \langle \mu_\kappa P_{XYZ}, \mu_\kappa P_{XY} P_Z \rangle_{\mathcal{H}_\kappa} \cdots$$
A kernel test statistic using Lancaster Measure

Table: $V$-statistic estimators of $\langle \mu_\kappa \nu, \mu_\kappa \nu' \rangle_{\mathcal{H}_\kappa}$ (without terms $P_X P_Y P_Z$). $H$ is centering matrix $I - n^{-1}$

<table>
<thead>
<tr>
<th>$\nu' \setminus \nu$</th>
<th>$P_{XYZ}$</th>
<th>$P_{XY} P_Z$</th>
<th>$P_{XZ} P_Y$</th>
<th>$P_{YZ} P_X$</th>
<th>$P_X P_Y P_Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{XYZ}$</td>
<td>$(K \circ L \circ M)_{++}$</td>
<td>$((K \circ L) M)_{++}$</td>
<td>$((K \circ M) L)_{++}$</td>
<td>$((M \circ L) K)_{++}$</td>
<td>$tr(K_+ \circ L_+ \circ M_+)$</td>
</tr>
<tr>
<td>$P_{XY} P_Z$</td>
<td>$(K \circ L)<em>{++} M</em>{++}$</td>
<td>$(MKL)_{++}$</td>
<td>$(KLM)_{++}$</td>
<td>$(KL)<em>{++} M</em>{++}$</td>
<td></td>
</tr>
<tr>
<td>$P_{XZ} P_Y$</td>
<td></td>
<td>$(K \circ M)<em>{++} L</em>{++}$</td>
<td>$(KML)_{++}$</td>
<td>$(KM)<em>{++} L</em>{++}$</td>
<td></td>
</tr>
<tr>
<td>$P_{YZ} P_X$</td>
<td></td>
<td></td>
<td>$(L \circ M)<em>{++} K</em>{++}$</td>
<td>$(LM)<em>{++} K</em>{++}$</td>
<td></td>
</tr>
<tr>
<td>$P_X P_Y P_Z$</td>
<td></td>
<td></td>
<td></td>
<td>$K_{++} L_{++} M_{++}$</td>
<td></td>
</tr>
</tbody>
</table>

\[
\lVert \mu_\kappa (\Delta_L P) \rVert_{\mathcal{H}_\kappa}^2 = \frac{1}{n^2} \left( H K H \circ H L H \circ H M H \right)_{++}.
\]

Lancaster interaction statistic: Sejdinovic, G, Bergsma, NIPS13

Empirical joint central moment in the feature space
A kernel test statistic using Lancaster Measure

<table>
<thead>
<tr>
<th>$\nu \setminus \nu'$</th>
<th>$P_{XYZ}$</th>
<th>$P_{XY}P_Z$</th>
<th>$P_{XZ}P_Y$</th>
<th>$P_{YZ}P_X$</th>
<th>$P_XP_YP_Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{XYZ}$</td>
<td>$(K \circ L \circ M)_{++}$</td>
<td>$((K \circ L) M)_{++}$</td>
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<td>$tr(K_+ \circ L_+ \circ M_+)$</td>
</tr>
<tr>
<td>$P_{XY}P_Z$</td>
<td>$(K \circ L)<em>{++} M</em>{++}$</td>
<td>$(MKL)_{++}$</td>
<td>$(KLM)_{++}$</td>
<td>$(KL)<em>{++} M</em>{++}$</td>
<td></td>
</tr>
<tr>
<td>$P_{XZ}P_Y$</td>
<td>$(K \circ M)<em>{++} L</em>{++}$</td>
<td>$(KML)_{++}$</td>
<td>$(KM)<em>{++} L</em>{++}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{YZ}P_X$</td>
<td>$(L \circ M)<em>{++} K</em>{++}$</td>
<td>$(LM)<em>{++} K</em>{++}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_XP_YP_Z$</td>
<td>$K_{++} L_{++} M_{++}$</td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Table: $V$-statistic estimators of $\langle \mu_\kappa \nu, \mu_\kappa \nu' \rangle_{\mathcal{H}_\kappa}$ (without terms $P_XP_YP_Z$). $H$ is centering matrix $I - n^{-1}$

**Lancaster interaction statistic:** Sejdinovic, G, Bergsma, NIPS13

$$||\mu_\kappa (\Delta_L P)||_{\mathcal{H}_\kappa}^2 = \frac{1}{n^2} \left( HKH \circ H LH \circ HMH \right)_{++}.$$

Empirical joint central moment in the feature space
Lancaster test, CI test for $X \perp Y | Z$ from Zhang et al. (2011), and a factorisation test, $n = 500$
Interaction for $D \geq 4$

Interaction measure valid for all $D$:

(Streitberg, 1990)

$$\Delta_S P = \sum_{\pi} (-1)^{|\pi|-1} (|\pi| - 1)! J_\pi P$$

- For a partition $\pi$, $J_\pi$ associates to the joint the corresponding factorisation, e.g., $J_{13|2|4} P = P_{X_1 X_3} P_{X_2} P_{X_4}$. 
Interaction for $D \geq 4$

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Co-authors

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Questions?