Lecture 2: Mappings of Probabilities to RKHS and Applications

Lille, 2014

Arthur Gretton

Gatsby Unit, CSML, UCL
Detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Detecting statistical dependence

- How do you detect dependence...?
- ...in a discrete domain?  [Read and Cressie, 1988]
Detecting statistical dependence

- How do you detect dependence...
- ...in a discrete domain? [Read and Cressie, 1988]
Detecting statistical dependence

- How do you detect dependence...
- ...in a discrete domain?  [Read and Cressie, 1988]

<table>
<thead>
<tr>
<th>P(A,T)</th>
<th>On time</th>
<th>Late</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alarm</td>
<td>0.27</td>
<td>0.03</td>
</tr>
<tr>
<td>No alarm</td>
<td>0.07</td>
<td>0.63</td>
</tr>
</tbody>
</table>
Detecting statistical dependence

- How do you detect dependence...
- ...in a discrete domain?  [Read and Cressie, 1988]

<table>
<thead>
<tr>
<th>P(A,T)</th>
<th>On time</th>
<th>Late</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alarm</td>
<td>0.10</td>
<td>0.20</td>
</tr>
<tr>
<td>No alarm</td>
<td>0.24</td>
<td>0.46</td>
</tr>
</tbody>
</table>
Detecting statistical dependence

- How do you detect dependence...
- ...in a discrete domain? [Read and Cressie, 1988]

$X_1$: Honourable senators, I have a question for the Leader of the Government in the Senate with regard to the support funding to farmers that has been announced. Most farmers have not received any money yet.

$X_2$: No doubt there is great pressure on provincial and municipal governments in relation to the issue of child care, but the reality is that there have been no cuts to child care funding from the federal government to the provinces. In fact, we have increased federal investments for early childhood development.

$Y_1$: Honorable senators, my question addresses the leader of the government in the Senate and pertains to the support funding that has been announced for farmers. Most farmers have not received any money yet.

$Y_2$: Il est évident que les ordres de gouvernements provinciaux et municipaux subissent de fortes pressions en ce qui concerne les services de garde, mais le gouvernement n’a pas réduit le financement qu’il verse aux provinces pour les services de garde. Au contraire, nous avons augmenté le financement fédéral pour le développement des jeunes enfants.

Are the French text extracts translations of the English ones?
Detecting statistical dependence, continuous domains

- How do you detect dependence...
- ...in a **continuous** domain?
Detecting statistical dependence, continuous domains

• How do you detect dependence...
• ...in a **continuous** domain?
Detecting statistical dependence, continuous domains

- How do you detect dependence... 
- ...in a **continuous** domain?
Detecting statistical dependence, continuous domains

- How do you detect dependence...

- ...in a continuous domain?

- **Problem**: fails even in “low” dimensions! \[^{[NIPS07a, ALT08]}\]
  - \(X\) and \(Y\) in \(\mathbb{R}^4\), statistic=Power divergence, samples= 1024, cases where dependence detected=0/500

- Too few points per bin
Detecting statistical dependence, continuous domains

- How do you detect dependence...
- ...in a **continuous** domain?
- **Problem**: fails even in “low” dimensions! [NIPS07a, ALT08]
  - $X$ and $Y$ in $\mathbb{R}^4$, statistic=Power divergence, samples=1024, cases where dependence detected=0/500
- Too few points per bin

Can we **represent** and **compare** distributions in high dimensions?
Further motivating questions

- Compare distributions with high dimension/low sample size/“complex” structure
  - Microarray data (aggregation problem)
  - Neuroscience: naturalistic stimulus, complex response
  - Images and text on web (kernels on structured data)
Outline

- **Kernel metric** on the space of **probability measures**
  - Function revealing differences in distributions
  - Distance between means in space of features (RKHS)

- **Characteristic kernels**: feature space mappings of probabilities **unique**
Outline

- **Kernel metric** on the space of probability measures
  - Function revealing differences in distributions
  - Distance between means in space of features (RKHS)
- **Characteristic kernels**: feature space mappings of probabilities *unique*
- **Dependence detection**
  - Covariance and Correlation in feature space
Outline

- **Kernel metric** on the space of probability measures
  - Function revealing differences in distributions
  - Distance between means in space of features (RKHS)
- **Characteristic kernels**: feature space mappings of probabilities unique
- **Dependence detection**
  - Covariance and Correlation in feature space
- **Advanced topics**
  - Testing for big data
  - Bayesian inference without models
  - Three way interactions
  - Energy distance/distance covariance is special case of RKHS distances
Kernel distance between distributions
**Feature mean difference**

- Simple example: 2 Gaussians with different means
- Answer: *t*-test

![Two Gaussians with different means](image-url)
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 and same variance
- Difference in means using higher order features...RKHS
Reminder: feature maps and the RKHS

- Feature map of $x \in \mathbb{R}^2$, written $\varphi_x$

$$
\varphi^{(p)}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1x_2\sqrt{2} \end{bmatrix} \quad \varphi^{(g)}(x) = \begin{bmatrix} \ldots \sqrt{\lambda_i}e_i(x) \ldots \end{bmatrix} \in \ell_2
$$
Reminder: feature maps and the RKHS

- **Feature map** of $x \in \mathbb{R}^2$, written $\varphi_x$

  \[
  \varphi^{(p)}(x) = \begin{bmatrix}
  x_1^2 & x_2^2 & x_1 x_2 \sqrt{2}
  \end{bmatrix}
  \]

  \[
  \varphi^{(g)}(x) = \begin{bmatrix}
  \ldots \sqrt{\lambda_i} e_i(x) \ldots
  \end{bmatrix} \in \ell_2
  \]

- **Inner product** between feature maps:

  \[
  \langle \varphi^{(p)}(x), \varphi^{(p)}(y) \rangle_{\mathcal{F}} = \langle x, y \rangle^2
  \]

  \[
  \langle \varphi^{(g)}(x), \varphi^{(g)}(y) \rangle_{\mathcal{F}} = \exp \left( -\lambda \|x - y\|^2 \right)
  \]
Reminder: feature maps and the RKHS

- **Feature map** of $x \in \mathbb{R}^2$, written $\varphi_x$

  $\varphi^{(p)}(x) = \begin{bmatrix} x_1^2 & x_2^2 & x_1 x_2 \sqrt{2} \end{bmatrix}$

  $\varphi^{(g)}(x) = \begin{bmatrix} \ldots \sqrt{\lambda_i e_i(x)} \ldots \end{bmatrix} \in \ell_2$

- **Inner product** between feature maps:

  $\langle \varphi^{(p)}(x), \varphi^{(p)}(y) \rangle_{\mathcal{F}} = \langle x, y \rangle^2$

  $\langle \varphi^{(g)}(x), \varphi^{(g)}(y) \rangle_{\mathcal{F}} = \exp \left( -\lambda \|x - y\|^2 \right)$

- In general,

  $\langle \varphi_{x_1}, \varphi_{x_2} \rangle_{\mathcal{F}} = k(x_1, x_2)$

  for positive definite $k(x, y)$

**Kernels are inner products of feature maps**
Reminder: feature view of RKHS functions

- Reproducing property:

\[
f(x) = \sum_{i=1}^{m} \alpha_i k(x_i, x) = \sum_{i=1}^{m} \alpha_i \langle \varphi(x_i), \varphi(x) \rangle_F = \langle f(\cdot), \varphi(x) \rangle_F
\]

\[
f(\cdot) = \sum_{i=1}^{m} \alpha_i \varphi(x_i)
\]
For **finite dimensional feature spaces**, we can define expectations in terms of inner products.

\[ \phi(x) = k(\cdot, x) = \begin{bmatrix} x \\ x^2 \end{bmatrix} \quad f(\cdot) = \begin{bmatrix} a \\ b \end{bmatrix} \]

Then

\[ f(x) = \begin{bmatrix} a \\ b \end{bmatrix}^\top \begin{bmatrix} x \\ x^2 \end{bmatrix} = \langle f(\cdot), \phi(x) \rangle_{\mathcal{F}}. \]
The mean in feature space

For finite dimensional feature spaces, we can define expectations in terms of inner products.

\[ \phi(x) = k(\cdot, x) = \begin{bmatrix} x \\ x^2 \end{bmatrix} \quad f(\cdot) = \begin{bmatrix} a \\ b \end{bmatrix} \]

Then

\[ f(x) = \begin{bmatrix} a \\ b \end{bmatrix}^\top \begin{bmatrix} x \\ x^2 \end{bmatrix} = \langle f(\cdot), \phi(x) \rangle_{\mathcal{F}}. \]

Consider random variable \( x \sim \mathbf{P} \)

\[ \mathbf{E}_\mathbf{P} f(x) = \mathbf{E}_\mathbf{P} \left( \begin{bmatrix} a \\ b \end{bmatrix}^\top \begin{bmatrix} x \\ x^2 \end{bmatrix} \right) = \begin{bmatrix} a \\ b \end{bmatrix}^\top \begin{bmatrix} \mathbf{E}_\mathbf{P} x \\ \mathbf{E}_\mathbf{P} (x^2) \end{bmatrix} =: \begin{bmatrix} a \\ b \end{bmatrix}^\top \mu_\mathbf{P}. \]

Does this reasoning translate to infinite dimensions?
Does the feature space mean exist?

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

$$
\mathbb{E}_\mathcal{P} f(x) = \langle f(\cdot), \mu_\mathcal{P} (\cdot) \rangle_{\mathcal{F}} \quad \forall f \in \mathcal{F}
$$
Does there exist an element \( \mu_P \in \mathcal{F} \) such that

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

Recall the concept of **bounded operator**: a linear operator \( A : \mathcal{F} \to \mathbb{R} \) is bounded when \( \forall f \in \mathcal{F} \),

\[
|Af| \leq \lambda_A \|f\|_{\mathcal{F}}.
\]

**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 \( g_A \in \mathcal{F} \),

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

Existence of mean embedding: If $\mathbb{E}_P \sqrt{k(x,x)} < \infty$ then $\mu_P \in \mathcal{F}$.

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

$$|T_P f| \leq |\mathbb{E}_P f(x)| \leq \mathbb{E}_P |f(x)| = \mathbb{E}_P |\langle f(\cdot), \phi(x) \rangle_{\mathcal{F}}| \leq \mathbb{E}_P \left( \sqrt{k(x,x)} \|f\|_{\mathcal{F}} \right).$$

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

$$T_P f = \langle f(\cdot), \mu_P(\cdot) \rangle_{\mathcal{F}}.$$
Embedding of $P$ to feature space

- Mean embedding $\mu_P \in \mathcal{F}$
  \[
  \langle \mu_P(\cdot), f(\cdot) \rangle_{\mathcal{F}} = E_P f(x).
  \]
- What does prob. feature map look like?
  \[
  \mu_P(x) = \langle \mu_P(\cdot), \varphi(x) \rangle_{\mathcal{F}}
  \]
  \[
  = \langle \mu_P(\cdot), k(\cdot, x) \rangle_{\mathcal{F}} = E_P k(x, x).
  \]

**Expectation of kernel!**

- Empirical estimate:
  \[
  \hat{\mu}_P(x) = \frac{1}{m} \sum_{i=1}^m k(x_i, x) \quad x_i \sim P
  \]
\( \mu_P \) is feature map of probability

Embedding of \( P \) to feature space

- Mean embedding \( \mu_P \in \mathcal{F} \)

\[
\langle \mu_P(\cdot), f(\cdot) \rangle_{\mathcal{F}} = E_P f(x).
\]

- What does prob. feature map look like?

\[
\mu_P(x) = \langle \mu_P(\cdot), \varphi(x) \rangle_{\mathcal{F}} = \langle \mu_P(\cdot), k(\cdot, x) \rangle_{\mathcal{F}} = E_P k(x, x).
\]

Expectation of kernel!

- Empirical estimate:

\[
\hat{\mu}_P(x) = \frac{1}{m} \sum_{i=1}^{m} k(x_i, x) \quad x_i \sim P
\]
Function Showing Difference in Distributions

- Are $P$ and $Q$ different?
Function Showing Difference in Distributions

- Are $P$ and $Q$ different?
Function Showing Difference in Distributions

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

$$
MMD(P, Q; F) := \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(y) \right].
$$
Function Showing Difference in Distributions

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

$$\text{MMD}(P, Q; F) := \sup_{f \in F} \left[ E_P f(x) - E_Q f(y) \right].$$
• What if the function is not smooth?

\[
\text{MMD}(P, Q; F) := \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(y) \right].
\]
• What if the function is not smooth?

\[
\text{MMD}(\mathcal{P}, \mathcal{Q}; F) := \sup_{f \in F} \mathbb{E}_P f(x) - \mathbb{E}_Q f(y).
\]
Function Showing Difference in Distributions

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

\[
\text{MMD}(P, Q; F) := \sup_{f \in F} [E_P f(x) - E_Q f(y)].
\]

- Gauss \( P \) vs Laplace \( Q \)

![Graph showing Witness f for Gauss and Laplace densities](image_url)
Function Showing Difference in Distributions

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

  $$\text{MMD}(P, Q; F) := \sup_{f \in F} [E_P f(x) - E_Q f(y)].$$

- **Classical results**: $\text{MMD}(P, Q; F) = 0$ iff $P = Q$, when
  - $F =$ bounded continuous [Dudley, 2002]
  - $F =$ bounded variation 1 (Kolmogorov metric) [Müller, 1997]
  - $F =$ bounded Lipschitz (Earth mover’s distances) [Dudley, 2002]
Function Showing Difference in Distributions

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

  \[
  \text{MMD}(P, Q; F) := \sup_{f \in F} [E_P f(x) - E_Q f(y)].
  \]

- **Classical results**: $\text{MMD}(P, Q; F) = 0$ iff $P = Q$, when
  
  - $F =$ bounded continuous [Dudley, 2002]
  - $F =$ bounded variation 1 (Kolmogorov metric) [Müller, 1997]
  - $F =$ bounded Lipschitz (Earth mover’s distances) [Dudley, 2002]

- $\text{MMD}(P, Q; F) = 0$ iff $P = Q$ when $F =$ the unit ball in a characteristic RKHS $\mathcal{F}$ [ISMB06, NIPS06a, NIPS07b, NIPS08a, JMLR10]
Function Showing Difference in Distributions

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

\[
\text{MMD}(P, Q; F) := \sup_{f \in F} [E_P f(x) - E_Q f(y)].
\]

- **Classical results:** $\text{MMD}(P, Q; F) = 0$ iff $P = Q$, when
  - $F =$ bounded continuous [Dudley, 2002]
  - $F =$ bounded variation 1 (Kolmogorov metric) [Müller, 1997]
  - $F =$ bounded Lipschitz (Earth mover’s distances) [Dudley, 2002]

- $\text{MMD}(P, Q; F) = 0$ iff $P = Q$ when $F =$ the unit ball in a characteristic RKHS $\mathcal{F}$ [ISMB06, NIPS06a, NIPS07b, NIPS08a, JMLR10]

How do smooth functions relate to feature maps?
Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

\[
\text{MMD}^2(P, Q; F) = \left( \sup_{f \in F} [\mathbb{E}_P f(x) - \mathbb{E}_Q f(y)] \right)^2
\]

![Witness f for Gauss and Laplace densities](image)
The (kernel) MMD: [ISMB06, NIPS06a]

\[
\text{MMD}^2(P, Q; F) = \left( \sup_{f \in F} [\mathbb{E}_P f(x) - \mathbb{E}_Q f(y)] \right)^2
\]

use

\[
\mathbb{E}_P(f(x)) =: \langle \mu_P, f \rangle_F
\]
Function view vs feature mean view

- The (kernel) MMD: [ISMB06, NIPS06a]

\[
\text{MMD}^2(P, Q; F) = \left( \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(y) \right] \right)^2
\]

use

\[
\mathbb{E}_P(f(x)) =: \langle \mu_P, f \rangle_{\mathcal{F}}
\]
Function view vs feature mean view

- **The (kernel) MMD:** [ISMB06, NIPS06a]

\[
\text{MMD}^2(P, Q; F) = \left( \sup_{f \in F} \left[ \mathbb{E}_P f(x) - \mathbb{E}_Q f(y) \right] \right)^2
\]

use

\[
\|\theta\|_\mathcal{F} = \sup_{f \in F} \langle f, \theta \rangle_\mathcal{F}
\]

\[
\|\mu_P - \mu_Q\|_\mathcal{F}^2
\]

Function view and feature view equivalent
Empirical estimate of MMD

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^m \sim \mathbf{P} \) and \( \{y_i\}_{i=1}^m \sim \mathbf{Q} \),

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

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^{m} \sim P \) and \( \{y_i\}_{i=1}^{m} \sim Q \),

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

- Proof:

\[
\|\mu_P - \mu_Q\|^2_F = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_F = \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle
\]
Empirical estimate of MMD

- An unbiased empirical estimate: for $\{x_i\}_{i=1}^{m} \sim P$ and $\{y_i\}_{i=1}^{m} \sim Q$,

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

- Proof:

$$\| \mu_P - \mu_Q \|^2_F = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_F$$

$$= \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle$$
Empirical estimate of MMD

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^{m} \sim P \) and \( \{y_i\}_{i=1}^{m} \sim Q \),

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

- Proof:

\[
\|\mu_P - \mu_Q\|_F^2 = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_F = \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle = \langle E_P \varphi(x), E_P \varphi(x) \rangle + \ldots
\]
Empirical estimate of MMD

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^m \sim \mathbf{P} \) and \( \{y_i\}_{i=1}^m \sim \mathbf{Q} \),

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

- Proof:

\[
\|\mu_P - \mu_Q\|_{\mathcal{F}}^2 = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_{\mathcal{F}} \\
= \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle \\
= \langle \mathbf{E}_P \varphi(x), \mathbf{E}_P \varphi(x) \rangle + \ldots \\
= \mathbf{E}_P \langle \varphi(x), \varphi(x') \rangle + \ldots
\]
Empirical estimate of MMD

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^m \sim P \) and \( \{y_i\}_{i=1}^m \sim Q \),

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

- Proof:

\[
\|\mu_P - \mu_Q\|_F^2 = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_F
= \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle
= \langle E_P \varphi(x), E_P \varphi(x) \rangle + \ldots
= E_P \langle \varphi(x), \varphi(x') \rangle + \ldots
= E_P k(x, x') + E_Q k(y, y') - 2E_{P,Q} k(x, y)
\]
Empirical estimate of MMD

- An unbiased empirical estimate: for \( \{x_i\}_{i=1}^m \sim P \) and \( \{y_i\}_{i=1}^m \sim Q \),

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

- Proof:

\[
\|\mu_P - \mu_Q\|^2_\mathcal{F} = \langle \mu_P - \mu_Q, \mu_P - \mu_Q \rangle_\mathcal{F} \\
= \langle \mu_P, \mu_P \rangle + \langle \mu_Q, \mu_Q \rangle - 2 \langle \mu_P, \mu_Q \rangle \\
= \langle E_P \varphi(x), E_P \varphi(x) \rangle + \ldots \\
= \langle \varphi(x), \varphi(x') \rangle + \ldots \\
= E_P k(x, x') + E_Q k(y, y') - 2E_{P,Q} k(x, y)
\]

Then \( \hat{E}k(x, x') = \frac{1}{m(m-1)} \sum_{i=1}^m \sum_{j \neq i}^m k(x_i, x_j) \)
MMD for independence

- Dependence measure: [ALT05, NIPS07a, ALT07, ALT08, JMLR10]

\[
\left( \sup_f \left[ \mathbb{E}_{P_{XY}} f - \mathbb{E}_{P_X P_Y} f \right] \right)^2 = \sup_{\|f\| \leq 1} \langle f, \mu_{P_{XY}} - \mu_{P_X P_Y} \rangle_{\mathcal{F} \times \mathcal{G}} \]

\[
= \left\| \mu_{P_{XY}} - \mu_{P_X P_Y} \right\|_{\mathcal{F} \times \mathcal{G}}^2 := HSIC(P_{XY}, P_X P_Y)
\]
MMD for independence

- Dependence measure: [ALT05, NIPS07a, ALT07, ALT08, JMLR10]

\[
\left( \sup_f \left( E_{P_{XY}} f - E_{P_X P_Y} f \right) \right)^2 = \sup_{\|f\| \leq 1} \langle f, \mu_{P_{XY}} - \mu_{P_X P_Y} \rangle_{F \times G} \\
= \|\mu_{P_{XY}} - \mu_{P_X P_Y}\|_{F \times G}^2 := HSIC(P_{XY}, P_X P_Y)
\]

\[
\begin{align*}
&k(\begin{array}{c} 1 \\ 2 \end{array}) & l(\begin{array}{c} 1 \\ 2 \end{array}) \\
\Rightarrow & k(\begin{array}{c c} 1 & 1 \\ 2 & 2 \end{array}) = k(\begin{array}{c} 1 \\ 2 \end{array}) \times l(\begin{array}{c} 1 \\ 2 \end{array})
\end{align*}
\]
Characteristic kernels (Version 1: Via Universality)
Characteristic Kernels (via universality)

Characteristic: MMD a metric (MMD = 0 iff $P = Q$) [NIPS07b, COLT08]
Characteristic: MMD a metric (MMD = 0 iff $P = Q$) [NIPS07b, COLT08]

Classical result: $P = Q$ if and only if $E_P(f(x)) = E_Q(f(y))$ for all $f \in C(\mathcal{X})$, the space of bounded continuous functions on $\mathcal{X}$ [Dudley, 2002]
Characteristic Kernels (via universality)

Characteristic: MMD a metric (MMD = 0 iff $P = Q$) [NIPS07b, COLT08]

Classical result: $P = Q$ if and only if $E_P(f(x)) = E_Q(f(y))$ for all $f \in C(\mathcal{X})$, the space of bounded continuous functions on $\mathcal{X}$ [Dudley, 2002]

Universal RKHS: $k(x, x')$ continuous, $\mathcal{X}$ compact, and $\mathcal{F}$ dense in $C(\mathcal{X})$ with respect to $L_\infty$ [Steinwart, 2001]
Characteristic Kernels (via universality)

Characteristic: MMD a metric (MMD = 0 iff $P = Q$) \[\text{[NIPS07b, COLT08]}\]

Classical result: $P = Q$ if and only if $\mathbb{E}_P(f(x)) = \mathbb{E}_Q(f(y))$ for all $f \in C(\mathcal{X})$, the space of bounded continuous functions on $\mathcal{X}$ \[\text{[Dudley, 2002]}\]

Universal RKHS: $k(x, x')$ continuous, $\mathcal{X}$ compact, and $\mathcal{F}$ dense in $C(\mathcal{X})$ with respect to $L_{\infty}$ \[\text{[Steinwart, 2001]}\]

If $\mathcal{F}$ universal, then $\text{MMD} \{P, Q; F\} = 0$ iff $P = Q$
Proof:
First, it is clear that $P = Q$ implies $\text{MMD}\{P, Q; F\}$ is zero.

Converse: by the universality of $\mathcal{F}$, for any given $\epsilon > 0$ and $f \in C(\mathcal{X})$ \exists $g \in \mathcal{F}$

$$\|f - g\|_{\infty} \leq \epsilon.$$
Characteristic Kernels (via universality)

Proof:
First, it is clear that $P = Q$ implies $\text{MMD} \{P, Q; F\}$ is zero.

Converse: by the universality of $\mathcal{F}$, for any given $\epsilon > 0$ and $f \in C(\mathcal{X})$ $\exists g \in \mathcal{F} \ni \|f - g\|_{\infty} \leq \epsilon$.

We next make the expansion

$$|E_P f(x) - E_Q f(y)| \leq |E_P f(x) - E_P g(x)| + |E_P g(x) - E_Q g(y)| + |E_Q g(y) - E_Q f(y)|.$$

The first and third terms satisfy

$$|E_P f(x) - E_P g(x)| \leq E_P |f(x) - g(x)| \leq \epsilon.$$
Characteristic Kernels (via universality)

Proof (continued):

Next, write

\[ \mathbb{E}_P g(x) - \mathbb{E}_Q g(y) = \langle g(\cdot), \mu_P - \mu_Q \rangle_F = 0, \]

since MMD \( \{P, Q; F\} = 0 \) implies \( \mu_P = \mu_Q \). Hence

\[ |\mathbb{E}_P f(x) - \mathbb{E}_Q f(y)| \leq 2\epsilon \]

for all \( f \in C(X) \) and \( \epsilon > 0 \), which implies \( P = Q \).
Characteristic kernels (Version 2: Via Fourier)
Reminder: Fourier series

- Function \([-\pi, \pi]\) with periodic boundary.

\[
f(x) = \sum_{\ell=-\infty}^{\infty} \hat{f}_\ell \exp(\imath \ell x) = \sum_{\ell=-\infty}^{\infty} \hat{f}_\ell (\cos(\ell x) + \imath \sin(\ell x)) .
\]
Characteristic Kernels (via Fourier)

**Reminder:** Fourier series of kernel

\[ k(x, y) = k(x - y) = k(z), \quad k(z) = \sum_{\ell = -\infty}^{\infty} \hat{k}_\ell \exp (i \ell z), \]

E.g. Gaussian, \( k(x) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left( -\frac{x^2}{2\sigma^2} \right), \quad \hat{k}_\ell = \frac{1}{2\pi} \exp \left( -\frac{\sigma^2 \ell^2}{2} \right). \)
Characteristic Kernels (via Fourier)

Maximum mean embedding via Fourier series:

- Fourier series for $P$ is characteristic function $\phi_P$
- Fourier series for mean embedding is product of fourier series! (convolution theorem)

$$\mu_P(x) = E_P k(x - x) = \int_{-\pi}^{\pi} k(x - t)dP(t)$$

$$\hat{\mu}_{P,\ell} = \hat{k}_\ell \times \phi_{P,\ell}$$
Characteristic Kernels (via Fourier)

Maximum mean embedding via Fourier series:

- Fourier series for $\mathbf{P}$ is characteristic function $\phi_\mathbf{P}$
- Fourier series for mean embedding is product of fourier series! (convolution theorem)

\[
\mu_{\mathbf{P}}(x) = E_\mathbf{P} k(x - x) = \int_{-\pi}^{\pi} k(x - t) d\mathbf{P}(t) \quad \hat{\mu}_{\mathbf{P},\ell} = \hat{k}_\ell \times \phi_{\mathbf{P},\ell}
\]

- MMD can be written in terms of Fourier series:

\[
\text{MMD}(\mathbf{P}, \mathbf{Q}; \mathcal{F}) := \left\| \sum_{\ell=-\infty}^{\infty} \left[ (\phi_{\mathbf{P},\ell} - \phi_{\mathbf{Q},\ell}) \hat{k}_\ell \right] \exp(\imath \ell x) \right\|_{\mathcal{F}}
\]

- **Characteristic**: MMD a metric (MMD = 0 iff $\mathbf{P} = \mathbf{Q}$) \cite{NIPS07b, COLT08, JMLR10}
Example

- Example: $P$ differs from $Q$ at one frequency
Example: $P$ differs from $Q$ at (roughly) one frequency

\begin{align*}
P(x) &\quad \xrightarrow{F} \quad \phi_{P,\ell} \\
Q(x) &\quad \xrightarrow{F} \quad \phi_{Q,\ell}
\end{align*}
- Example: $P$ differs from $Q$ at (roughly) one frequency
Is the **Gaussian** kernel characteristic?

\[
MMD(\mathcal{P}, \mathcal{Q}; F) := \left\| \sum_{\ell = -\infty}^{\infty} \left[ (\phi_{\mathcal{P}, \ell} - \phi_{\mathcal{Q}, \ell}) \hat{k}_\ell \right] \exp(\imath \ell x) \right\|_F
\]
Is the Gaussian kernel characteristic? **YES**

\[
MMD(P, Q; F) := \left\| \sum_{\ell=-\infty}^{\infty} \left[ (\phi_P,\ell - \phi_Q,\ell) \hat{k}_\ell \right] \exp(i\ell x) \right\|_F
\]
Example

Is the triangle kernel characteristic?

\[
\text{MMD}(P, Q; F) := \left\| \sum_{\ell = -\infty}^{\infty} \left[ (\phi_{P,\ell} - \phi_{Q,\ell}) \hat{k}_{\ell} \right] \exp(i\ell x) \right\|_F
\]
Example

Is the triangle kernel characteristic? NO

\[ \text{MMD}(\mathbf{P}, \mathbf{Q}; F) := \left\| \sum_{\ell=-\infty}^{\infty} \left( \phi_{\mathbf{P},\ell} - \phi_{\mathbf{Q},\ell} \right) \hat{k}_\ell \exp(i\ell x) \right\|_F \]
Can we prove characteristic on $\mathbb{R}^d$?
Characteristic Kernels (via Fourier)

- Can we prove characteristic on $\mathbb{R}^d$?
- Characteristic function of $P$ via Fourier transform

$$\phi_P(\omega) = \int_{\mathbb{R}^d} e^{ix^\top \omega} dP(x)$$
Characteristic Kernels (via Fourier)

- Can we prove characteristic on $\mathbb{R}^d$?
- Characteristic function of $P$ via Fourier transform
  \[
  \phi_P(\omega) = \int_{\mathbb{R}^d} e^{ix^\top \omega} dP(x)
  \]
- Translation invariant kernels: $k(x, y) = k(x - y) = k(z)$
- Bochner’s theorem:
  \[
  k(z) = \int_{\mathbb{R}^d} e^{-iz^\top \omega} d\Lambda(\omega)
  \]
  - $\Lambda$ finite non-negative Borel measure
Characteristic Kernels (via Fourier)

- Can we prove characteristic on $\mathbb{R}^d$?
- **Characteristic function** of $P$ via Fourier transform

$$
\phi_P(\omega) = \int_{\mathbb{R}^d} e^{ix^\top \omega} dP(x)
$$

- **Translation invariant kernels**: $k(x, y) = k(x - y) = k(z)$
- **Bochner’s theorem**:

$$
k(z) = \int_{\mathbb{R}^d} e^{-iz^\top \omega} d\Lambda(\omega)
$$

  - $\Lambda$ finite non-negative Borel measure
Characteristic Kernels (via Fourier)

- Fourier representation of MMD:

$$\text{MMD}(P, Q; F) := \| \left[ (\bar{\phi}_P(\omega) - \bar{\phi}_Q(\omega)) \Lambda(\omega) \right]^\vee \|_F$$

- \(\phi_P\) characteristic function of \(P\)
- \(f^\wedge\) is Fourier transform, \(f^\vee\) is inverse Fourier transform
- \(\mu_P := \int k(\cdot, x) \, dP(x)\)
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency
Example

• Example: $P$ differs from $Q$ at (roughly) one frequency
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency

Gaussian kernel

Difference $|\phi_P - \phi_Q|$
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency
Example

- Example: \( P \) differs from \( Q \) at (roughly) one frequency

**Sinc kernel**

Difference \( |\phi_P - \phi_Q| \)
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency

NOT characteristic
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency

Triangle (B-spline) kernel

Difference $|\phi_P - \phi_Q|$
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency
Example

- Example: $P$ differs from $Q$ at (roughly) one frequency
Choosing the kernel

- **Gaussian** kernel example

- MMD vs frequency of perturbation to $P$
Why does MMD decay with increasing perturbation freq.?

- Fourier series argument (notationally easier, for periodic domains only):

\[
MMD(P, Q; F) := \left\| \sum_{\ell=-\infty}^{\infty} \left[ (\phi_P, \ell - \phi_Q, \ell) \hat{k}_\ell \right] \exp(\imath \ell x) \right\|_F
\]

- The squared norm of a function \( f \) in \( \mathcal{F} \) is:

\[
\| f \|_{\mathcal{F}}^2 = \langle f, f \rangle_{\mathcal{F}} = \sum_{\ell=-\infty}^{\infty} \frac{|\hat{f}_\ell|^2}{\hat{k}_\ell}.
\]

- Squared MMD is

\[
MMD(P, Q; F) = \sum_{\ell=-\infty}^{\infty} \frac{[|\phi_P, \ell - \phi_Q, \ell| \hat{k}_\ell]^2}{\hat{k}_\ell} = \sum_{\ell=-\infty}^{\infty} |\phi_P, \ell - \phi_Q, \ell| \hat{k}_\ell
\]
Choosing the kernel

• B-spline kernel example

• MMD vs frequency of perturbation to $P$
Summary: Characteristic Kernels

- **Characteristic kernel:** \( (\text{MMD} = 0 \iff \mathbb{P} = \mathbb{Q}) \) [NIPS07b, COLT08]
- **Main theorem:** \( k \) characteristic for prob. measures on \( \mathbb{R}^d \) if and only if \( \text{supp}(\Lambda) = \mathbb{R}^d \) [COLT08, JMLR10]
Summary: Characteristic Kernels

- **Characteristic kernel**: \( \text{MMD} = 0 \text{ iff } \mathbf{P} = \mathbf{Q} \) \[\text{NIPS07b, COLT08}\]

- **Main theorem**: \( k \) characteristic for prob. measures on \( \mathbb{R}^d \) if and only if \( \text{supp}(\Lambda) = \mathbb{R}^d \) \[\text{COLT08, JMLR10}\]
  - Corollary: continuous, compactly supported \( k \) characteristic
Summary: Characteristic Kernels

- **Characteristic kernel**: \((\text{MMD} = 0 \iff \mathbf{P} = \mathbf{Q})\) \cite{NIPS07b, COLT08}

- **Main theorem**: \(k\) characteristic for prob. measures on \(\mathbb{R}^d\) if and only if \(\text{supp}(\Lambda) = \mathbb{R}^d\) \cite{COLT08, JMLR10}
  - Corollary: continuous, compactly supported \(k\) characteristic

- **Similar reasoning wherever extensions of Bochner’s theorem exist**: \cite{NIPS08a}
  - Locally compact Abelian groups (periodic domains, as we saw)
  - Compact, non-Abelian groups (orthogonal matrices)
  - The semigroup \(\mathbb{R}_n^+\) (histograms)
Statistical hypothesis testing
Reminder: detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Reminder: detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Reminder: detecting differences in brain signals

The problem: Do local field potential (LFP) signals change when measured near a spike burst?
Statistical test using MMD (1)

- Two hypotheses:
  - $H_0$: null hypothesis ($P = Q$)
  - $H_1$: alternative hypothesis ($P \neq Q$)
Statistical test using MMD (1)

- Two hypotheses:
  - $H_0$: null hypothesis ($P = Q$)
  - $H_1$: alternative hypothesis ($P \neq Q$)
- Observe samples $x := \{x_1, \ldots, x_n\}$ from $P$ and $y$ from $Q$
- If empirical $\text{MMD}(x, y; F')$ is
  - “far from zero”: reject $H_0$
  - “close to zero”: accept $H_0$
Statistical test using MMD (2)

- “far from zero” vs “close to zero” - threshold?
- **One answer:** asymptotic distribution of $\text{MMD}(\mathbf{x}, \mathbf{y}; F')$
Statistical test using MMD (2)

- “far from zero” vs “close to zero” - threshold?
- One answer: asymptotic distribution of \( \text{MMD}(\mathbf{x}, \mathbf{y}; F) \)
- An unbiased empirical estimate (quadratic cost):

\[
\text{MMD}(\mathbf{x}, \mathbf{y}; F) = \frac{1}{n(n-1)} \sum_{i \neq j} \left[ k(x_i, x_j) - k(x_i, y_j) - k(y_i, x_j) + k(y_i, y_j) \right] h((x_i, y_i), (x_j, y_j))
\]
Statistical test using MMD (2)

• “far from zero” vs “close to zero” - threshold?

• One answer: asymptotic distribution of $\text{MMD}(x, y; F)$

• An unbiased empirical estimate (quadratic cost):

$$\text{MMD}(x, y; F) = \frac{1}{n(n-1)} \sum_{i \neq j} \left[ k(x_i, x_j) - k(x_i, y_j) - k(y_i, x_j) + k(y_i, y_j) \right] h((x_i, y_i), (x_j, y_j))$$

• When $P \neq Q$, asymptotically normal [Hoeffding, 1948, Serfling, 1980]

• Expression for the variance: $z_i := (x_i, y_i)$

$$\sigma_u^2 = \frac{2^2}{n} \left( \mathbb{E}_z \left[ (\mathbb{E}_{z'} h(z, z'))^2 \right] - \left[ \mathbb{E}_{z,z'}(h(z, z')) \right]^2 \right) + O(n^{-2})$$
Statistical test using MMD (3)

- Example: laplace distributions with different variance
Statistical test using MMD (4)

- When $\mathbf{P} = \mathbf{Q}$, U-statistic degenerate: $\mathbb{E}_{z'}[h(z, z')] = 0$ [Anderson et al., 1994]

- Distribution is

$$n\text{MMD}(\mathbf{x}, \mathbf{y}; F') \sim \sum_{l=1}^{\infty} \lambda_l [z_l^2 - 2]$$

- where
  - $z_l \sim \mathcal{N}(0, 2)$ i.i.d
  - $\int_{\mathcal{X}} \tilde{k}(x, x') \psi_i(x) d\mathbf{P}(x) = \lambda_i \psi_i(x')$ centred
Statistical test using MMD (4)

- When $P = Q$, U-statistic degenerate: $\mathbb{E}_{z'}[h(z, z')] = 0$ [Anderson et al., 1994]
- Distribution is

$$n\text{MMD}(x, y; F') \sim \sum_{l=1}^{\infty} \lambda_l \left[ z_l^2 - 2 \right]$$

- where
  - $z_l \sim \mathcal{N}(0, 2)$ i.i.d
  - $\int_{X} \tilde{k}(x, x') \psi_i(x) dP(x) = \lambda_i \psi_i(x')$

![MMD density under H0](image)
Statistical test using MMD (5)

- Given $P = Q$, want threshold $T$ such that $P(\text{MMD} > T) \leq 0.05$
• Given $P = Q$, want threshold $T$ such that $P(\text{MMD} > T) \leq 0.05$

• **Permutation** for empirical CDF [Arcones and Giné, 1992]

• **Pearson curves** by matching first four moments [Johnson et al., 1994]

• **Large deviation bounds** [Hoeffding, 1963, McDiarmid, 1989]

• **Consistent test** using kernel eigenspectrum [NIPS09b]
Statistical test using MMD (5)

- Given $\mathbf{P} = \mathbf{Q}$, want threshold $T$ such that $\mathbf{P}(\text{MMD} > T) \leq 0.05$
- **Permutation** for empirical CDF [Arcones and Giné, 1992]
- **Pearson curves** by matching first four moments [Johnson et al., 1994]
- **Large deviation bounds** [Hoeffding, 1963, McDiarmid, 1989]
- **Consistent test** using kernel eigenspectrum [NIPS09b]
**Consistent test w/o bootstrap (not examinable)**

- **Maximum mean discrepancy (MMD):** distance between $\mathbf{P}$ and $\mathbf{Q}$

  \[
  \text{MMD}(\mathbf{P}, \mathbf{Q}; F) := \| \mu_{\mathbf{P}} - \mu_{\mathbf{Q}} \|^2_F
  \]

- Is $\widehat{\text{MMD}}$ significantly $> 0$?

- $\mathbf{P} = \mathbf{Q}$, null distrib. of $\widehat{\text{MMD}}$:

  \[
  n\widehat{\text{MMD}} \xrightarrow{D} \sum_{l=1}^{\infty} \lambda_l (z_l^2 - 2),
  \]

  - $\lambda_l$ is $l$th eigenvalue of
    kernel $\tilde{k}(x_i, x_j)$

**Use Gram matrix spectrum for $\hat{\lambda}_l$: consistent test without bootstrap**
Kernel dependence measures
Reminder: MMD can be used as a dependence measure

- **Dependence measure:** [ALT05, NIPS07a, ALT07, ALT08, JMLR10]

\[
\left( \sup_f \left[ \mathbb{E}_{p_{XY}} f - \mathbb{E}_{p_Xp_Y} f \right] \right)^2 = \sup_{\|f\| \leq 1} \left\langle f, \mu_{p_{XY}} - \mu_{p_Xp_Y} \right\rangle_{\mathcal{F} \times \mathcal{G}}^2 \\
= \|\mu_{p_{XY}} - \mu_{p_Xp_Y}\|_{\mathcal{F} \times \mathcal{G}}^2 := HSIC(p_{XY}, p_Xp_Y)
\]
Reminder: MMD can be used as a dependence measure

- Dependence measure: \([\text{ALT05, NIPS07a, ALT07, ALT08, JMLR10}]\)

\[
\left( \sup_f \left[ \mathbb{E}_{P_{XY}} f - \mathbb{E}_{P_X P_Y} f \right] \right)^2 = \sup_{\|f\| \leq 1} \langle f, \mu_{P_{XY}} - \mu_{P_X P_Y} \rangle_{\mathcal{F} \times \mathcal{G}}^2 = \|\mu_{P_{XY}} - \mu_{P_X P_Y}\|_{\mathcal{F} \times \mathcal{G}}^2 =: \text{HSIC}(P_{XY}, P_X P_Y)
\]
Distribution of HSIC at independence

• (Biased) empirical HSIC a v-statistic

\[ HSIC_b = \frac{1}{n^2} \text{trace}(KHLH) \]

– **Statistical testing:** How do we find when this is **larger enough** that the null hypothesis \( P = P_x P_y \) is unlikely?

– Formally: given \( P = P_x P_y \), what is the threshold \( T \) such that \( P(\text{HSIC} > T) < \alpha \) for small \( \alpha \)?
Distribution of HSIC at independence

- (Biased) empirical HSIC a v-statistic

\[ HSIC_b = \frac{1}{n^2} \text{trace}(KHLH) \]

- Associated U-statistic degenerate when \( P = P_xP_y \) [Serfling, 1980]:

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

\[ \lambda_l \psi_l(z_j) = \int h_{ijqr} \psi_l(z_i) dF_{i,q,r}, \quad h_{ijqr} = \frac{1}{4!} \sum_{(t,u,v,w)} k_{tu}l_{tu} + k_{tu}l_{vw} - 2k_{tu}l_{tv} \]
Distribution of HSIC at independence

- **(Biased) empirical HSIC** a \(v\)-statistic

\[
HSIC_b = \frac{1}{n^2} \text{trace}(KHLH)
\]

- Associated U-statistic **degenerate** when \(P = P_x P_y\) [Serfling, 1980]:

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

\[
\lambda_l \psi_l(z_j) = \int h_{ijqr} \psi_l(z_i) dF_{i,q,r}, \quad h_{ijqr} = \frac{1}{4!} \sum_{(t,u,v,w)} k_{tu}l_{tu} + k_{tu}l_{vw} - 2k_{tu}l_{tv}
\]

- **First two moments** [NIPS07b]

\[
\mathbb{E}(\text{HSIC}_b) = \frac{1}{n} \text{Tr}C_{xx} \text{Tr}C_{yy}
\]

\[
\text{var}(\text{HSIC}_b) = \frac{2(n-4)(n-5)}{(n)^4} \|C_{xx}\|_{\text{HS}}^2 \|C_{yy}\|_{\text{HS}}^2 + O(n^{-3}).
\]
Statistical testing with HSIC

- Given $P = P_x P_y$, what is the threshold $T$ such that $P(\text{HSIC} > T) < \alpha$ for small $\alpha$?

- Null distribution via permutation [Feuerverger, 1993]
  - 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 $T$ is $1 - \alpha$ quantile of empirical CDF
Statistical testing with HSIC

• Given $P = P_xP_y$, what is the threshold $T$ such that $P(\text{HSIC} > T) < \alpha$ for small $\alpha$?

• Null distribution via permutation [Feuerverger, 1993]
  - 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 $T$ is $1 - \alpha$ quantile of empirical CDF

• Approximate null distribution via moment matching [Kankainen, 1995]:

$$n\text{HSIC}_b(Z) \sim \frac{x^{\alpha-1}e^{-x/\beta}}{\beta^\alpha \Gamma(\alpha)}$$

where

$$\alpha = \frac{(\mathbf{E}(\text{HSIC}_b))^2}{\text{var}(\text{HSIC}_b)}, \quad \beta = \frac{\text{var}(\text{HSIC}_b)}{n\mathbf{E}(\text{HSIC}_b)}.$$
Experiment: dependence testing for translation

- (Biased) empirical HSIC:
  \[ HSIC_b = \frac{1}{n^2} \text{trace}(KHLH) \]

- Translation example: [NIPS07b] Canadian Hansard (agriculture)
- 5-line extracts,
  \( k \)-spectrum kernel, \( k = 10 \),
  repetitions=300,
  sample size 10

- \( k \)-spectrum kernel: average Type II error 0 (\( \alpha = 0.05 \))
Experiment: dependence testing for translation

- **(Biased) empirical HSIC:**
  \[
  HSIC_b = \frac{1}{n^2} \text{trace}(KHLH)
  \]

- **Translation example:** [NIPS07b]
  Canadian Hansard
  (agriculture)

  - 5-line extracts,
    \( k \)-spectrum kernel, \( k = 10 \),
    repetitions=300,
    sample size 10

- **\( k \)-spectrum kernel:** average Type II error 0 \((\alpha = 0.05)\)

- **Bag of words kernel:** average Type II error 0.18
Advanced topics

- Energy distance and the MMD
- Two-sample testing for big data
- Testing three-way interactions
- Bayesian inference without models
Summary

• **MMD** a distance between distributions [ISMB06, NIPS06a, JMLR10, JMLR12a]
  - high dimensionality
  - non- Euclidean data (*strings*, graphs)
  - Nonparametric hypothesis tests

• Measure and test **independence** [ALT05, NIPS07a, NIPS07b, ALT08, JMLR10, JMLR12a]

• **Characteristic RKHS**: MMD a **metric** [NIPS07b, COLT08, NIPS08a]
  - Easy to check: does spectrum cover \( \mathbb{R}^d \)
Co-authors

- **From UCL:**
  - Luca Baldassarre
  - Steffen Grunewalder
  - Guy Lever
  - Sam Patterson
  - Massimiliano Pontil
  - Dino Sejdinovic

- **External:**
  - Karsten Borgwardt, MPI
  - Wicher Bergsma, LSE
  - Kenji Fukumizu, ISM
  - Zaid Harchaoui, INRIA
  - Bernhard Schoelkopf, MPI
  - Alex Smola, CMU/Google
  - Le Song, Georgia Tech
  - Bharath Sriperumbudur, Cambridge
Selected references

Characteristic kernels and mean embeddings:


Two-sample, independence, conditional independence tests:


Energy distance, relation to kernel distances


Three way interaction

Selected references (continued)

Conditional mean embedding, RKHS-valued regression:

Kernel Bayes rule:
References


A. Miller. Interpolated probability metrics and their generalization classes of functions.
G. Székely, M. Rizzo, and N. Bakirov. Measuring and testing dependence by


G. Székely and M. Rizzo. A new test for multivariate normality. J. Multivariate

G. Székely and M. Rizzo. Testing for equal distributions in high dimension.

I. Steinwart. On the influence of the kernel on the consistency of support

R. Serfling. Approximation Theorems of Mathematical Statistics. Wiley, New York,
1980.

T. Read and N. Cressie. Goodness-of-Fit Statistics for Discrete Multivariate Anal-