Structured Data: Dependency, Testing

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∈ Structured Data: Learning, Prediction, Dependency, Testing
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Software (Python, Matlab)

- Dependency measures (KCCA, HSIC), divergences (MMD), etc.; several demos:

  https://bitbucket.org/szzoli/ite-in-python
  https://bitbucket.org/szzoli/ite/

- 2-sample, independence & goodness-of-fit tests (quadratic → linear-time methods):

  https://github.com/wittawatj/interpretable-test
  https://github.com/wittawatj/fsic-test
  https://github.com/wittawatj/kernel-gof

Outline

- Motivation:
    - Objective functions: from dependency measures.
    - Testing.

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  - Objective functions: from dependency measures.
  - Testing.
- Kernel, RKHS.
- Kernel canonical correlation analysis.
- Mean embedding:
  - Characteristic property,
  - Universality.
- Maximum mean discrepancy.
- Cross-covariance operator, HSIC.
- Hypothesis testing.

Dependency Measures as Objective Functions

Outlier-robust image registration [Kybic, 2004, Neemuchwala et al., 2007]

Given two images:

Goal: find the transformation which takes the right one to the left.

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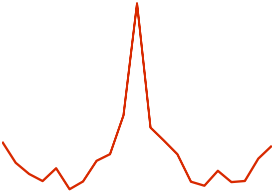


Goal: find the transformation which takes the right one to the left.

Outlier-robust image registration: equations

- Reference image: $\mathbf{y}_{\text{ref}}$,
- test image: $\mathbf{y}_{\text{test}}$,
- possible transformations: $\boldsymbol{\Theta}$.

Objective:

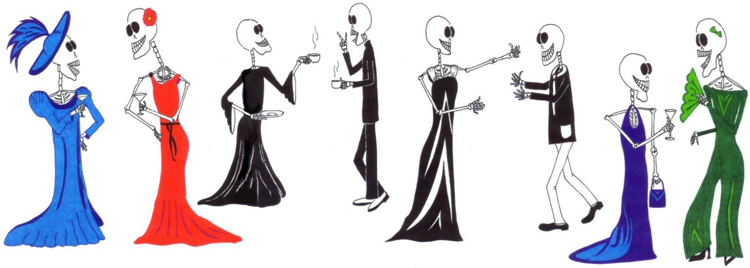
$$J(\boldsymbol{\theta}) = \underbrace{I(\mathbf{y}_{\text{ref}}, \mathbf{y}_{\text{test}}(\boldsymbol{\theta}))}_{\text{similarity}} \to \max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}},$$

In the example: I=KCCA.

Independent Subspace Analysis [Cardoso, 1998]

Cocktail party problem:

- independent groups of people / music bands,
- observation = mixed sources.



ISA equations

Observation:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t, \qquad \mathbf{s} = \left[\mathbf{s}^1; \ldots; \mathbf{s}^M\right].$$

Goal: $\hat{\mathbf{s}}$ from $\{\mathbf{x}_1, \ldots, \mathbf{x}_T\}$. Assumptions:

- independent groups: $I\left(\mathbf{s}^1, \ldots, \mathbf{s}^M\right) = 0$,
- $\mathbf{s}^m$-s: non-Gaussian,
- $\mathbf{A}$: invertible.

ISA solution

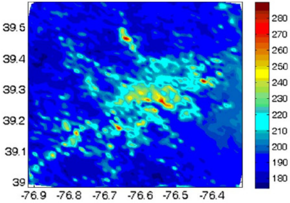
Find $\mathbf{W}$ which makes the estimated components independent:

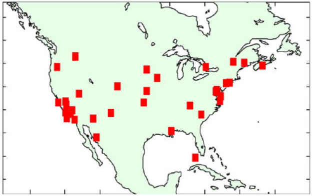
$$\mathbf{y} = \mathbf{W}\mathbf{x} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right],$$
$$J(\mathbf{W}) = I\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) \to \min_{\mathbf{W}}.$$

Distribution regression [Póczos et al., 2013, Szabó et al., 2016]. Sustainability

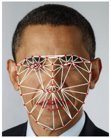
- **Goal**: aerosol prediction = air pollution → climate.

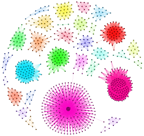
- Prediction using labelled bags:
  - bag := multi-spectral satellite measurements over an area,
  - label := local aerosol value.





Objects in the bags





- Examples:
  - time-series modelling: user = set of time-series,
  - computer vision: image = collection of patch vectors,
  - NLP: corpus = bag of documents,
  - network analysis: group of people = bag of friendship graphs, ...

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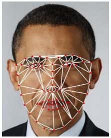

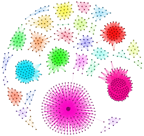

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  - NLP: corpus = bag of documents,
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- Wider context (statistics): point estimation tasks.

Regression on labelled bags

- Given:
  - labelled bags: $\hat{\mathbf{z}} = \left\{\left(\hat{P}_i, y_i\right)\right\}_{i=1}^{\ell}$, $\hat{P}_i$: bag from P_i, $N := |\hat{P}_i|$.
  - test bag: $\hat{P}$.

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$$f_{\hat{\mathbf{z}}}^{\lambda} = \arg\min_{f \in \mathcal{H}} \frac{1}{\ell} \sum_{i=1}^{\ell} \left[f\Big(\underbrace{\mu_{\hat{P}_i}}_{\text{feature of } \hat{P}_i}\Big) - y_i \right]^2 + \lambda \|f\|_{\mathcal{H}}^2 .$$

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$$\hat{y}\left(\hat{P}\right) = \mathbf{g}^T (\mathbf{G} + \ell\lambda\mathbf{I})^{-1}\mathbf{y},$$
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Challenge

Inner product of distributions: $K\left(\mu_{\hat{P}_i}, \mu_{\hat{P}_j}\right) = ?$

Feature selection

- **Goal**: find
  - the feature subset (# of rooms, criminal rate, local taxes)
  - most relevant for house price prediction (y).

Feature selection: equations

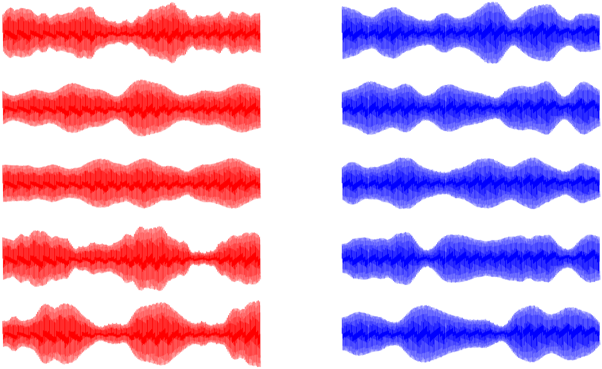
- Features: $x^1, \ldots, x^F$. Subset: $S \subseteq \{1, \ldots, F\}$.
- MaxRelevance - MinRedundancy principle [Peng et al., 2005]:

$$J(S) = \frac{1}{|S|} \sum_{i \in S} I\left(x^i, y\right) - \frac{1}{|S|^2} \sum_{i,j \in S} I\left(x^i, x^j\right) \rightarrow \max_{S \subseteq \{1,\ldots,F\}}.$$

Testing

Motivation: detecting differences in AM signals

- Amplitude modulation:
  - simple technique to transmit voice over radio.
  - in the example: 2 songs.
- Fragments from $\text{song}_1 \sim \mathbb{P}_x$, $\text{song}_2 \sim \mathbb{P}_y$.



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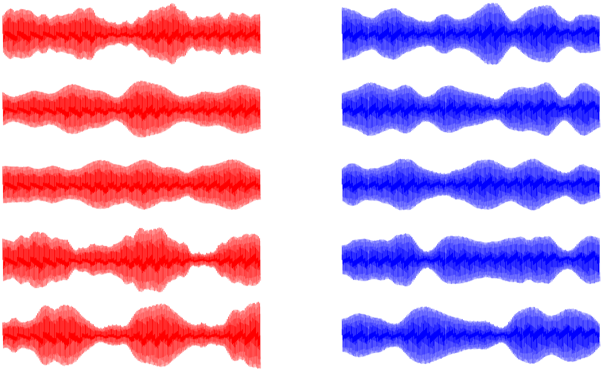

Question: $\mathbb{P}_x = \mathbb{P}_y$?

Motivation: discrete domain - 2-sample testing

- How do we compare distributions?
- Given: 2 sets of text fragments (fisheries, agriculture).

x_1: Now disturbing reports out of Newfoundland show that the fragile snow crab industry is in serious decline. First the west coast salmon, the east coast salmon and the cod, and now the snow crabs off Newfoundland.

x_2: To my pleasant surprise he responded that he had personally visited those wharves and that he had already announced money to fix them. What wharves did the minister visit in my riding and how much additional funding is he going to provide for Delaps Cove, Hampton, Port Lorne, ...

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y_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.

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Do $\{x_i\}$ and $\{y_j\}$ come from the same distribution, i.e. $\mathbb{P}_x = \mathbb{P}_y$?

Motivation: discrete domain - independence testing

- How do we detect dependency? (paired samples)

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.

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y_1: Honorables sénateurs, ma question s'adresse au leader du gouvernement au Sénat et concerne l'aide financiére qu'on a annoncée pour les agriculteurs. La plupart des agriculteurs n'ont encore rien reu de cet argent.

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.

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Are the French paragraphs translations of the English ones, or have nothing to do with it, i.e. $\mathbb{P}_{XY} = \mathbb{P}_X \otimes \mathbb{P}_Y$?

We will use kernels to tackle these problems

They exist essentially on any data type

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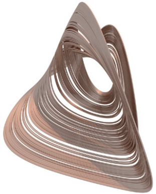
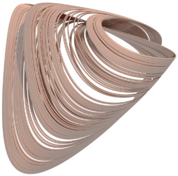
trees [Collins and Duffy, 2001, Kashima and Koyanagi, 2002], time series [Cuturi, 2011], strings [Lodhi et al., 2002], mixture models, hidden Markov models or linear dynamical systems [Jebara et al., 2004], sets [Haussler, 1999, Gärtner et al., 2002], fuzzy domains [Guevara et al., 2017], distributions [Hein and Bousquet, 2005, Martins et al., 2009, Muandet et al., 2011], groups [Cuturi et al., 2005] with specific constructions on permutations [Jiao and Vert, 2016], graphs [Vishwanathan et al., 2010, Kondor and Pan, 2016], . . .





Kernel Canonical Correlation Analysis (KCCA)

Independence measures

- Given: random variable $(x, y) \in \mathcal{X} \times \mathcal{Y}$, $(x, y) \sim \mathbb{P}_{xy}$.
- Goal: measure the dependence of x and y.

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- Goal: measure the dependence of x and y.
- Desiderata for a $Q(\mathbb{P}_{xy})$ independence measure [Rényi, 1959]:
  1. $Q(\mathbb{P}_{xy})$ is well-defined,
  2. $Q(\mathbb{P}_{xy}) \in [0, 1]$,
  3. $Q(\mathbb{P}_{xy}) = 0$ iff. $x \perp y$.
  4. $Q(\mathbb{P}_{xy}) = 1$ iff. $y = f(x)$ or $x = g(y)$.

Independence measures

- He showed:

$$Q(\mathbb{P}_{xy}) = \sup_{f,g:\ \text{measurable}} \operatorname{corr}(f(x), g(y)),$$

  satisfies 1-4.
- Too ambitious:
  - computationally intractable.
  - many measurable functions.

Independence measures: measurable → continuous

- $C_b(\mathcal{X}) = \{f : \mathcal{X} \text{ metric} \to \mathbb{R}, \text{ bounded continuous}\}$ would also work.
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- $C_b(\mathcal{X}) = \{f : \mathcal{X} \text{ metric} \to \mathbb{R}, \text{ bounded continuous}\}$ would also work.
- Still too large!
- Idea:
  - certain RKHS-s are dense in $C_b(\mathcal{X})$.
  - computionally tractable.

KCCA: definition

- Given: $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$.
- Associated:
  - feature maps $\varphi(x) = k(\cdot, x)$, $\psi(y) = \ell(\cdot, y)$,
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- KCCA measure of $(x, y) \in \mathcal{X} \times \mathcal{Y}$

$$\rho_{\text{KCCA}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \operatorname{corr}(f(x), g(y)),$$

$$\operatorname{corr}(f(x), g(y)) = \frac{\operatorname{cov}_{xy}(f(x), g(y))}{\sqrt{\operatorname{var}_x f(x) \operatorname{var}_y g(y)}}.$$

KCCA: notes

- Optimization domain: $\mathcal{H}_k \times \mathcal{H}_\ell \ni (f, g)$.
- By reproducing property: we will get a finite-D task.
- k,ℓ linear: traditional CCA.
- In practice: we have $\{(x_n, y_n)\}_{n=1}^N$ samples from (x, y).

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Recall the reproducing property

$$f(x) = \langle f, k(\cdot, x)\rangle_{\mathcal{H}_k} \quad \forall f \in \mathcal{H}_k, x \in \mathcal{X}.$$

KCCA: empirical estimate

$$\widehat{\mathrm{cov}}_{xy}(f(x),g(y)) = \frac{1}{N}\sum_{n=1}^{N}\Bigg[\underbrace{f(x_n) - \frac{1}{N}\sum_{i=1}^{N} f(x_i)}_{\left\langle f,\varphi(x_n)-\frac{1}{N}\sum_{i=1}^{N}\varphi(x_i)\right\rangle_{\mathcal{H}_k}}\Bigg]\Bigg[\underbrace{g(y_n) - \frac{1}{N}\sum_{i=1}^{N} g(y_i)}_{\left\langle g,\psi(y_n)-\frac{1}{N}\sum_{i=1}^{N}\psi(y_i)\right\rangle_{\mathcal{H}_\ell}}\Bigg]$$

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- $\forall$ component of f $\perp$

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has no affect in the objective.

Key idea

Enough to consider $f = \sum_{i=1}^N c_i\tilde{\varphi}(x_i)$, $g = \sum_{i=1}^N d_i\tilde{\psi}(y_i)$.

KCCA: empirical estimate

Using that $f = \sum_{i=1}^{N} c_i \tilde{\varphi}(x_i)$, $g = \sum_{i=1}^{N} d_i \tilde{\psi}(y_i)$:

$$\langle f, \tilde{\varphi}(x_n) \rangle_{\mathcal{H}_k} = \sum_{i=1}^{N} c_i \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_n) \rangle_{\mathcal{H}_k}$$

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$$\left\langle g, \tilde{\psi}(y_n)\right\rangle_{\mathcal{H}_\ell} = (\mathbf{d}^T \tilde{\mathbf{G}}_y)_n,$$

with the centered kernels ($\tilde{k}$, $\tilde{\ell}$) and Gram matrices ($\tilde{\mathbf{G}}_x$, $\tilde{\mathbf{G}}_y$).

Until now

All the objective terms can be expressed by $\mathbf{c}$, $\mathbf{d}$, $\tilde{\mathbf{G}}_x$, $\tilde{\mathbf{G}}_y$.

KCCA: empirical estimate

$$\widehat{\text{cov}}_{xy}(f(x), g(y)) = \frac{1}{N}\sum_{n=1}^{N} \langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k} \left\langle g, \tilde{\psi}(y_n)\right\rangle_{\mathcal{H}_\ell},$$

$$\widehat{\text{var}}_x f(x) = \frac{1}{N}\sum_{n=1}^{N} \langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k}{}^2, \widehat{\text{var}}_y g(y) = \frac{1}{N}\sum_{n=1}^{N} \left\langle g, \tilde{\psi}(y_n)\right\rangle_{\mathcal{H}_\ell}{}^2,$$

and we have

$$\langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k} = (\mathbf{c}^T \tilde{\mathbf{G}}_x)_n, \qquad \left\langle g, \tilde{\psi}(y_n)\right\rangle_{\mathcal{H}_\ell} = (\mathbf{d}^T \tilde{\mathbf{G}}_y)_n.$$

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and we have

$$\langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k} = (\mathbf{c}^T \tilde{\mathbf{G}}_x)_n, \qquad \left\langle g, \tilde{\psi}(y_n)\right\rangle_{\mathcal{H}_\ell} = (\mathbf{d}^T \tilde{\mathbf{G}}_y)_n.$$

Thus,

$$\widehat{\mathrm{cov}}_{xy}(f(x), g(y)) = \frac{1}{N}\mathbf{c}^T \tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \mathbf{d},$$

$$\widehat{\mathrm{var}}_x f(x) = \frac{1}{N}\mathbf{c}^T (\tilde{\mathbf{G}}_x)^2 \mathbf{c}, \quad \widehat{\mathrm{var}}_y g(y) = \frac{1}{N}\mathbf{d}^T (\tilde{\mathbf{G}}_y)^2 \mathbf{d}.$$

KCCA: finite-D form

Empirical estimate of KCCA:

$$\widehat{\rho_{\text{KCCA}}}^{\text{temp}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell) = \sup_{\mathbf{c}\in\mathbb{R}^N, \mathbf{d}\in\mathbb{R}^N} \frac{\mathbf{c}^T \tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \mathbf{d}}{\sqrt{\mathbf{c}^T (\tilde{\mathbf{G}}_x)^2 \mathbf{c}} \sqrt{\mathbf{d}^T (\tilde{\mathbf{G}}_y)^2 \mathbf{d}}}.$$

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In practice ($\kappa > 0$):

$$\widehat{\rho_{\text{KCCA}}}(x, y) := \widehat{\rho_{\text{KCCA}}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa)$$

$$= \sup_{\mathbf{c}\in\mathbb{R}^N, \mathbf{d}\in\mathbb{R}^N} \frac{\mathbf{c}^T \tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \mathbf{d}}{\sqrt{\mathbf{c}^T \left(\tilde{\mathbf{G}}_x + \kappa \mathbf{I}_N\right)^2 \mathbf{c}} \sqrt{\mathbf{d}^T \left(\tilde{\mathbf{G}}_y + \kappa \mathbf{I}_N\right)^2 \mathbf{d}}}.$$

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Question

How do we solve it?

KCCA: solution

Stationary points of $\widehat{\rho_{\text{KCCA}}}(x,y)$:

$$\mathbf{0}=\frac{\partial \widehat{\rho_{\text{KCCA}}}(x,y)}{\partial \mathbf{c}}, \qquad \mathbf{0}=\frac{\partial \widehat{\rho_{\text{KCCA}}}(x,y)}{\partial \mathbf{d}},$$

which simplifies to

$$\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d}=\frac{(\mathbf{c}^T\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d})(\tilde{\mathbf{G}}_x+\kappa\mathbf{I}_N)^2\mathbf{c}}{\mathbf{c}^T(\tilde{\mathbf{G}}_x+\kappa\mathbf{I}_N)^2\mathbf{c}}, \quad \tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x\mathbf{c}=\frac{(\mathbf{d}^T\tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x\mathbf{c})(\tilde{\mathbf{G}}_y+\kappa\mathbf{I}_N)^2\mathbf{d}}{\mathbf{d}^T(\tilde{\mathbf{G}}_y+\kappa\mathbf{I}_N)^2\mathbf{d}}.$$

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Stationary points of $\widehat{\rho_{\text{KCCA}}}(x, y)$:

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$$\tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \mathbf{d} = \frac{(\mathbf{c}^T \tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \mathbf{d})(\tilde{\mathbf{G}}_x + \kappa \mathbf{I}_N)^2 \mathbf{c}}{\mathbf{c}^T (\tilde{\mathbf{G}}_x + \kappa \mathbf{I}_N)^2 \mathbf{c}}, \quad \tilde{\mathbf{G}}_y \tilde{\mathbf{G}}_x \mathbf{c} = \frac{(\mathbf{d}^T \tilde{\mathbf{G}}_y \tilde{\mathbf{G}}_x \mathbf{c})(\tilde{\mathbf{G}}_y + \kappa \mathbf{I}_N)^2 \mathbf{d}}{\mathbf{d}^T (\tilde{\mathbf{G}}_y + \kappa \mathbf{I}_N)^2 \mathbf{d}}.$$

Normalization:

- $(\mathbf{c}, \mathbf{d})$: solution $\Rightarrow$ $(a\mathbf{c}, b\mathbf{d})$: solution $a, b \in \mathbb{R}, \neq 0$.
- denominators $:= 1$.

KCCA: final task

Find the maximal eigenvalue, $\lambda := \mathbf{c}^T\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d}$, of the generalized eigenvalue problem:

$$\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y \\ \tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \mathbf{c}^T\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d} \begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_y + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

$$\mathbf{Az} = \lambda\mathbf{Bz}.$$

KCCA as an independence measure

If $x \perp y$, then $\rho_{\text{KCCA}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = 0$. Opposite direction:

- For 'rich' $\mathcal{H}_k$, $\mathcal{H}_\ell$
  [Bach and Jordan, 2002, Gretton et al., 2005b].

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- For 'rich' $\mathcal{H}_k$, $\mathcal{H}_\ell$
  [Bach and Jordan, 2002, Gretton et al., 2005b].
- Enough: universal kernel on a compact metric domain (later).
- Example ($\gamma > 0$):
  - Gaussian: $k(x, x') = e^{-\gamma \|x - x'\|_2^2}$.
  - Laplacian kernel: $k(x, x') = e^{-\gamma \|x - x'\|_2}$.

KCCA: regularization

In fact, we estimated

$$\rho_{\mathrm{KCCA}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \operatorname{corr}(f(x), g(y); \kappa),$$

$$\operatorname{corr}(f(x), g(y); \kappa) = \frac{\operatorname{cov}_{xy}(f(x), g(y))}{\sqrt{\operatorname{var}_x f(x) + \kappa \|f\|^2_{\mathcal{H}_k}}\sqrt{\operatorname{var}_y g(y) + \kappa \|g\|^2_{\mathcal{H}_\ell}}}.$$

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- Regularization is important: With $\kappa = 0$, $\lambda \in \{0, \pm 1\} \Rightarrow$

$$\rho_{\text{KCCA}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = 1$$

would be data-independently [Gretton et al., 2005b], [Bach and Jordan, 2002].

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$$\rho_{\text{KCCA}}(x, y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \operatorname{corr}(f(x), g(y); \kappa),$$

$$\operatorname{corr}(f(x), g(y); \kappa) = \frac{\operatorname{cov}_{xy}(f(x), g(y))}{\sqrt{\operatorname{var}_x f(x) + \kappa \|f\|^2_{\mathcal{H}_k}} \sqrt{\operatorname{var}_y g(y) + \kappa \|g\|^2_{\mathcal{H}_\ell}}}.$$

- For consistent KCCA estimate:
  - $\kappa_N \to 0$ [Leurgans et al., 1993](spline-RKHS), [Fukumizu et al., 2007] (general RKHS).
  - analysis: covariance operators (later).

KCCA: symmetry, other form

For

$$\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y \\ \tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \mathbf{c}^T\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d} \begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_y + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

$([\mathbf{c}, \mathbf{d}], \lambda)$ solution $\Rightarrow$ $([-\mathbf{c}; \mathbf{d}], -\lambda)$: solution. Thus, eigenvalues:

$$\{\lambda_1, -\lambda_1, \ldots, \lambda_N, -\lambda_N\}.$$

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$$\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y \\ \tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \mathbf{c}^T\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y\mathbf{d} \begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_y + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

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Adding the r.h.s. to both sides:

$$\begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 & \tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y \\ \tilde{\mathbf{G}}_y\tilde{\mathbf{G}}_x & (\tilde{\mathbf{G}}_\mathbf{y} + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = (1+\lambda) \begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_x + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

with eigenvalues $\{1+\lambda_1, 1-\lambda_1, \ldots, 1+\lambda_N, 1-\lambda_N\}$.

KCCA: M-variables

2-variables $[(x, y)]$:

$$\begin{bmatrix} (\tilde{\mathbf{G}}_{\mathbf{x}} + \kappa \mathbf{I}_N)^2 & \tilde{\mathbf{G}}_x \tilde{\mathbf{G}}_y \\ \tilde{\mathbf{G}}_y \tilde{\mathbf{G}}_x & (\tilde{\mathbf{G}}_{\mathbf{y}} + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = (1 + \lambda) \begin{bmatrix} (\tilde{\mathbf{G}}_x + \kappa \mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_x + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

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For M-variables (pairwise dependence):

$$\begin{bmatrix} (\tilde{\mathbf{G}}_1 + \kappa \mathbf{I}_N)^2 & \tilde{\mathbf{G}}_1 \tilde{\mathbf{G}}_2 & \ldots & \tilde{\mathbf{G}}_1 \tilde{\mathbf{G}}_M \\ \tilde{\mathbf{G}}_2 \tilde{\mathbf{G}}_1 & (\tilde{\mathbf{G}}_2 + \kappa \mathbf{I}_N)^2 & \ldots & \tilde{\mathbf{G}}_2 \tilde{\mathbf{G}}_M \\ \vdots & \vdots & & \vdots \\ \tilde{\mathbf{G}}_M \tilde{\mathbf{G}}_1 & \tilde{\mathbf{G}}_M \tilde{\mathbf{G}}_2 & \ldots & (\tilde{\mathbf{G}}_M + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{bmatrix} =$$

$$\gamma \begin{bmatrix} (\tilde{\mathbf{G}}_1 + \kappa \mathbf{I}_N)^2 & \mathbf{0} & \ldots & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_2 + \kappa \mathbf{I}_N)^2 & \ldots & \mathbf{0} \\ \vdots & \vdots & & \\ \mathbf{0} & \mathbf{0} & \ldots & (\tilde{\mathbf{G}}_M + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{bmatrix}.$$

Centered Gram matrix

In short

$\tilde{\mathbf{G}}_x = \mathbf{H}\mathbf{G}_x\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N\times N}$.

$$(\tilde{\mathbf{G}}_x)_{ij} = \tilde{k}(x_i, x_j) = \left\langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \right\rangle_{\mathcal{H}_k}$$

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$$
\begin{aligned}
(\tilde{\mathbf{G}}_x)_{ij} &= \tilde{k}(x_i, x_j) = \left\langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \right\rangle_{\mathcal{H}_k} \\
&= \left\langle \varphi(x_i) - \frac{1}{N}\sum_{n=1}^{N} \varphi(x_n), \varphi(x_j) - \frac{1}{N}\sum_{m=1}^{N} \varphi(x_m) \right\rangle_{\mathcal{H}_k} \\
&= (\mathbf{G}_x)_{ij} - \frac{1}{N}\sum_{m=1}^{N} (\mathbf{G}_x)_{im} - \frac{1}{N}\sum_{n=1}^{N} (\mathbf{G}_x)_{ni} + \frac{1}{N^2}\sum_{n,m=1}^{N} (\mathbf{G}_x)_{nm}
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&= \left(\mathbf{G}_x - \mathbf{G}_x \frac{\mathbf{E}_N}{N} - \frac{\mathbf{E}_N}{N}\mathbf{G}_x + \frac{\mathbf{E}_N}{N}\mathbf{G}_x\frac{\mathbf{E}_N}{N} \right)_{ij},
\end{aligned}$$

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&= \left(\mathbf{G}_x - \mathbf{G}_x\frac{\mathbf{E}_N}{N} - \frac{\mathbf{E}_N}{N}\mathbf{G}_x + \frac{\mathbf{E}_N}{N}\mathbf{G}_x\frac{\mathbf{E}_N}{N}\right)_{ij}, \\
&= (\mathbf{H}\mathbf{G}_x\mathbf{H})_{ij},
\end{aligned}
$$

$\mathbf{H}$: symmetric ($\mathbf{H} = \mathbf{H}^T$), idempotent ($\mathbf{H}^2 = \mathbf{H}$).

KCCA: finished.

Mean embedding

Mean embedding: pioneers

- Nonparametric probability distribution representation.
- Late 70s-; survey in [Berlinet and Thomas-Agnan, 2004].

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- Late 70s-; survey in [Berlinet and Thomas-Agnan, 2004].
- Pioneers in ML: Bharath Sriperumbudur, Arthur Gretton, Kenji Fukumizu, Alex Smola, Bernhard Schölkopf, Le Song.

Mean embedding: further pointers

- Names+: Ingo Steinwart, Francis Bach, Dino Sejdinovic, Wittawat Jitkrittum, Krikamol Maundet, Kacper P. Chwialkowski, Ilya Tolstikhin, Carl Johann Simon-Gabriel, David Lopez-Paz, Dougal Sutherland, Aaditya Ramdas, Karsten Borgwardt, Me;)

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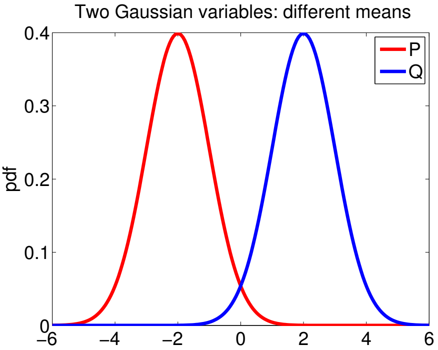
- Wiki: `https://en.wikipedia.org/wiki/Kernel_embedding_of_distributions`.
- Recent review: [Muandet et al., 2017].

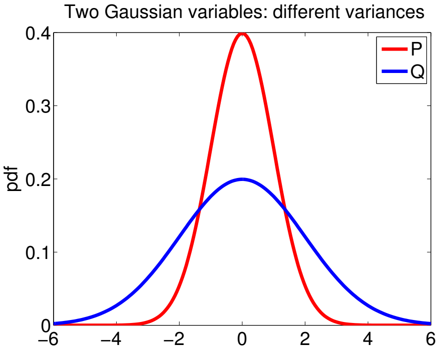
Towards representations of distributions: $\mathbb{E}X$

- Given: 2 Gaussians with different means.
- Solution: *t*-test.



Towards representations of distributions: $\mathbb{E}X^2$

- Setup: 2 Gaussians; same means, different variances.
- Idea: look at the 2nd-order features of RVs.



Towards representations of distributions: $\mathbb{E}X^2$

- Setup: 2 Gaussians; same means, different variances.
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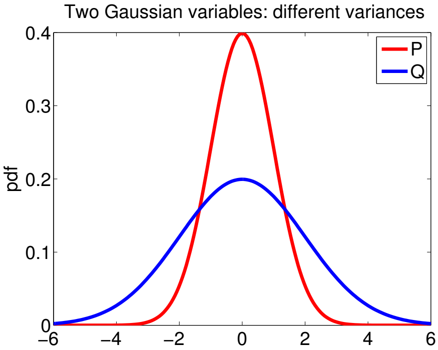
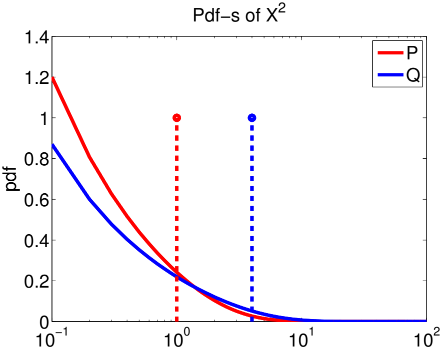
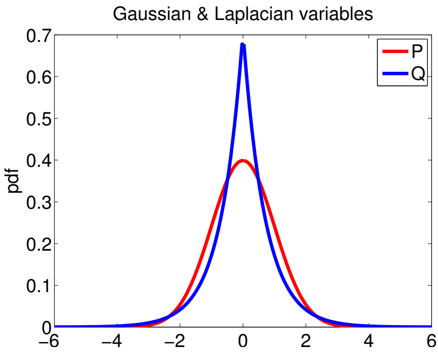
- $\varphi_x = x^2 \Rightarrow$ difference in $\mathbb{E}X^2$.





Towards representations of distributions: further moments

- Setup: a Gaussian and a Laplacian distribution.
- Challenge: their means *and* variances are the same.
- Idea: look at higher-order features.



Let us consider feature representations!

From kernel trick to mean trick

- Recall:
  - $\varphi(x) \in \mathcal{H}_k$: feature of $x \in \mathcal{X}$.
  - Kernel: $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}_k}$.

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  - Feature of $\mathbb{P}$:

$$\mu_{\mathbb{P}} = \mathbb{E}_{x \sim \mathbb{P}}[\varphi(x)] \in \mathcal{H}_k.$$

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Commonly used construction

$\mu_{\mathbb{P}} = \mathbb{E}_{x\sim\mathbb{P}}[\varphi(x)]$. Indeed. . .

Distribution Representation via Functions

- Cumulative density function:

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$\mathbb{P} \mapsto \mu_{\mathbb{P}} = \int_{\mathcal{X}} \varphi(x)\mathrm{d}\mathbb{P}(x)$, in our case: $\varphi(x) = k(\cdot, x)$.

Bochner integral: quick summary [Diestel and Uhl, 1977, Dinculeanu, 2000, Steinwart and Christmann, 2008]

- Given:
  - $(\mathcal{X}, \mathcal{A}, \mu)$: σ-finite measure space,
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- f measurable function is Bochner μ-integrable if
  - $\exists$ (f_n) measurable step functions: $\lim_{n\to\infty} \int_{\mathcal{X}} \|f - f_n\|_B \, \mathrm{d}\mu = 0$.
  - In this case $\lim_{n\to\infty} \int_{\mathcal{X}} f_n \mathrm{d}\mu$ exists, $=: \int_{\mathcal{X}} f \mathrm{d}\mu$.

Bochner integral: properties

- $f : \mathcal{X} \to B$ is Bochner integrable $\Leftrightarrow \int_{\mathcal{X}} \|f\|_B \, d\mu < \infty$.

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- If
  - $S : B \to B_2$: bounded linear operator,
  - $f : X \to B$: Bochner integrable, then

  $S \circ f : X \to B_2$ is Bochner integrable and

$$S\left(\int_{\mathcal{X}} f \mathrm{d}\mu\right) = \int_{\mathcal{X}} Sf \mathrm{d}\mu.$$

Bochner integral: properties

- $f:\mathcal{X}\to B$ is Bochner integrable $\Leftrightarrow \int_{\mathcal{X}}\|f\|_B\,\mathrm{d}\mu<\infty$.
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In short

$\left|\int f\mathrm{d}\mu\right|\leqslant\int|f|\mathrm{d}\mu$ and $c\int f\mathrm{d}\mu=\int cf\mathrm{d}\mu$ generalize nicely.

Mean embedding: $\exists$, $\mathbb{E}_{\mathbb{P}}$-reproducing property

Given:

- $(\mathcal{X}, \mathcal{A})$ measurable space,
- $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ kernel.

Theorem

$\mu_{\mathbb{P}} := \int_{\mathcal{X}} k(\cdot, x)\mathrm{d}\mathbb{P}(x)$ *exists,* $\mu_{\mathbb{P}} \in \mathcal{H}_k$*, and*

$$\mathbb{P}f := \mathbb{E}_{x\sim\mathbb{P}} f(x) = \langle f, \mu_{\mathbb{P}} \rangle_{\mathcal{H}_k} \ \forall f \in \mathcal{H}_k$$

under mild conditions:

- $\mathbb{E}_{x\sim\mathbb{P}}\sqrt{k(x,x)} < \infty$, *and*
- $y \mapsto k(y,x)$ *is measurable for any* $x \in \mathcal{X}$.

Existence of $\mu_{\mathbb{P}}$: proof

- $\exists \int_{\mathcal{X}} k(\cdot, x) \mathrm{d}\mathbb{P}(x)$ ($\& \in \mathcal{H}_k$) $\Leftrightarrow$

$$\infty > \int_{\mathcal{X}} \|k(\cdot, x)\|_{\mathcal{H}_k} \mathrm{d}\mathbb{P}(x) = \mathbb{E}_{x\sim\mathbb{P}}\sqrt{k(x,x)}.$$

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  - reproducing property of k,
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    - reproducing property of k,
    - $g \in \mathcal{H}_k \mapsto \langle f, g\rangle \in \mathbb{R}$: bounded linear ($S \leftrightarrow \int$).
- Measurability of $x \in \mathcal{X} \mapsto k(\cdot,x) \in \mathcal{H}_k$: $\Leftrightarrow$ $y \mapsto k(y,x)$ is measurable $\forall x$ [Berlinet and Thomas-Agnan, 2004].

Mean embedding: specific cases

For

- $k(x, x') = e^{\langle x, x' \rangle}$: $\mu_{\mathbb{P}}$ = moment generating function of $\mathbb{P}$.
- $k(x, y) = e^{i\langle x, y \rangle}$: $\mu_{\mathbb{P}}$ = characteristic function of $\mathbb{P}$.
  - Only formally: $k(x, y) = k(y, x)^*$ fails.
- $\mathbb{P} = \delta_x$, $\mu_{\mathbb{P}} = k(\cdot, x)$.

Mean embedding: conditions

Condition:

- $y \mapsto k(y,x)$ is measurable $\forall x$: super-mild.
- $\mathbb{E}_{x\sim\mathbb{P}}\sqrt{k(x,x)} < \infty$: holds for bounded kernels, i.e. when

$$\sup_{x,x'\in\mathcal{X}} k(x,x') \leqslant B_k < \infty.$$

Mean embedding: empirical estimate

- $\mu_{\mathbb{P}}$: typically analytically not available.
- Empirical estimate: from $\{x_i\}_{i=1}^n \overset{i.i.d.}{\sim} \mathbb{P}$

$$\widehat{\mu_{\mathbb{P}}} = \frac{1}{n}\sum_{i=1}^n k(\cdot, x_i) = \mu_{\mathbb{P}_n} \in \mathcal{H}_k,$$

where $\mathbb{P}_n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$ is the empirical measure.

Empirical mean embedding: finite-sample guarantees

Theorem ([Altun and Smola, 2006])

For a k bounded kernel [$\sup_{x,y\in\mathcal{X}} k(x,y) \leqslant B_k$], *with probability* $\geqslant 1-\delta$

$$\|\mu_{\mathbb{P}} - \mu_{\mathbb{P}_n}\|_{\mathcal{H}_k} \leqslant \frac{\left[1+\sqrt{\log\left(\frac{1}{\delta}\right)}\right]\sqrt{2B_k}}{\sqrt{n}}.$$

Finite-sample guarantee: proof idea

- $g(x_1,\ldots,x_n) = \|\mu_{\mathbb{P}} - \mu_{\mathbb{P}_n}\|_{\mathcal{H}_k}$: bounded difference property $\Rightarrow$
- McDiarmid inequality: concentration around $\mathbb{E}g$.
- $\mathbb{E}g \leqslant$ expected kernel values (B_k appears).

Finite-sample guarantee: note

Alternative of

$$\mathbb{P}\left(\|\mu_{\mathbb{P}}-\mu_{\mathbb{P}_n}\|_{\mathcal{H}_k} \leqslant \frac{\left[1+\sqrt{\log\left(\frac{1}{\delta}\right)}\right]\sqrt{2B_k}}{\sqrt{n}}\right) \geqslant 1-\delta.$$

Directly by the Bernstein inequality [Caponnetto and De Vito, 2007]:

$$\mathbb{P}\left(\|\mu_{\mathbb{P}}-\mu_{\mathbb{P}_n}\|_{\mathcal{H}_k} \leqslant 2\sqrt{B_k}\left[\frac{2}{n}+\frac{1}{\sqrt{n}}\log\left(\frac{2}{\delta}\right)\right]\right) \geqslant 1-\delta$$

would give a bit worse dependence.

MMD: preview

- Mean embeddings define a semi-metric (MMD):

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- d_k is metric $\Leftrightarrow \mathbb{P} \mapsto \mu_{\mathbb{P}}$ is injective.
- Characteristic kernel [Fukumizu et al., 2004, Fukumizu et al., 2008]:
  - characteristic function analogy.
  - L-order polynomial kernel: encodes moments $\leqslant L$. (not)

Mean embedding: universality (k)

Universal kernel

Let $C(\mathcal{X}) = \{f : \mathcal{X} \to \mathbb{R} \text{ continuous}\}$.

Definition

Assume:

- $\mathcal{X}$: compact metric space.
- k: continuous kernel on $\mathcal{X}$.

k is called *(c)-universal* [Steinwart, 2001] if $\mathcal{H}_k$ is dense in $(C(\mathcal{X}), \|\cdot\|_\infty)$.

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$\mathcal{X}$ assumption $\Rightarrow$

$C(\mathcal{X}) = C_b(\mathcal{X}) = \{f : \mathcal{X} \to \mathbb{R} \text{ continuous bounded}\}$

Universal kernel

$\mathcal{H}_k \subset C(\mathcal{X})$? Non-compact spaces?

Notes:

- k: continuous, $\mathcal{X}$: compact $\Rightarrow$ k: bounded.
- k: continuous, bounded $\Rightarrow$ $\mathcal{H}_k \subset C(\mathcal{X})$ [Steinwart and Christmann, 2008].

Universal kernel

$\mathcal{H}_k \subset C(\mathcal{X})$? Non-compact spaces?

Notes:

- Extensions of c-universality to non-compact spaces:
  - c_0-universality, cc-universality, …[Carmeli et al., 2010, Sriperumbudur et al., 2010a, Simon-Gabriel and Schölkopf, 2018].

k: universal $\Rightarrow$ k: characteristic

$\geqslant 3$ different proof options:

1. [Micchelli et al., 2006]: k is c-universal $\Leftrightarrow$ μ is injective on $\mathcal{M}_b(\mathcal{X})$, the set of finite signed Borel measures on $\mathcal{X}$.

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Let us construct some *examples* first! (then prove 1-2)

Properties of universal kernels [Steinwart, 2001, Steinwart and Christmann, 2008]

If k is universal, then

- $k(x, x) > 0$ for all $x \in \mathcal{X}$.

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  is a metric.
- The normalized kernel (recall: corr)

$$\tilde{k}(x,y) := \frac{k(x,y)}{\sqrt{k(x,x)k(y,y)}}$$

  is universal.

Universal Taylor kernels [Steinwart, 2001, Steinwart and Christmann, 2008]

- For an $C^\infty \ni f : (-r, r) \to \mathbb{R}$

$$f(t) = \sum_{n=0}^{\infty} a_n t^n \quad t \in (-r, r), \;\; r \in (0, \infty].$$

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$$f(t) = \sum_{n=0}^{\infty} a_n t^n \quad t \in (-r, r), \; r \in (0, \infty].$$

- If $a_n > 0 \; \forall n$, then

$$k(x, y) = f(\langle x, y \rangle)$$

is universal on $\mathcal{X} := \left\{x \in \mathbb{R}^d : \|x\|_2 \leqslant \sqrt{r}\right\}$.

Universal kernels on compact subsets of $\mathbb{R}^d$, $\alpha > 0$

- $k(x,y) = e^{\alpha\langle x,y\rangle}$: previous result with $f(t) = e^{\alpha t} \Rightarrow a_n = \frac{\alpha^n}{n!}$.

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- $k(x,y) = e^{-\alpha\|x-y\|_2^2}$: exp. kernel & normalization.

Universal kernels on compact subsets of $\mathbb{R}^d$, $\alpha > 0$

- $k(x, y) = (1 - \langle x, y \rangle)^{-\alpha}$ binomial kernel
  - on $\mathcal{X}$ compact $\subset \{x \in \mathbb{R}^d : \|x\|_2 < 1\}$.
  - $f(t) = (1 - t)^{-\alpha} = \sum_{n=0}^{\infty} \underbrace{\binom{-\alpha}{n}(-1)^n}_{>0} t^n \quad (|t| < 1)$,

where $\binom{b}{n} = \sum_{i=1}^{n} \frac{b-i+1}{i}$.

Universal ⇒ characteristic: proof-1

Injectivity on finite signed measures (proof):

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$$\{0\} = H^{\perp} := \{F \in C' : \forall f \in H, F(f) = 0\}.$$

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$$= \{\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) : \mu_{\mathbb{F}} = 0\}.$$

Universal $\Rightarrow$ characteristic: proof-2

Direct reasoning: We have already 'mentioned' [Dudley, 2004]:

- Let $\mathcal{X}$: metric space, $\mathbb{P}, \mathbb{Q} \in \mathcal{M}_1^+(\mathcal{X})$.
- Then $\mathbb{P} = \mathbb{Q}$ (Borel probability measures) $\Leftrightarrow$

$$\mathbb{P}f = \mathbb{Q}f \left(:= \int_{\mathcal{X}} f(x) \mathrm{d}\mathbb{Q}(x) \right) \quad \forall f \in C_b(\mathcal{X}).$$

We have a characterization of $\mathbb{P} = \mathbb{Q}$ in terms of expectations.

Universal $\Rightarrow$ characteristic: proof-2

- Goal: $\mu_{\mathbb{P}} = \mu_{\mathbb{Q}} \Rightarrow \mathbb{P} = \mathbb{Q}$ [$\Leftrightarrow \mathbb{P}f = \mathbb{Q}f$, $\forall f \in C_b(\mathcal{X})$].

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- $\mathcal{H}_k \ni$ g:= ϵ-approximation of f,

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$$|\mathbb{P}g - \mathbb{Q}g| = |\underbrace{\langle g, \mu_{\mathbb{P}}\rangle_{\mathcal{H}_k} - \langle g, \mu_{\mathbb{Q}}\rangle_{\mathcal{H}_k}}_{\left\langle g, \underbrace{\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}}_{=0} \right\rangle_{\mathcal{H}_k}}| = 0.$$ Thus $|\mathbb{P}f - \mathbb{Q}f| \leqslant 2\epsilon$.

Universality: finished. Now: characteristic property.

$d_k(\mathbb{P},\mathbb{Q})$ (=MMD) in terms of kernel evaluations

[Gretton et al., 2007]:

$$d_k^2(\mathbb{P},\mathbb{Q}) = \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}^2 = \left\| \int_{\mathcal{X}} k(\cdot,x)\mathrm{d}\mathbb{P}(x) - \int_{\mathcal{X}} k(\cdot,y)\mathrm{d}\mathbb{Q}(y) \right\|_{\mathcal{H}_k}^2$$

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&= \langle a - b, a - b \rangle_{\mathcal{H}_k} \\
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&= \int_{\mathcal{X}} \int_{\mathcal{X}} k(x, x') \mathrm{d}\mathbb{P}(x) \mathrm{d}\mathbb{P}(x') + \int_{\mathcal{X}} \int_{\mathcal{X}} k(y, y') \mathrm{d}\mathbb{Q}(y) \mathrm{d}\mathbb{Q}(y') \\
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&= \int_{\mathcal{X}}\int_{\mathcal{X}} k(x,x')\mathrm{d}\mathbb{P}(x)\mathrm{d}\mathbb{P}(x') + \int_{\mathcal{X}}\int_{\mathcal{X}} k(y,y')\mathrm{d}\mathbb{Q}(y)\mathrm{d}\mathbb{Q}(y') \\
&\quad - 2\int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathrm{d}\mathbb{P}(x)\mathrm{d}\mathbb{Q}(y) \\
&= \int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathrm{d}(\mathbb{P}-\mathbb{Q})(x)\mathrm{d}(\mathbb{P}-\mathbb{Q})(y).
\end{aligned}
$$

$\Rightarrow$ Polynomial kernels are *not* characteristic

[Sriperumbudur et al., 2010b]:

- $k(x, y) = \langle x, y \rangle$: linear kernel ($L = 1$).

$$d_k^2(\mathbb{P}, \mathbb{Q}) = \|m_{\mathbb{P}} - m_{\mathbb{Q}}\|_2^2, \qquad m_{\mathbb{P}} = \int_{\mathcal{X}} x \mathrm{d}\mathbb{P}(x).$$

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- $k(x,y) = (\langle x,y\rangle + 1)^2$ ($L=2$):

$$d_k^2(\mathbb{P},\mathbb{Q}) = 2\left\| m_{\mathbb{P}} - m_{\mathbb{Q}} \right\|_2^2 + \left\| \Sigma_{\mathbb{P}} - \Sigma_{\mathbb{Q}} + m_{\mathbb{P}} m_{\mathbb{P}}^T - m_{\mathbb{Q}} m_{\mathbb{Q}}^T \right\|_F^2,$$

where $\|\cdot\|_F$: Frobenious norm; $\Sigma_{\mathbb{P}}$: cov. matrix w.r.t. $\mathbb{P}$.

Characteristic property

Well-understood for

1. Continuous bounded shift-invariant kernels on $\mathbb{R}^d$:

$$k(x,y) = k_0(x-y),\ k_0 \in C_b\left(\mathbb{R}^d\right).$$

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1. Continuous bounded shift-invariant kernels on $\mathbb{R}^d$:

$$k(x,y) = k_0(x-y),\ k_0 \in C_b\left(\mathbb{R}^d\right).$$

2. Continuous bounded radial kernels on $\mathbb{R}^d$:

$$k(x,y) = k_0(\|x-y\|_2), \quad k_0 \in C_b\left(\mathbb{R}^d\right),$$
$$k_0(z) = \int_{[0,\infty)} e^{-tz^2} \mathrm{d}\nu(t)$$

$\nu \in \mathcal{M}_b^+[0,\infty)$, i.e. it is a finite measure on $[0,\infty)$.

Bochner's theorem

We focus on continuous bounded shift-invariant kernels:

Theorem (Bochner's theorem [Wendland, 2005], $k \leftrightarrow \Lambda$)

$$k_0(z) = \int_{\mathbb{R}^d} e^{-i\langle z,\omega\rangle} \mathrm{d}\Lambda(\omega),$$

where Λ is a finite Borel measure (w.l.o.g. probability).

MMD in terms of characteristic functions

Using Bochner's theorem:

$$d_k^2(\mathbb{P}, \mathbb{Q}) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} k(x, y) \mathrm{d}(\mathbb{P} - \mathbb{Q})(x) \mathrm{d}(\mathbb{P} - \mathbb{Q})(y)$$

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&= \int_{\mathbb{R}^d} \underbrace{\left[\int_{\mathbb{R}^d} e^{-i\langle x,\omega\rangle}\mathrm{d}(\mathbb{P}-\mathbb{Q})(x)\right]}_{\overline{\phi_{\mathbb{P}}(\omega)-\phi_{\mathbb{Q}}(\omega)}} \underbrace{\left[\int_{\mathbb{R}^d} e^{i\langle y,\omega\rangle}\mathrm{d}(\mathbb{P}-\mathbb{Q})(y)\right]}_{\phi_{\mathbb{P}}(\omega)-\phi_{\mathbb{Q}}(\omega)}\mathrm{d}\Lambda(\omega)
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Continuous bounded translation-invariant kernels

Theorem ([Sriperumbudur et al., 2010b])

They are characteristic iff. $supp(\Lambda) = \mathbb{R}^d$.

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- Example: Gaussian, Laplacian, Matérn kernel, B-spline kernel.

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- Example: Gaussian, Laplacian, Matérn kernel, B-spline kernel.
- Similar characterization ∃ on 'Bochner domains' (LCA groups [Berg et al., 1984], orthogonal matrices, $\mathbb{R}_+^d$) [Fukumizu et al., 2009b].

Matérn kernel

$$k(x,y) = k_0(x-y) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}\,\|x-y\|_2}{\sigma} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}\,\|x-y\|_2}{\sigma} \right),$$

where K_ν: modified Bessel function of the second kind of order ν

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$$k(x,y) = k_0(x-y) = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2v}\,\|x-y\|_2}{\sigma}\right)^{v} K_v\left(\frac{\sqrt{2v}\,\|x-y\|_2}{\sigma}\right),$$

$$\widehat{k_0}(\omega) = \frac{2^{d+v}\pi^{\frac{d}{2}}\Gamma(v+d/2)v^v}{\Gamma(v)\sigma^{2v}}\left(\frac{2v}{\sigma^2}+4\pi^2\|\omega\|_2^2\right)^{-(v+d/2)} > 0 \quad \forall\omega\in\mathbb{R}^d,$$

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- For $v = \frac{1}{2}$: one gets $k(x,y) = e^{-\frac{\|x-y\|_2}{\sigma}}$.
- Gaussian kernel: $v \to \infty$.

Shift-invariant kernels on $\mathbb{R}$ [Sriperumbudur et al., 2010b]

For Poisson kernel: $\sigma \in (0,1)$.

kernel name	k_0	$\widehat{k_0}(\omega)$	$supp(\widehat{k_0})$
Gaussian	$e^{-\frac{x^2}{2\sigma^2}}$	$\sigma e^{-\frac{\sigma^2\omega^2}{2}}$	$\mathbb{R}$
Laplacian	$e^{-\sigma\|x\|}$	$\sqrt{\frac{2}{\pi}}\frac{\sigma}{\sigma^2+\omega^2}$	$\mathbb{R}$
B_{2n+1}-spline	$*^{2n+2}\chi_{\left[-\frac{1}{2},\frac{1}{2}\right]}(x)$	$\frac{4^{n+1}}{\sqrt{2\pi}}\frac{\sin^{2n+2}\left(\frac{\omega}{2}\right)}{\omega^{2n+2}}$	$\mathbb{R}$
Sinc	$\frac{\sin(\sigma x)}{x}$	$\sqrt{\frac{\pi}{2}}\chi_{[-\sigma,\sigma]}(\omega)$	$[-\sigma,\sigma]$
Poisson	$\frac{1-\sigma^2}{\sigma^2-2\sigma\cos(x)+1}$	$\sqrt{2\pi}\sum_{j=-\infty}^{\infty}\sigma^{\|j\|}\delta(\omega-j)$	$\mathbb{Z}$
Dirichlet	$\frac{\sin\left(\frac{(2n+1)x}{2}\right)}{\sin\left(\frac{x}{2}\right)}$	$\sqrt{2\pi}\sum_{j=-\infty}^{\infty}\delta(\omega-j)$	$\{0,\pm 1,\pm 2,\ldots,\pm n\}$
Fejér	$\frac{1}{n+1}\frac{\sin^2\frac{(n+1)x}{2}}{\sin^2\left(\frac{x}{2}\right)}$	$\sqrt{2\pi}\sum_{j=-n}^{n}\left(1-\frac{\|j\|}{n+1}\right)\delta(\omega-j)$	$\{0,\pm 1,\pm 2,\ldots,\pm n\}$
Cosine	$\cos(\sigma x)$	$\sqrt{\frac{\pi}{2}}\left[\delta(\omega-\sigma)+\delta(\omega+\sigma)\right]$	$\{-\sigma,\sigma\}$

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For $x \in \mathbb{R}^d$: $k_0(x) = \prod_{j=1}^{d} k_0(x_j)$, $\widehat{k_0}(\omega) = \prod_{j=1}^{d} \widehat{k_0}(\omega_j)$.

B-spline kernel type kernels

- Still k: continuous, bounded, shift-invariant.
- B-spline kernel: $supp(k_0)$ is compact $\leftarrow$ practically relevant.
- Note: $supp(f) := \overline{\{x \in \mathbb{R}^d : f(x) \neq 0\}}$.

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- More generally

Theorem ([Sriperumbudur et al., 2010b])

$supp(k_0)$: compact $\Rightarrow$ k is characteristic.

Construction of new characteristic kernels: $+$, $\times$

Theorem ([Sriperumbudur et al., 2010b])

If k, k_1, k_2: continuous, bounded, shift-invariant; k: characteristic, $k_2 \neq 0$. Then $k + k_1$, kk_2 is also characteristic.

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Proof.

We focus on $k + k_1$ (product: similarly):

$$(k + k_1)(x, y) := k(x, y) + k_1(x, y) = k_0(x - y) + (k_1)_0(x - y)$$
$$= \int_{\mathbb{R}^d} e^{-i\langle x-y,\omega\rangle} \mathrm{d}(\Lambda + \Lambda_1)(\omega).$$

□

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- k: characteristic $\Rightarrow$ $supp(\Lambda) = \mathbb{R}^d$.

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- k: characteristic $\Rightarrow supp(\Lambda) = \mathbb{R}^d$.
- Since $supp(\Lambda) \subseteq supp(\Lambda + \Lambda_1)$, we get $supp(\Lambda + \Lambda_1) = \mathbb{R}^d$; hence $k + k_1$ is characteristic.

□

Radial, bounded, continuous kernels on $\mathbb{R}^d$

Recall (radial kernel):

$$k(x,y) = k_0(\|x-y\|_2), \qquad k_0(z) = \int_{[0,\infty)} e^{-tz^2} \mathrm{d}\nu(t).$$

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Theorem ([Sriperumbudur et al., 2010b])

k is characteristic iff. $\mathrm{supp}(\nu) \neq \{0\}$.

More general spaces

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Definition

A $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ bounded, measurable kernel is called *integrally strictly positive definite (ispd)* if

$$\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) \mathrm{d}\mathbb{F}(x)\mathbb{F}(y) > 0 \quad \forall 0 \neq \mathbb{F} \in \mathcal{M}_b(\mathcal{X}).$$

Sufficient condition: ispd

Theorem ([Sriperumbudur et al., 2010b])

Ispd kernels are characteristic on an $\mathcal{X}$ topological space.

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- Dirichlet kernel: characteristic, though not ispd.
- ispd property: checking might not be easy.

Ispd: constructions

Shift-variant ispd from shift-invariant ispd kernel:

$$k_0(x, y) = f(x)k(x, y)f(y), \quad f \in C_b(\mathcal{X}).$$

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Example (exponential ← Gaussian): $k_0(x, y) = e^{\sigma\langle x,y\rangle}$, $\mathcal{X} \subset \mathbb{R}^d$ compact

$$k(x, y) = e^{-\sigma\frac{\|x-y\|^2}{2}}, \qquad f(x) = e^{\sigma\frac{\|x\|^2}{2}}.$$

Denseness in L^r

Theorem ([Fukumizu et al., 2008, Fukumizu et al., 2009a])

Let $r \geqslant 1$.

- *Sufficient condition: A $k : (\mathcal{X}, \mathcal{A}) \times (\mathcal{X}, \mathcal{A}) \to \mathbb{R}$ bounded measurable kernel is characteristic if $\mathcal{H}_k + \mathbb{R}$ is dense in $L^r(\mathcal{X}, \mathcal{A}, \mathbb{P})$ for all $\mathbb{P} \in \mathcal{M}_1^+(\mathcal{X})$.*

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Let us prove this theorem. . .

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  1. using the max. difference of $\mathbb{P}$ and $\mathbb{Q}$ $\Rightarrow$ TV of $\mathbb{P} - \mathbb{Q}$,

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  2. exploit denseness for $\chi_A \in \underbrace{L^r(\mathcal{X}, \mathcal{A}, |\mathbb{P} - \mathbb{Q}|)}_{=:L^r(|\mathbb{P}-\mathbb{Q}|)}$.

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$$\overset{(*)}{=} |\mathbb{P}\chi_A - \mathbb{Q}\chi_A|.$$

(*): $\mathbb{P}f = \mathbb{Q}f$ for any $f \in \mathcal{H}_k$ since $\mu_{\mathbb{P}} = \mu_{\mathbb{Q}}$.

Denseness in L^2 is necessary: proof

If $\mathcal{H}_k + \mathbb{R}$ is *not dense* in $L^2(\mathbb{P}) := L^2(\mathcal{X}, \mathcal{A}, \mathbb{P})$, then

- goal: $\underbrace{\exists \mathbb{Q}_1 \neq \mathbb{Q}_2 \in \mathcal{M}_1^+(\mathcal{X}) \text{ s.t. } \mu_{\mathbb{Q}_1} = \mu_{\mathbb{Q}_2}}_{\mu \text{ is not injective}}$.

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- Hahn-Banach: $0 \neq f \in L^2(\mathbb{P})$ s.t. $f \perp 1, \mathcal{H}_k$, thus

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- We define $\mathbb{Q}_1$, $\mathbb{Q}_2 \in \mathcal{M}_1^+(\mathcal{X})$ from f ($f \neq 0 \Rightarrow \mathbb{Q}_1 \neq \mathbb{Q}_2$):

$$\mathbb{Q}_1(A) = c \int_A |f| \mathrm{d}\mathbb{P}, \quad \mathbb{Q}_2(A) = c \int_A (\underbrace{|f| - f}_{\geqslant 0}) \mathrm{d}\mathbb{P}, \quad c = \frac{1}{\int_{\mathcal{X}} |f| \mathrm{d}\mathbb{P}}.$$

Denseness in L^2 is necessary: proof continued

We arrive at

$$\mu_{\mathbb{Q}_1} - \mu_{\mathbb{Q}_2} = \int_{\mathcal{X}} k(\cdot, x)\mathrm{d}\mathbb{Q}_1(x) - \int_{\mathcal{X}} k(\cdot, x)\mathrm{d}\mathbb{Q}_2(x)$$

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(\mu_{\mathbb{Q}_1} - \mu_{\mathbb{Q}_2})(y) &= c \int_{\mathcal{X}} f(x) k(y, x) \mathrm{d}\mathbb{P}(x) \\
&= c \Big\langle f, \underbrace{k(y, \cdot)}_{\in \mathcal{H}_k} \Big\rangle_{L^2(\mathbb{P})} = 0 \quad (\forall y \in \mathcal{X}).
\end{aligned}$$

We arrive at

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Thus $\mu_{\mathbb{Q}_1} - \mu_{\mathbb{Q}_2} = 0$ despite $\mathbb{Q}_1 \neq \mathbb{Q}_2$.

Infinitely divisible distributions: quick summary

U: random variable.

Question

Can it be decomposed to the sum of 2 i.i.d. random variables?

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Question

Can it be decomposed to the sum of n i.i.d. random variables for any $n \in \mathbb{Z}^+$?

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- Poisson, negative binomial, Gamma distribution, student t.

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Counterexamples:

- uniform, binomial distribution $\xleftarrow{\text{spec.}}$ $\forall$ any distribution with bounded (finite) support.

Symmetric infinitely divisible on $\mathbb{R}^d \Rightarrow$ characteristic

Theorem ([Nishiyama and Fukumizu, 2016])

Assume

- $k(x, y) = k_0(x - y)$, $k_0 \in C_b(\mathbb{R}^d)$, k_0 *is the pdf of*
- *an infinitely divisible, symmetric distribution.*

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Then k is characteristic.

Examples: Gaussian, Matérn kernel, α-stable kernels, student t-kernels, ...

Characteristic kernels: finished.

Local summary

- Dependency measure applications.
- KCCA. Mean embedding: $\mu_{\mathbb{P}} = \int_X k(\cdot, x) \mathrm{d}\mathbb{P}(x) \in \mathcal{H}_k$.
- Injectivity of μ on
  - probability distributions: characteristic property.
  - finite signed measures: universality ($\mathcal{X}$: compact metric).
- By definition: injectivity of μ $\Leftrightarrow$

$$d_k(\mathbb{P}, \mathbb{Q}) := \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}$$

is a metric.

Maximum mean discrepancy (MMD)

MMD is a specific integral probability metric (IPM)

- $\mathcal{F} = \left\{ f \in \mathcal{H}_k : \|f\|_{\mathcal{H}_k} = 1 \right\}$: unit ball in $\mathcal{H}_k$.

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- IPMs [Zolotarev, 1983, Müller, 1997].

- $\mathcal{F} = C_b(\mathcal{X})$ with $\mathcal{X}$ metric space.

IPM: other $\mathcal{F}$ examples giving metric

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- $\mathcal{F} = \left\{f : \|f\|_L := \sup_{x\neq y} \frac{|f(x)-f(y)|}{\rho(x,y)} \leqslant 1\right\}$:
  - Kantorovich metric $\xrightarrow{\mathcal{X}\text{: separable metric}}$ Wasserstein distance.

IPM: other $\mathcal{F}$ examples giving metric

- $\mathcal{F} = \{f : \|f\|_\infty := \sup_{x\in\mathcal{X}} |f(x)| \leqslant 1\}$:
  - bounded functions.
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TV upper bounds MMD [Sriperumbudur et al., 2010b]:

$$d_k(\mathbb{P},\mathbb{Q}) \leqslant \sup_{x\in\mathcal{X}} \sqrt{k(x,x)}\, TV(\mathbb{P},\mathbb{Q}).$$

IPM: other $\mathcal{F}$ examples giving metric – continued

- $\mathcal{F} = \{f : \|f\|_{BL} := \|f\|_\infty + \|f\|_L \leqslant 1\}$
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- $\mathcal{F} = \left\{\chi_{(-\infty,t]} : t \in \mathbb{R}^d\right\}$:
  - indicator functions of half-intervals.
  - Kolmogorov distance.

Empirical estimation of IPMs

[Sriperumbudur et al., 2012]:

- Kantorovich, Dudley metric: linear programming task.
- MMD (d_k): easier.

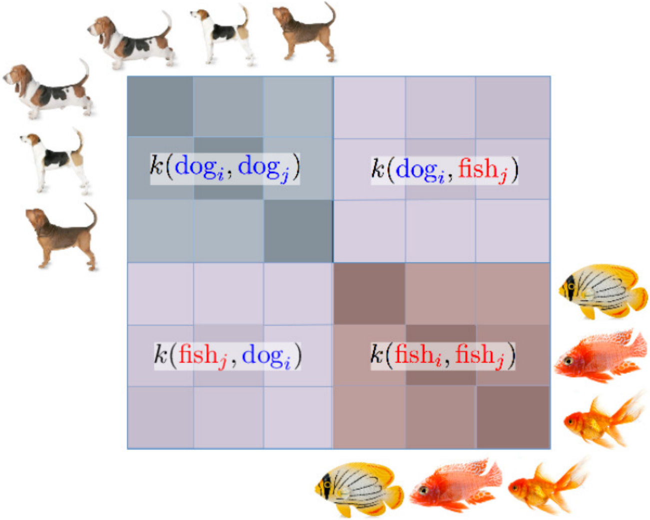
MMD estimators

MMD estimator: intuition

 $\sim P$

 $\sim Q$

MMD estimator: intuition



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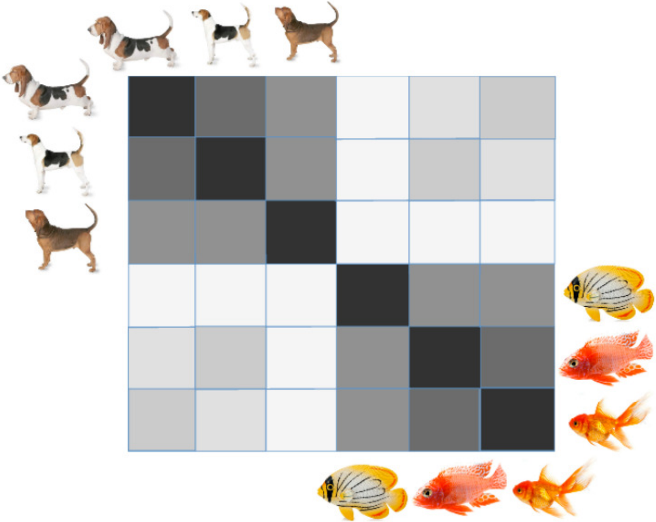

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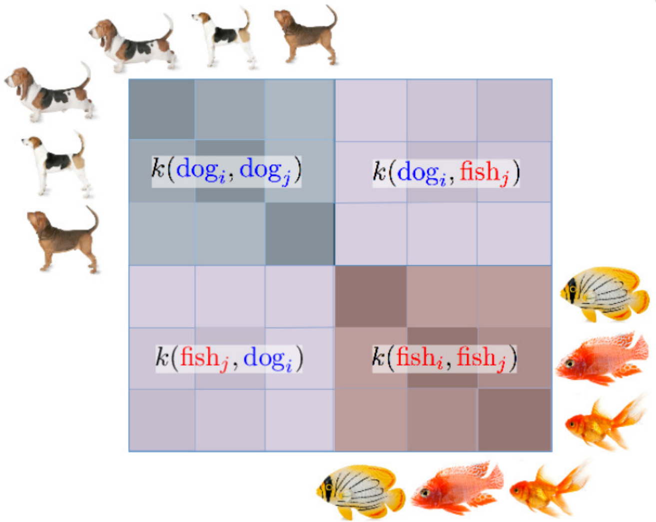

$$\widehat{\text{MMD}}^2(\mathbb{P}, \mathbb{Q}) = \overline{G_{\mathbb{P},\mathbb{P}}} + \overline{G_{\mathbb{Q},\mathbb{Q}}} - 2\overline{G_{\mathbb{P},\mathbb{Q}}}$$ (without diagonals in $\overline{G_{\mathbb{P},\mathbb{P}}}$, $\overline{G_{\mathbb{Q},\mathbb{Q}}}$)

† $\widehat{\text{MMD}}$ & $\widehat{\text{HSIC}}$ illustration credit: Arthur Gretton

MMD estimator-1

Recall: MMD = squared difference between feature means:

$$\mathrm{MMD}^2(\mathbb{P},\mathbb{Q}) := d_k^2(\mathbb{P},\mathbb{Q}) = \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}^2 = \\ = \mathbb{E}_{x\sim\mathbb{P},x'\sim\mathbb{P}} k(x,x') + \mathbb{E}_{y\sim\mathbb{Q},y'\sim\mathbb{Q}} k(y,y') \\ - 2\mathbb{E}_{x\sim\mathbb{P},y\sim\mathbb{Q}} k(x,y).$$

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Unbiased empirical estimator using $\{x_i\}_{i=1}^m \sim \mathbb{P}$, $\{y_j\}_{j=1}^n \sim \mathbb{Q}$:

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We plug in the empirical measures ($\mathbb{P}_m$, $\mathbb{Q}_n$):

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$$\langle \mu_{\mathbb{P}_m}, \mu_{\mathbb{Q}_n}\rangle_{\mathcal{H}_k} = \left\langle \frac{1}{m}\sum_{i=1}^m k(\cdot, x_i), \frac{1}{n}\sum_{j=1}^n k(\cdot, y_j)\right\rangle_{\mathcal{H}_k}$$

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$$\widehat{\mathrm{MMD}}_b^2(\mathbb{P},\mathbb{Q}) = \underbrace{\frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m}k(x_i,x_j)}_{\text{V-statistic-1}} + \underbrace{\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}k(y_i,y_j)}_{\text{V-statistic-2}} - \underbrace{\frac{2}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}k(x_i,y_j)}_{\text{sample average}}.$$

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- Computational complexity: $\mathcal{O}\left((m+n)^2\right)$, quadratic.

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- Other valid $K(\mu_{\mathbb{P}}, \mu_{\mathbb{Q}})$ examples $\rightarrow$ distribution classification [Póczos et al., 2012, Muandet et al., 2011] / distribution regression [Szabó et al., 2016].

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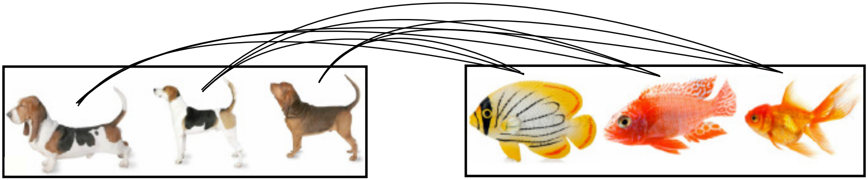
Let us see the details.

Set kernel

Convolution kernels [Haussler, 1999] ∋ set kernel [Gärtner et al., 2002]:

$$K(\mathbb{P}_m, \mathbb{Q}_n) := \langle \mu_{\mathbb{P}_m}, \mu_{\mathbb{Q}_n} \rangle_{\mathcal{H}_k} = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k(x_i, y_j).$$



Other valid K examples [Christmann and Steinwart, 2010], [Szabó et al., 2015] → distribution regression

Recall: $K(\mathbb{P},\mathbb{Q}) = \langle \mu_{\mathbb{P}}, \mu_{\mathbb{Q}} \rangle_{\mathcal{H}_k}$, linear kernel.

K_G	K_e	K_C
$e^{-\frac{\left\|\mu_{\mathbb{P}}-\mu_{\mathbb{Q}}\right\|^2_{\mathcal{H}_k}}{2\theta^2}}$	$e^{-\frac{\left\|\mu_{\mathbb{P}}-\mu_{\mathbb{Q}}\right\|_{\mathcal{H}_k}}{2\theta^2}}$	$\left(1+\left\|\mu_{\mathbb{P}}-\mu_{\mathbb{Q}}\right\|^2_{\mathcal{H}_k}/\theta^2\right)^{-1}$

K_t	K_i
$\left(1+\left\|\mu_{\mathbb{P}}-\mu_{\mathbb{Q}}\right\|^{\theta}_{\mathcal{H}_k}\right)^{-1}$	$\left(\left\|\mu_{\mathbb{P}}-\mu_{\mathbb{Q}}\right\|^2_{\mathcal{H}_k}+\theta^2\right)^{-\frac{1}{2}}$

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Functions of $\left\Vert \mu_{\mathbb{P}}-\mu_{\mathbb{Q}} \right\Vert_{\mathcal{H}_k}$ ⇒ computation: similar to set kernel.

Few analytic expressions exist: examples [Gretton et al., 2007, Muandet et al., 2011]

Assume: $\mathbb{P} = N(m_1, \Sigma_1)$, $\mathbb{Q} = N(m_2, \Sigma_2)$.

$k(x,y)$	$K(\mu_{\mathbb{P}}, \mu_{\mathbb{Q}}) = \langle \mu_{\mathbb{P}}, \mu_{\mathbb{Q}} \rangle_{\mathcal{H}_k}$
$e^{-\frac{\gamma}{2}\|x-y\|_2^2}$	$\frac{e^{-\frac{1}{2}(m_1-m_2)^T(\Sigma_1+\Sigma_2+\gamma I)^{-1}(m_1-m_2)}}{\|\gamma\Sigma_1+\gamma\Sigma_2+I\|^{\frac{1}{2}}}$

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$(1+\langle x,y\rangle)^3$	$(1+\langle m_1,m_2\rangle)^3 + 6m_1^T\Sigma_1\Sigma_2 m_2 + 3(1+\langle m_1,m_2\rangle) \times [\mathrm{tr}(\Sigma_1\Sigma_2) + m_1\Sigma_2 m_1 + m_2\Sigma_1 m_2]$

RKBS definition

Definition ([Zhang et al., 2009])

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Notes:

- Generally, $\mathcal{B} \subseteq \mathcal{B}''$.
- For $\mathcal{B} = \mathcal{H}$ Hilbert: $(\mathcal{H}')' = \mathcal{H}$ (Riesz representation theorem).

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  - $\mu_{\mathbb{P}} = \int_{\mathcal{X}} \underbrace{k(\cdot, x)}_{\in \mathcal{B}', \text{ see Bochner integral}} \mathrm{d}\mathbb{P}(x) \in \mathcal{B}'$ [Sriperumbudur et al., 2011].

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RKBS: computational intractability

Key for RKHS $\mathcal{H}_k$:

$$d_k{}^2(\mathbb{P},\mathbb{Q}) = \int_{\mathcal{X}}\int_{\mathcal{X}} k(x,y)\mathrm{d}(\mathbb{P}-\mathbb{Q})(x)\mathrm{d}(\mathbb{P}-\mathbb{Q})(y).$$

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For RKBS $\mathcal{B}$:

- d_k: not expressible in terms of $k(x,y)$,
- associated distances and estimators: no closed form expressions.

MMD: finished

Covariance operator

Idea: (un)centered cross-covariance

$$C_{xy}^{u} = \mathbb{E}_{xy}\left[xy^T\right],$$

u: uncentered, c: centered.

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u: uncentered, c: centered. In short, $xy^{T} \to \varphi(x) \otimes \psi(y)$.

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Question

What is $\varphi(x) \otimes \psi(y)$ and $\|\cdot\|_{HS}$?

Intuition of $a \otimes b$, goal: $a := \varphi(x) \in \mathcal{H}_k$, $b := \psi(y) \in \mathcal{H}_\ell$

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- $\mathcal{H}_1 \otimes \mathcal{H}_2$: completion of $\mathcal{L}$.

$a_1 \otimes \ldots \otimes a_M$, $\mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_M$ would work similarly

Tensor product of M Hilbert spaces:

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$\Rightarrow$ HSIC for M-variables: ✓

$\langle \cdot, \cdot \rangle$: well-defined & pos. definite [Reed and Simon, 1980]

Well-definedness: $\langle \lambda, \lambda' \rangle$ is expansion-independent, i.e.

$$\lambda_1 = \sum_{i=1}^{n_1} c_i a_i \otimes b_i = \lambda_2 = \sum_{j=1}^{n_2} c'_j a'_j \otimes b'_j,$$

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- In short, $\langle \lambda, \lambda \rangle = 0 \Rightarrow c_{ij} = 0$ $(\forall i, j)$, i.e. $\lambda = 0$.

Tensor product of RKHSs

Theorem ([Berlinet and Thomas-Agnan, 2004])

- *Given:* $\mathcal{H}_1 = \mathcal{H}_k$, $\mathcal{H}_2 = \mathcal{H}_\ell$ *RKHSs with kernel* k *and* ℓ.
- *Then* $\mathcal{H}_1 \otimes \mathcal{H}_2$ *is RKHS with kernel*

$$k \otimes \ell : (\mathcal{X} \times \mathcal{Y}) \times (\mathcal{X} \times \mathcal{Y}) \to \mathbb{R},$$
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Intuition:

- inner product on $\mathcal{X}$ and $\mathcal{Y}$ $\to$ inner product on $\mathcal{X} \times \mathcal{Y}$.
- $\mathcal{X}$ = animal images, $\mathcal{Y}$ = descriptions of animals.

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Hilbert-Schmidt operators: quick summary

- An $L: \mathcal{H}_1 \to \mathcal{H}_2$ bounded linear operator is called Hilbert-Schmidt if

$$\|L\|_{HS}^2 := \sum_i \underbrace{\|Le_i\|_{\mathcal{H}_2}^2}_{=\sum_j \left\langle Le_i, f_j \right\rangle_{\mathcal{H}_2}^2} < \infty.$$

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- $\mathcal{H}_1, \mathcal{H}_2$: separable $\Rightarrow I, J$: countable, i.e. 'sums'.
- $\langle L_1, L_2 \rangle_{HS}$: well-defined (independent of the chosen basis).
- For RKHSs ($\mathcal{H}_i$): $\mathcal{X}$: separable, k: continuous $\Rightarrow \mathcal{H}_k$: separable [Steinwart and Christmann, 2008].

$a \otimes b$ is Hilbert-Schmidt: linear & bounded

For $a \otimes b$ with $a \in \mathcal{H}_1$, $b \in \mathcal{H}_2$:

- linearity: ✓
- boundedness ($c \in \mathcal{H}_2$):

$$\left\|(a \otimes b)c\right\|_{\mathcal{H}_1} = \left\|a \left\langle b, c\right\rangle_{\mathcal{H}_2}\right\|_{\mathcal{H}_1}$$

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- linearity: ✓
- boundedness ($c \in \mathcal{H}_2$):

$$\|(a \otimes b)c\|_{\mathcal{H}_1} = \left\| a \langle b, c \rangle_{\mathcal{H}_2} \right\|_{\mathcal{H}_1} = \left| \langle b, c \rangle_{\mathcal{H}_2} \right| \|a\|_{\mathcal{H}_1}$$

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Thus $\|a \otimes b\| \leqslant \|a\|_{\mathcal{H}_1} \|b\|_{\mathcal{H}_2} < \infty$.

$a \otimes b$ is a Hilbert-Schmidt operator

Let $(e_i)_{i \in I} \subset \mathcal{H}_2$ ONB,

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In short

$$\|a \otimes b\|_{HS}^2 = \|a\|_{\mathcal{H}_1}^2 \|b\|_{\mathcal{H}_2}^2.$$

Uncentered cross-covariance operator

$$C_{xy}^{u} := \mathbb{E}_{xy}\Big[\underbrace{\varphi(x)\otimes\psi(y)}_{\in HS(\mathcal{H}_\ell,\mathcal{H}_k)}\Big] \in HS\left(\mathcal{H}_\ell, \mathcal{H}_k\right).$$

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- $\|\varphi(x) \otimes \psi(y)\|_{HS} = \|\varphi(x)\|_{\mathcal{H}_k} \|\psi(y)\|_{\mathcal{H}_\ell} = \sqrt{k(x,x)}\sqrt{\ell(y,y)}$.
- Sufficient condition: k and ℓ are bounded.

Centered covariance operator [Baker, 1973]

Let $\mu_x := \mu_{\mathbb{P}_x}$, $\mu_y := \mu_{\mathbb{P}_y}$. $\mathbb{P}_x, \mathbb{P}_y$: marginals of $\mathbb{P}_{xy}$.

$$C_{xy}^c = \mathbb{E}_{xy}\left[\left(\varphi(x) - \underbrace{\mathbb{E}_x\varphi(x)}_{\mu_x}\right) \otimes \left(\psi(y) - \underbrace{\mathbb{E}_y\psi(y)}_{\mu_y}\right)\right]$$

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Hilbert-Schmidt independence criterion (HSIC)

HSIC [Fukumizu et al., 2004, Gretton et al., 2005a]:

$$\mathrm{HSIC}(x, y; \mathcal{H}_k, \mathcal{H}_\ell) := \left\| C_{xy}^c \right\|_{HS}.$$

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Question

When does HSIC characterize independence?

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Question

When does HSIC characterize independence?
We will discuss it later (after HSIC ⇔ distance covariance).

How do covariance operators encode covariance?

Let $g \in \mathcal{H}_\ell$, $f \in \mathcal{H}_k$, $HS := HS(\mathcal{H}_\ell, \mathcal{H}_k)$.

$$\left\langle f, C^u_{xy} g \right\rangle_{\mathcal{H}_k} = \left\langle C^u_{xy}, f \otimes g \right\rangle_{HS}$$

Cheating:

- next slide.
- Enough $f \in \mathcal{H}_1$, $g \in \mathcal{H}_2$, $L \in HS\left(\mathcal{H}_2, \mathcal{H}_1\right)$

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$$= \mathbb{E}_{xy} \underbrace{\langle \varphi(x) \otimes \psi(y), f \otimes g \rangle_{HS}}_{= f(x) g(y)}$$

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Proof: $(b_i)_{i \in I}$ ONB in $\mathcal{H}_2$,

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With $L := a \otimes b$

$$\langle a \otimes b, f \otimes g\rangle_{HS(\mathcal{H}_2,\mathcal{H}_1)} = \langle f, (a \otimes b)g\rangle_{\mathcal{H}_1}$$

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Remember: we have seen this for $a = f$, $b = g$ (when proving $a \otimes b$ is HS).

Effect of the centered cross-covariance operator

Using that $C_{xy}^c = C_{xy}^u - \mu_x \otimes \mu_y$

$$\left\langle f, C_{xy}^c g \right\rangle_{\mathcal{H}_k} = \left\langle f, C_{xy}^u g \right\rangle_{\mathcal{H}_k} - \langle f, (\mu_x \otimes \mu_y) g \rangle_{\mathcal{H}_k}$$

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$$\stackrel{\otimes}{=} \mathbb{E}_{xy}[f(x)g(y)] - \underbrace{\langle f, \mu_x \rangle_{\mathcal{H}_k}}_{\mathbb{E}_x f(x)} \underbrace{\langle g, \mu_y \rangle_{\mathcal{H}_\ell}}_{\mathbb{E}_y g(y)}$$

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$$
\begin{aligned}
\left\langle f, C^c_{xy} g \right\rangle_{\mathcal{H}_k} &= \left\langle f, C^u_{xy} g \right\rangle_{\mathcal{H}_k} - \left\langle f, (\mu_x \otimes \mu_y) g \right\rangle_{\mathcal{H}_k} \\
&\overset{\otimes}{=} \mathbb{E}_{xy}[f(x)g(y)] - \underbrace{\langle f, \mu_x \rangle_{\mathcal{H}_k}}_{\mathbb{E}_x f(x)} \underbrace{\langle g, \mu_y \rangle_{\mathcal{H}_\ell}}_{\mathbb{E}_y g(y)} \\
&= cov(f(x), g(y)).
\end{aligned}
$$

Three notes

- KCCA formulation: using C^c_{xy}, C^c_{xx}, C^c_{yy}.

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Three notes

- KCCA formulation: using C^c_{xy}, C^c_{xx}, C^c_{yy}.
- HSIC: captures $\mathbb{P}_{xy} \stackrel{?}{=} \mathbb{P}_x \otimes \mathbb{P}_y$ in $\mathcal{H}_k \otimes \mathcal{H}_\ell$.
- Link to distance covariance, energy distance.

In other words, ...

KCCA formulation with cross-covariance operators

$$\rho_{\mathrm{KCCA}}(x,y) = \sup_{f\in\mathcal{H}_k, g\in\mathcal{H}_\ell} \operatorname{corr}(f(x), g(y)) \Leftrightarrow$$

$$\sup_{f\in\mathcal{H}_k, g\in\mathcal{H}_\ell} \left\langle f, C^c_{xy} g\right\rangle_{\mathcal{H}_k} \text{ s.t. } \begin{cases} \left\langle f, C^c_{xx} f\right\rangle_{\mathcal{H}_k} & = 1, \\ \left\langle g, C^c_{yy} g\right\rangle_{\mathcal{H}_\ell} & = 1. \end{cases}$$

KCCA: with κ-regularization

$$\rho_{\text{KCCA}}(x, y, \kappa) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \operatorname{corr}(f(x), g(y); \kappa),$$

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Empirically,

$$\sup_{f\in\mathcal{H}_k, g\in\mathcal{H}_\ell} \left\langle f, \widehat{C^c_{xy}} g \right\rangle_{\mathcal{H}_k} \text{ s.t. } \begin{cases} \left\langle f, \left(\widehat{C^c_{xx}} + \kappa I\right) f \right\rangle_{\mathcal{H}_k} & = 1, \\ \left\langle g, \left(\widehat{C^c_{yy}} + \kappa I\right) g \right\rangle_{\mathcal{H}_\ell} & = 1. \end{cases}$$

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KCCA consistency analysis [Fukumizu et al., 2007]

using this formulation & the convergence of $\widehat{C^c_{xy}}$, $\widehat{C^c_{xx}}$, $\widehat{C^c_{yy}}$.

HSIC: $\mathbb{P}_{xy} \stackrel{?}{=} \mathbb{P}_x \otimes \mathbb{P}_y$ in $\mathcal{H}_k \otimes \mathcal{H}_\ell$

We saw $h((x,y),(x',y')) = k(x,x')\ell(y,y')$ is the kernel of $\mathcal{H}_k \otimes \mathcal{H}_\ell$. Let

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$$= \left\| \mathbb{E}_{xy}\left[\varphi(x) \otimes \psi(y)\right] - \mu_x \otimes \mu_y \right\|_{\mathcal{H}_h} = \mathrm{HSIC}(x,y)$$

using $\mathcal{H}_1 \otimes \mathcal{H}_2 \simeq HS(\mathcal{H}_2, \mathcal{H}_1)$.

Distance covariance

- Characteristic functions: ϕ_{xy}, ϕ_x, ϕ_y.

Distance covariance

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- $x \perp y$ iff. $dCov(x,y) = 0$.

Distance covariance: $\alpha = 1$

Alternative form in terms of pairwise distances:

$$dCov^2(x, y) = \mathbb{E}_{xy}\mathbb{E}_{x'y'}\left\|x - x'\right\|_2\left\|y - y'\right\|_2 + \mathbb{E}_{xx'}\left\|x - x'\right\|_2 \mathbb{E}_{yy'}\left\|y - y'\right\|_2 - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}\left\|x - x'\right\|_2 \mathbb{E}_{y'}\left\|y - y'\right\|_2\right].$$

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Extension [Lyons, 2013]:

$$dCov^2(x,y) = \mathbb{E}_{xy}\mathbb{E}_{x'y'}\rho_1(x,x')\rho_2(y,y') + \mathbb{E}_{xx'}(x,x')\,\mathbb{E}_{yy'}(y,y') - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}\rho_1(x,x')\,\mathbb{E}_{y'}\rho_2(y,y')\right],$$

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$(\mathcal{X},\rho_1)$, $(\mathcal{Y},\rho_2)$: metric spaces of negative type (def & examples: in a moment).

Distance covariance vs. HSIC

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Similarly to MMD (see later at $\widehat{\mathrm{HSIC}}$):

$$\mathrm{HSIC}^2(x,y) = \mathbb{E}_{xy}\mathbb{E}_{x'y'}k(x,x')\ell(y,y') + \mathbb{E}_{xx'}k(x,x')\mathbb{E}_{yy'}\ell(y,y') - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}k(x,x')\mathbb{E}_{y'}\ell(y,y')\right].$$

+extension to semi-metric spaces of negative type:

Theorem ([Sejdinovic et al., 2013b])

$dCov^2(x,y;\rho_1,\rho_2) = 4\mathrm{HSIC}^2(x,y;\mathcal{H}_k,\mathcal{H}_\ell)$, *where*

$$\rho_1(x,x') = k(x,x) + k(x',x') - 2k(x,x'),$$
$$\rho_2(y,y') = \ell(y,y) + \ell(y',y') - 2\ell(y,y').$$

Metric space

Definition

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- $\mathcal{X} = \mathbb{R}^d$, $\rho(x, y) = \|x - y\|_p = \left(\sum_{i=1}^d |x_i - y_i|^p\right)^{\frac{1}{p}}$, $p \geqslant 1$.

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- $\mathcal{X} = C[a, b]$, $\rho(x, y) = \max_{z \in [a,b]} |x(z) - y(z)|$.
- $\mathcal{X}$ any set. $\rho(x, y) = \delta_{x=y}$.

Semi-metric space: no triangle inequality

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It is called negative type if in addition

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \rho(x_i, x_j) \leqslant 0$$

for $\forall n \geqslant 2$, $\forall x_1, \ldots, x_n \in \mathcal{X}$ and $\forall a_1, \ldots, a_n \in \mathbb{R}$ with $\sum_{i=1}^{n} a_i = 0$.

Semi-metric space of negative type

[Berg et al., 1984]:

- $\rho : \checkmark \Rightarrow \rho^a : \checkmark$ for $\forall a \in (0, 1)$.

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- $+$1st part $\Rightarrow \rho(x,y) = \|x-y\|_2^q \checkmark$ with $q \in (0,2)$.
- Specifically: $\rho(x,y) = \|x-y\|_2$ is OK.

Energy distance [Székely and Rizzo, 2004, Baringhaus and Franz, 2004, Székely and Rizzo, 2005]

$x, x' \sim \mathbb{P}$, $y, y' \sim \mathbb{Q}$:

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- $EnDist(\mathbb{P}, \mathbb{Q}) \geqslant 0$ with ρ metric of negative-type.
- $EnDist(\mathbb{P}, \mathbb{Q}) = 0 \Leftrightarrow \mathbb{P} = \mathbb{Q}$ for $(\mathcal{X}, \rho)$ strictly negative spaces; example: $(\mathbb{R}^d, \|\cdot\|_2)$.

Strict negativity

In addition:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j \rho(x_i, x_j) < 0$$

if x_i-s are distinct and $\exists a_i \neq 0$.

Energy distance vs. MMD

Energy distance: also called N-distance
[Zinger et al., 1992, Klebanov, 2005],

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MMD (recall):

$$\mathrm{MMD}^2(\mathbb{P}, \mathbb{Q}) = \mathbb{E}_{x,x'}k(x,x') + \mathbb{E}_{y,y'}k(y,y') - 2\mathbb{E}_{xy}k(x,y).$$

MMD $\Leftrightarrow$ energy distance

Theorem ([Sejdinovic et al., 2013b])

$$EnDist(\mathbb{P}, \mathbb{Q}; \rho) = 2\mathrm{MMD}^2(\mathbb{P}, \mathbb{Q}; \mathcal{H}_k),$$

where

$$\rho(x, y) = k(x, x) + k(y, y) - 2k(x, y).$$

Central in applications: characteristic property

- HSIC, $k = \otimes_{m=1}^{M} k_m$, $x = (x_m)_{m=1}^{M}$:

$$\text{HSIC}_k(\mathbb{P}) := \text{MMD}_k\left(\mathbb{P}, \otimes_{m=1}^{M}\mathbb{P}_m\right), \quad k(x, x') := \prod_{m=1}^{M} k_m(x_m, x'_m).$$

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$\otimes_{m=1}^{M} k_m$: universal $\Rightarrow$ characteristic $\Rightarrow$ $\mathcal{I}$-characteristic.
Relation? Conditions in terms of k_m-s?

$$\otimes_{m=1}^M k_m : \quad \mathcal{I}\text{-char} \Longleftarrow \text{char} \Longleftarrow \text{universal}$$

$$(k_m)_{m=1}^M : \quad \text{char} \underset{\text{[Sriperumbudur et al., 2011]}}{\overset{\text{[Sriperumbudur et al., 2011]}}{\not\Longrightarrow \atop \Longleftarrow}} \text{-universal}$$

Existing Results, $M = 2$

- [Blanchard et al., 2011, Waegeman et al., 2012, Gretton, 2015]:
  $k_1 \& k_2$: universal $\Rightarrow k_1 \otimes k_2$: universal ($\Rightarrow \mathcal{I}$-characteristic).

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Extension to $M \geqslant 2$.

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Extension to $M \geqslant 2$.

Main Challenge

'$\otimes k_m$: $\mathcal{I}$-characteristic $\Leftrightarrow k_m$: characteristic $(\forall m)$' does NOT hold.

Results [Szabó and Sriperumbudur, 2017]

Proposition (characteristic property)

- $\otimes_{m=1}^{M} k_m$: *characteristic* $\Rightarrow$ $(k_m)_{m=1}^{M}$ *are characteristic.*
- $\not\Leftarrow$ *[* $|\mathcal{X}_m| = 2,\ k_m(x, x') = 2\delta_{x,x'} - 1$ *]*

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Results: continued

Proposition ($\mathcal{X}_m = \mathbb{R}^{d_m}$, k_m: continuous, shift-invariant, bounded)

$(k_m)_{m=1}^M$-s are characteristic $\Leftrightarrow$ $\otimes_{m=1}^M k_m$: $\mathcal{I}$-characteristic $\Leftrightarrow$ $\otimes_{m=1}^M k_m$: characteristic.

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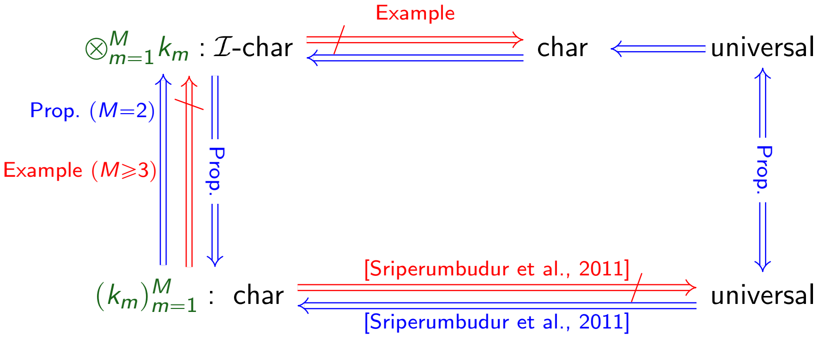
Proposition (Universality)

$\otimes_{m=1}^M k_m$: universal $\Leftrightarrow$ $(k_m)_{m=1}^M$ are universal.



Example
$\otimes_{m=1}^{M} k_m$: $\mathcal{I}$-char
char
universal
Prop. (M=2)
Example ($M \geqslant 3$)
Prop.
Prop.
$(k_m)_{m=1}^{M}$: char
[Sriperumbudur et al., 2011]
universal
[Sriperumbudur et al., 2011]

Covariance operator: finished.

Recall

- KCCA: independence measure,

$$\rho_{\mathsf{KCCA}}(x,y) = \sup_{f\in\mathcal{H}_k, g\in\mathcal{H}_\ell} \operatorname{corr}(f(x), g(y)).$$

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$$\mathrm{HSIC}(x,y) = \left\|C_{xy}^c\right\|_{HS}.$$

No density estimation

Thus,

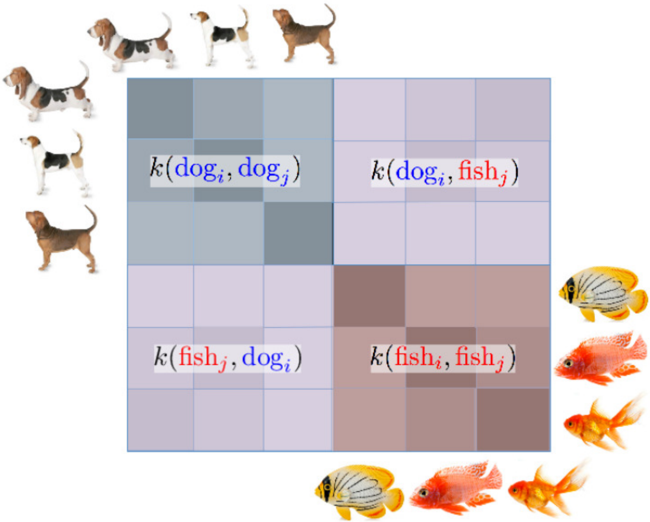
- independence measure,
- distance,
- inner product

measures/estimates on probability distributions

without density estimation!

HSIC estimators

Recall: MMD estimator



$\widehat{\text{MMD}}_u^2(\mathbb{P}, \mathbb{Q}) = \overline{G_{\mathbb{P},\mathbb{P}}} + \overline{G_{\mathbb{Q},\mathbb{Q}}} - 2\overline{G_{\mathbb{P},\mathbb{Q}}}$ (without diagonals in $\overline{G_{\mathbb{P},\mathbb{P}}}$, $\overline{G_{\mathbb{Q},\mathbb{Q}}}$)

HSIC: intuition. $\mathcal{X}$: images, $\mathcal{Y}$: descriptions.

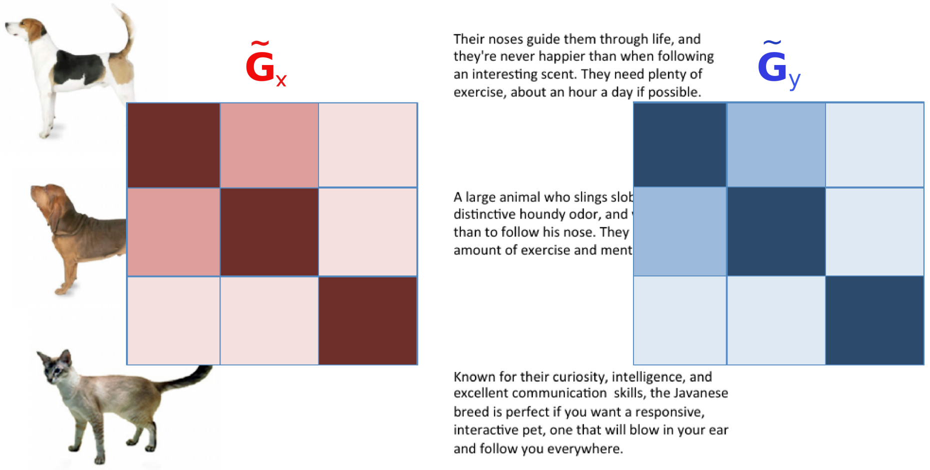
Their noses guide them through life, and they're never happier than when following an interesting scent. They need plenty of exercise, about an hour a day if possible.

A large animal who slings slobber, exudes a distinctive houndy odor, and wants nothing more than to follow his nose. They need a significant amount of exercise and mental stimulation.

Known for their curiosity, intelligence, and excellent communication skills, the Javanese breed is perfect if you want a responsive, interactive pet, one that will blow in your ear and follow you everywhere.

Text from dogtime.com and petfinder.com

HSIC intuition: Gram matrices



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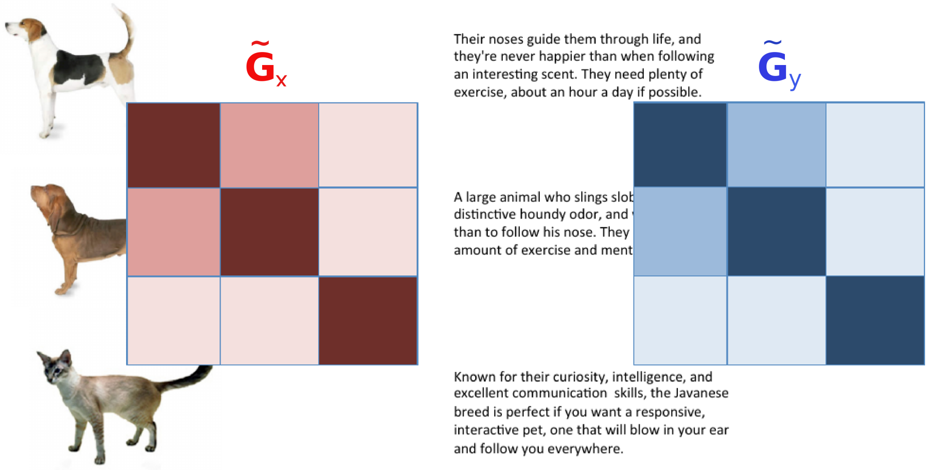
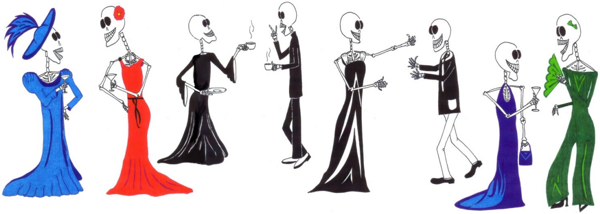


Empirical estimate:

$$\widehat{\mathrm{HSIC}^2} = \frac{1}{n^2}\left\langle \tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y \right\rangle_F.$$

Cocktail party: HSIC demo



ISA reminder

$$\mathbf{x} = \mathbf{A}\mathbf{s}, \qquad \mathbf{s} = \left[\mathbf{s}^1; \ldots; \mathbf{s}^M\right],$$

where $\mathbf{s}^m$-s are non-Gaussian & independent.

- Goal: $\{\mathbf{x}_t\}_{t=1}^T \to \mathbf{W} = \mathbf{A}^{-1}, \{\mathbf{s}_t\}_{t=1}^T,$

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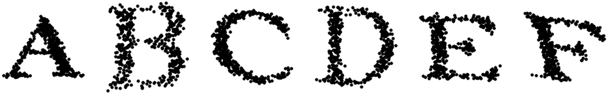
- Goal: $\{\mathbf{x}_t\}_{t=1}^T \rightarrow \mathbf{W} = \mathbf{A}^{-1}, \{\mathbf{s}_t\}_{t=1}^T$,
- Objective function:

$$\hat{\mathbf{s}} = \mathbf{W}\mathbf{x},$$
$$J(\mathbf{W}) = I\left(\hat{\mathbf{s}}^1, \ldots, \hat{\mathbf{s}}^M\right) \rightarrow \min_{\mathbf{W}}.$$

ISA: source, observation

- Hidden sources ($\mathbf{s}$):



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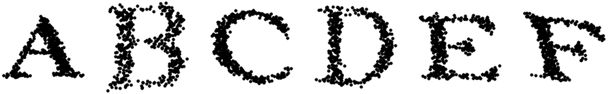
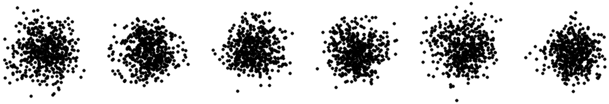


- Observation (**x**):



ISA: estimated sources using HSIC, ambiguity

- Estimated sources ($\hat{\mathbf{s}}$):

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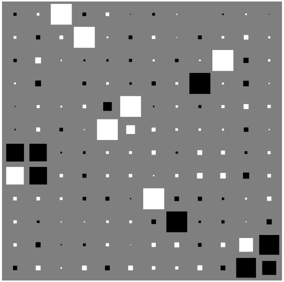
- Performance ($\hat{\mathbf{W}}\mathbf{A}$), ambiguity:



Conjecture: ISA separation theorem [Cardoso, 1998]

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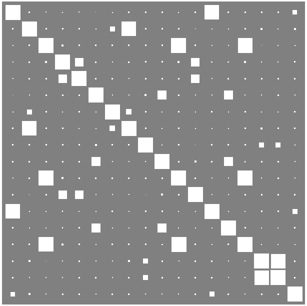

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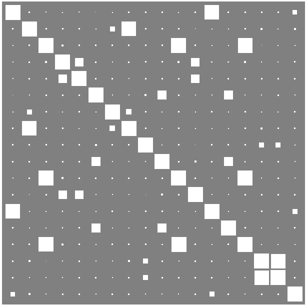

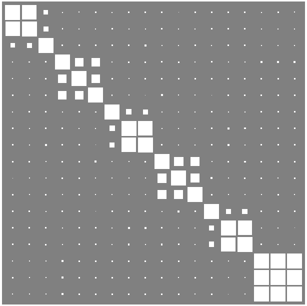

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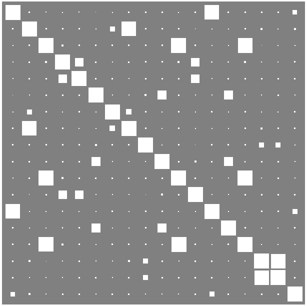

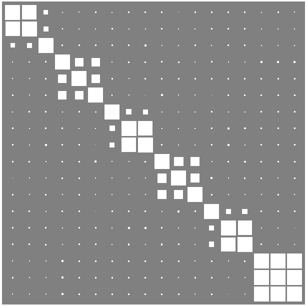

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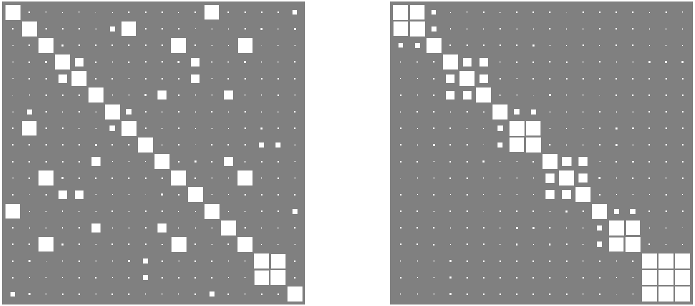
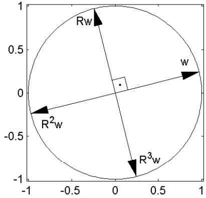
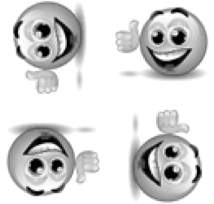


- Basis of the state-of-the-art ISA solvers.
- Sufficient conditions [Szabó et al., 2012]:
  - $\mathbf{s}^m$: spherical [Fang et al., 1990].

ISA s … $\mathbf{s}^m) = 2$ less is enough.

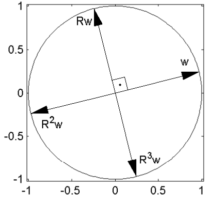


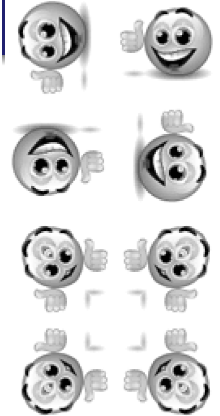


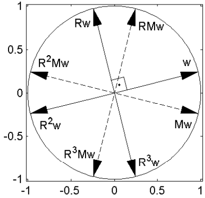
Invariance to

- 90° rotation: $f(u_1,u_2) = f(-u_2,u_1) = f(-u_1,-u_2) = f(u_2,-u_1)$.

ISA s … ough.







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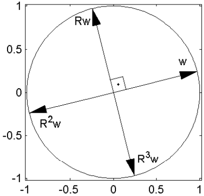

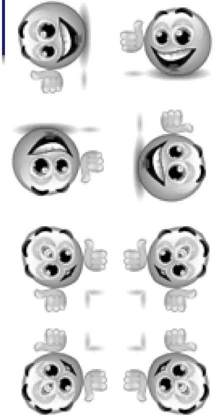

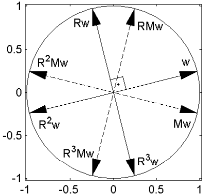

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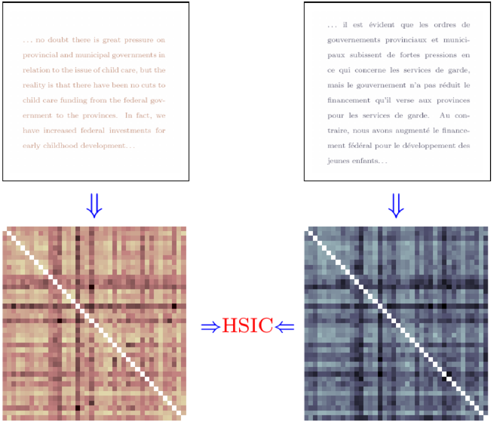
- L^p-spherical: $f(u_1, u_2) = h\left(\sum_i |u_i|^p\right) \quad (p > 0)$.

Another HSIC demo: translation

- 5-line extracts.
- representation, kernel: bag-of-words, r-spectrum ($r = 5$).
- sample size: $n = 10$. repetitions: 300.



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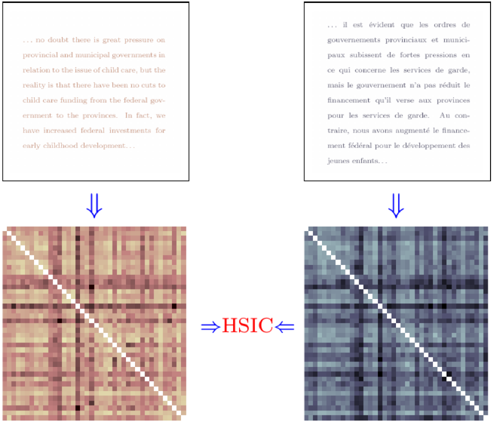
Results:

- r-spectrum: average Type-II error $= 0$ ($\alpha = 0.05$),
- bag-of-words: 0.18.



Recall: MMD in terms of kernel evaluations

$$\begin{aligned}\mathrm{MMD}^2(\mathbb{P},\mathbb{Q}) &= \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|^2_{\mathcal{H}_k} = \\ &= \mathbb{E}_{x\sim\mathbb{P},x'\sim\mathbb{P}} k(x,x') + \mathbb{E}_{y\sim\mathbb{Q},y'\sim\mathbb{Q}} k(y,y') \\ &\quad - 2\mathbb{E}_{x\sim\mathbb{P},y\sim\mathbb{Q}} k(x,y).\end{aligned}$$

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Question

Can we rewrite HSIC in terms of expected kernel values?

HSIC in terms of kernel evaluations [Gretton et al., 2005a]

$$\mathrm{HSIC}^2(x,y) = \left\| C_{xy}^c \right\|_{HS}^2 = \left\| C_{xy}^u - \mu_x \otimes \mu_y \right\|_{HS}^2$$

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First term:

$$\left\| C_{xy}^u \right\|_{HS}^2 = \left\langle \mathbb{E}_{xy}\left[\varphi(x) \otimes \psi(y)\right], \mathbb{E}_{x'y'}\left[\varphi(x') \otimes \psi(y')\right] \right\rangle_{HS}$$

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$$\langle e_1 \otimes f_1, e_2 \otimes f_2 \rangle_{HS(\mathcal{H}_2,\mathcal{H}_1)} = \langle e_1, e_2 \rangle_{\mathcal{H}_1} \langle f_1, f_2 \rangle_{\mathcal{H}_2}.$$

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HSIC: second term

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\begin{aligned}
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&= \mathbb{E}_{xx'} k(x, x') \mathbb{E}_{yy'} \ell(y, y').
\end{aligned}
$$

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HSIC: after gathering the terms

$$\begin{aligned}\mathrm{HSIC}^2(x,y) &= \mathbb{E}_{xy}\mathbb{E}_{x'y'}k(x,x')\ell(y,y') + \mathbb{E}_{xx'}k(x,x')\mathbb{E}_{yy'}\ell(y,y') \\ &\quad - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}k(x,x')\mathbb{E}_{y'}\ell(y,y')\right]. \\ &=: a + b - 2c.\end{aligned}$$

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- Let us estimate C_{xy}^u, μ_x, μ_y empirically.

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Result

$\widehat{\mathrm{HSIC}_b^2}(x,y) = \frac{1}{n^2}\left\langle \tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y \right\rangle_F$: see the intuition. The details...

First term:

$$a = \left\| C^u_{xy} \right\|^2_{HS} = \mathbb{E}_{xy}\mathbb{E}_{x'y'} k(x,x')\ell(y,y'),$$

$$\hat{a} = \left\| \widehat{C^u_{xy}} \right\|^2_{HS} =$$

First term:

$$a = \left\| C_{xy}^u \right\|_{HS}^2 = \mathbb{E}_{xy}\mathbb{E}_{x'y'} k(x,x')\ell(y,y'),$$

$$\hat{a} = \left\| \widehat{C_{xy}^u} \right\|_{HS}^2 = \left\langle \frac{1}{n}\sum_{i=1}^n \varphi(x_i) \otimes \psi(y_i), \frac{1}{n}\sum_{j=1}^n \varphi(x_j) \otimes \psi(y_j) \right\rangle_{HS}$$

HSIC estimation: from $\widehat{C_{xy}^u}, \hat{\mu}_x, \hat{\mu}_y$

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$$= \frac{1}{n^2} \sum_{i,j=1}^n (\mathbf{G}_x)_{ij} (\mathbf{G}_y)_{ij}$$

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First term:

$$a = \left\| C_{xy}^u \right\|_{HS}^2 = \mathbb{E}_{xy}\mathbb{E}_{x'y'} k(x,x')\ell(y,y'),$$

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$$= \frac{1}{n^2}\sum_{i,j=1}^n (\mathbf{G}_x)_{ij}(\mathbf{G}_y)_{ij} = \frac{1}{n^2}\left\langle \mathbf{G}_x, \mathbf{G}_y \right\rangle_F = \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y).$$

HSIC estimation: 2nd term

$b = \|\mu_x \otimes \mu_y\|_{HS}^2 = \mathbb{E}_{xx'} k(x, x') \mathbb{E}_{yy'} \ell(y, y')$.

$\hat{b} = \|\hat{\mu}_x \otimes \hat{\mu}_y\|_{HS}^2$

HSIC estimation: 2nd term

$$b = \|\mu_x \otimes \mu_y\|_{HS}^2 = \mathbb{E}_{xx'} k(x,x') \mathbb{E}_{yy'} \ell(y,y').$$

$$\hat{b} = \|\hat{\mu}_x \otimes \hat{\mu}_y\|_{HS}^2 = \langle \hat{\mu}_x \otimes \hat{\mu}_y, \hat{\mu}_x \otimes \hat{\mu}_y \rangle_{HS}$$

HSIC estimation: 2nd term

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$$\hat{b} = \|\hat{\mu}_x \otimes \hat{\mu}_y\|_{HS}^2 = \langle \hat{\mu}_x \otimes \hat{\mu}_y, \hat{\mu}_x \otimes \hat{\mu}_y \rangle_{HS}$$

$$= \left\langle \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right], \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right] \right\rangle_{HS}$$

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$$= \left\langle \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right], \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right] \right\rangle_{HS}$$

$$= \left[\frac{1}{n^2}\sum_{i,j=1}^n k(x_i, x_j)\right]\left[\frac{1}{n^2}\sum_{i,j=1}^n \ell(x_i, x_j)\right]$$

HSIC estimation: 2nd term

$$b = \|\mu_x \otimes \mu_y\|_{HS}^2 = \mathbb{E}_{xx'} k(x,x') \mathbb{E}_{yy'} \ell(y,y').$$

$$\hat{b} = \|\hat{\mu}_x \otimes \hat{\mu}_y\|_{HS}^2 = \langle \hat{\mu}_x \otimes \hat{\mu}_y, \hat{\mu}_x \otimes \hat{\mu}_y \rangle_{HS}$$

$$= \left\langle \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right], \left[\frac{1}{n}\sum_{i=1}^n \varphi(x_i)\right] \otimes \left[\frac{1}{n}\sum_{j=1}^n \psi(y_j)\right] \right\rangle_{HS}$$

$$= \left[\frac{1}{n^2}\sum_{i,j=1}^n k(x_i,x_j)\right] \left[\frac{1}{n^2}\sum_{i,j=1}^n \ell(x_i,x_j)\right] = \frac{1}{n^4}\left(\mathbf{1}^T \mathbf{G}_x \mathbf{1}\right)\left(\mathbf{1}^T \mathbf{G}_y \mathbf{1}\right).$$

HSIC estimation: 3rd term (without '−2')

$$c = \left\langle C_{xy}^u, \mu_x \otimes \mu_y \right\rangle_{HS},$$

$$\hat{c} = \left\langle \widehat{C_{xy}^u}, \hat{\mu}_x \otimes \hat{\mu}_y \right\rangle_{HS}$$

HSIC estimation: 3rd term (without '−2')

$$c = \left\langle C_{xy}^u, \mu_x \otimes \mu_y \right\rangle_{HS},$$

$$\hat{c} = \left\langle \widehat{C_{xy}^u}, \hat{\mu}_x \otimes \hat{\mu}_y \right\rangle_{HS}$$

$$= \left\langle \frac{1}{n}\sum_{i=1}^{n} \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^{n} \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^{n} \psi(y_b)\right] \right\rangle_{HS}$$

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$$= \frac{1}{n}\sum_{i=1}^{n} \left\langle \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^{n} \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^{n} \psi(y_b)\right] \right\rangle_{HS}$$

HSIC estimation: 3rd term (without '−2')

$$
\begin{aligned}
c &= \left\langle C_{xy}^u, \mu_x \otimes \mu_y \right\rangle_{HS}, \\
\hat{c} &= \left\langle \widehat{C_{xy}^u}, \hat{\mu}_x \otimes \hat{\mu}_y \right\rangle_{HS} \\
&= \left\langle \frac{1}{n} \sum_{i=1}^n \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n} \sum_{a=1}^n \varphi(x_a) \right] \otimes \left[\frac{1}{n} \sum_{b=1}^n \psi(y_b) \right] \right\rangle_{HS} \\
&= \frac{1}{n} \sum_{i=1}^n \left\langle \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n} \sum_{a=1}^n \varphi(x_a) \right] \otimes \left[\frac{1}{n} \sum_{b=1}^n \psi(y_b) \right] \right\rangle_{HS} \\
&= \frac{1}{n} \sum_{i=1}^n \underbrace{\left\langle \varphi(x_i), \frac{1}{n} \sum_{a=1}^n \varphi(x_a) \right\rangle_{\mathcal{H}_k}}_{\frac{1}{n}\sum_{a=1}^n k(x_i,x_a)} \underbrace{\left\langle \psi(y_i), \frac{1}{n} \sum_{b=1}^n \psi(y_b) \right\rangle_{\mathcal{H}_\ell}}_{\frac{1}{n}\sum_{b=1}^n \ell(y_i,y_b)}
\end{aligned}
$$

HSIC estimation: 3rd term (without '−2')

$$c = \left\langle C_{xy}^u, \mu_x \otimes \mu_y \right\rangle_{HS},$$

$$\begin{aligned}
\hat{c} &= \left\langle \widehat{C_{xy}^u}, \hat{\mu}_x \otimes \hat{\mu}_y \right\rangle_{HS} \\
&= \left\langle \frac{1}{n}\sum_{i=1}^n \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^n \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^n \psi(y_b)\right] \right\rangle_{HS} \\
&= \frac{1}{n}\sum_{i=1}^n \left\langle \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^n \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^n \psi(y_b)\right] \right\rangle_{HS} \\
&= \frac{1}{n}\sum_{i=1}^n \underbrace{\left\langle \varphi(x_i), \frac{1}{n}\sum_{a=1}^n \varphi(x_a) \right\rangle_{\mathcal{H}_k}}_{\frac{1}{n}\sum_{a=1}^n k(x_i,x_a)} \underbrace{\left\langle \psi(y_i), \frac{1}{n}\sum_{b=1}^n \psi(y_b) \right\rangle_{\mathcal{H}_\ell}}_{\frac{1}{n}\sum_{b=1}^n \ell(y_i,y_b)} \\
&= \frac{1}{n^3}\sum_{a,b=1}^n \underbrace{\left[\sum_{i=1}^n k(x_i,x_a)\ell(y_i,y_b)\right]}_{(\mathbf{G}_x\mathbf{G}_y)_{a,b}}
\end{aligned}$$

HSIC estimation: 3rd term (without '−2')

$$c = \left\langle C_{xy}^u, \mu_x \otimes \mu_y \right\rangle_{HS},$$

$$\hat{c} = \left\langle \widehat{C_{xy}^u}, \hat{\mu}_x \otimes \hat{\mu}_y \right\rangle_{HS}$$

$$= \left\langle \frac{1}{n}\sum_{i=1}^n \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^n \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^n \psi(y_b)\right] \right\rangle_{HS}$$

$$= \frac{1}{n}\sum_{i=1}^n \left\langle \varphi(x_i) \otimes \psi(y_i), \left[\frac{1}{n}\sum_{a=1}^n \varphi(x_a)\right] \otimes \left[\frac{1}{n}\sum_{b=1}^n \psi(y_b)\right] \right\rangle_{HS}$$

$$= \frac{1}{n}\sum_{i=1}^n \underbrace{\left\langle \varphi(x_i), \frac{1}{n}\sum_{a=1}^n \varphi(x_a) \right\rangle_{\mathcal{H}_k}}_{\frac{1}{n}\sum_{a=1}^n k(x_i,x_a)} \underbrace{\left\langle \psi(y_i), \frac{1}{n}\sum_{b=1}^n \psi(y_b) \right\rangle_{\mathcal{H}_\ell}}_{\frac{1}{n}\sum_{b=1}^n \ell(y_i,y_b)}$$

$$= \frac{1}{n^3}\sum_{a,b=1}^n \underbrace{\left[\sum_{i=1}^n k(x_i,x_a)\ell(y_i,y_b)\right]}_{(\mathbf{G}_x\mathbf{G}_y)_{a,b}} = \frac{1}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1}.$$

HSIC estimation: putting together

$$\widehat{\mathrm{HSIC}}_b^2(x, y) =: \hat{a} + \hat{b} - 2\hat{c}$$

HSIC estimation: putting together

$$\widehat{\mathrm{HSIC}}_b^2(x, y) =: \hat{a} + \hat{b} - 2\hat{c}$$
$$= \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1}$$

HSIC estimation: putting together

$$\begin{aligned}\widehat{\mathrm{HSIC}}_b^2(x,y) &=: \hat{a} + \hat{b} - 2\hat{c}\\ &= \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1}\\ &= \frac{1}{n^2}\operatorname{tr}\underbrace{\left(\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y + \frac{1}{n^2}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{1}\mathbf{1}^T\mathbf{G}_y\right)}_{\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_x\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_y}\end{aligned}$$

HSIC estimation: putting together

$$\widehat{\mathrm{HSIC}}_b^2(x,y) =: \hat{a} + \hat{b} - 2\hat{c}$$
$$= \frac{1}{n^2}\mathrm{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1}$$
$$= \frac{1}{n^2}\mathrm{tr}\,\underbrace{\left(\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y + \frac{1}{n^2}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{1}\mathbf{1}^T\mathbf{G}_y\right)}_{\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_x\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_y}$$
$$= \frac{1}{n^2}\mathrm{tr}\left(\mathbf{H}\mathbf{G}_x\mathbf{H}\mathbf{G}_y\right)$$

HSIC estimation: putting together

$$
\begin{aligned}
\widehat{\mathrm{HSIC}}_b^2(x,y) &=: \hat{a} + \hat{b} - 2\hat{c} \\
&= \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1} \\
&= \frac{1}{n^2}\operatorname{tr}\underbrace{\left(\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y + \frac{1}{n^2}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{1}\mathbf{1}^T\mathbf{G}_y\right)}_{\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_x\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_y} \\
&= \frac{1}{n^2}\operatorname{tr}(\mathbf{H}\mathbf{G}_x\mathbf{H}\mathbf{G}_y) = \frac{1}{n^2}\operatorname{tr}\left(\underbrace{\mathbf{H}\mathbf{G}_x\mathbf{H}}_{\tilde{\mathbf{G}}_x}\underbrace{\mathbf{H}\mathbf{G}_y\mathbf{H}}_{\tilde{\mathbf{G}}_y}\right)
\end{aligned}
$$

HSIC estimation: putting together

$$
\begin{aligned}
\widehat{\mathrm{HSIC}}_b^2(x,y) &=: \hat{a} + \hat{b} - 2\hat{c} \\
&= \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1} \\
&= \frac{1}{n^2}\operatorname{tr}\underbrace{\left(\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y + \frac{1}{n^2}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{1}\mathbf{1}^T\mathbf{G}_y\right)}_{\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_x\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_y} \\
&= \frac{1}{n^2}\operatorname{tr}\left(\mathbf{H}\mathbf{G}_x\mathbf{H}\mathbf{G}_y\right) = \frac{1}{n^2}\operatorname{tr}\left(\underbrace{\mathbf{H}\mathbf{G}_x\mathbf{H}}_{\tilde{\mathbf{G}}_x}\underbrace{\mathbf{H}\mathbf{G}_y\mathbf{H}}_{\tilde{\mathbf{G}}_y}\right) = \frac{1}{n^2}\left\langle\tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y\right\rangle_F.
\end{aligned}
$$

HSIC estimation: putting together

$$\widehat{\mathrm{HSIC}}_b^2(x,y) =: \hat{a} + \hat{b} - 2\hat{c}$$
$$= \frac{1}{n^2}\operatorname{tr}(\mathbf{G}_x\mathbf{G}_y) + \frac{1}{n^4}\left(\mathbf{1}^T\mathbf{G}_x\mathbf{1}\right)\left(\mathbf{1}^T\mathbf{G}_y\mathbf{1}\right) - \frac{2}{n^3}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y\mathbf{1}$$
$$= \frac{1}{n^2}\operatorname{tr}\underbrace{\left(\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y - \frac{1}{n}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{G}_y + \frac{1}{n^2}\mathbf{1}\mathbf{1}^T\mathbf{G}_x\mathbf{1}\mathbf{1}^T\mathbf{G}_y\right)}_{\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_x\left(\mathbf{I}_n - \frac{\mathbf{E}_n}{n}\right)\mathbf{G}_y}$$
$$= \frac{1}{n^2}\operatorname{tr}(\mathbf{H}\mathbf{G}_x\mathbf{H}\mathbf{G}_y) = \frac{1}{n^2}\operatorname{tr}\left(\underbrace{\mathbf{H}\mathbf{G}_x\mathbf{H}}_{\tilde{\mathbf{G}}_x}\underbrace{\mathbf{H}\mathbf{G}_y\mathbf{H}}_{\tilde{\mathbf{G}}_y}\right) = \frac{1}{n^2}\left\langle\tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y\right\rangle_F.$$

Bias of $\widehat{\mathrm{HSIC}}_b$: $\mathcal{O}\left(\frac{1}{n}\right)$.

Reminder: MMD^2, $\widehat{\text{MMD}}_b^2$, $\widehat{\text{MMD}}_u^2$

$$\text{MMD}^2(\mathbb{P},\mathbb{Q}) := \mathbb{E}_{xx'}k(x,x') + \mathbb{E}_{yy'}k(y,y') - 2\mathbb{E}_{xy}k(x,y),$$

$$\widehat{\text{MMD}}_b^2(\mathbb{P},\mathbb{Q}) = \frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m}k(x_i,x_j) + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}k(y_i,y_j) - \frac{2}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}k(x_i,y_j),$$

$$\widehat{\text{MMD}}_u^2(\mathbb{P},\mathbb{Q}) = \frac{1}{m(m-1)}\sum_{i=1}^{m}\sum_{j\neq i}^{m}k(x_i,x_j) + \frac{1}{n(n-1)}\sum_{i=1}^{n}\sum_{j\neq i}k(y_i,y_j) - \frac{2}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}k(x_i,y_j).$$

$\widehat{\mathrm{HSIC}}_b^2$ until now

$$\mathrm{HSIC}^2(x, y) = \mathbb{E}_{xy}\mathbb{E}_{x'y'}k(x, x')\ell(y, y') + \mathbb{E}_{xx'}k(x, x')\mathbb{E}_{yy'}\ell(y, y') - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}k(x, x')\mathbb{E}_{y'}\ell(y, y')\right],$$

$$\widehat{\mathrm{HSIC}}_b^2(x, y) = \frac{1}{n^2}\sum_{i,j=1}^{n} k(x_i, x_j)\ell(y_i, y_j) + \ldots.$$

$\widehat{\mathrm{HSIC}}_b^2$ until now

$$\mathrm{HSIC}^2(x,y) = \mathbb{E}_{xy}\mathbb{E}_{x'y'}k(x,x')\ell(y,y') + \mathbb{E}_{xx'}k(x,x')\mathbb{E}_{yy'}\ell(y,y') - 2\mathbb{E}_{xy}\left[\mathbb{E}_{x'}k(x,x')\mathbb{E}_{y'}\ell(y,y')\right],$$

$$\widehat{\mathrm{HSIC}}_b^2(x,y) = \frac{1}{n^2}\sum_{i,j=1}^{n} k(x_i,x_j)\ell(y_i,y_j) + \ldots.$$

- x, x' should be independent, but
- with plug-in: $i = j$, it introduces bias.

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{ij} \ell_{ij},$$

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{ij}\ell_{ij}, \qquad \hat{a}_u = \frac{1}{n(n-1)} \sum_{i \neq j} k_{ij}\ell_{ij}$$

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{ij}\ell_{ij}, \qquad \hat{a}_u = \underbrace{\frac{1}{n(n-1)} \sum_{i \neq j} k_{ij}\ell_{ij}}_{\frac{1}{(n)_2} \sum_{(i,j) \in I_2^n} k_{ij}\ell_{ij}},$$

$I_p^n = \{(i_1, \ldots, i_p) : i_j \in \{1, \ldots, n\}$ *without* replacement$\}$, $(n)_p = \left|I_p^n\right|$.

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2}\sum_{i,j=1}^{n} k_{ij}\ell_{ij}, \qquad \hat{a}_u = \underbrace{\frac{1}{n(n-1)}\sum_{i\neq j} k_{ij}\ell_{ij}}_{\frac{1}{(n)_2}\sum_{(i,j)\in I_2^n} k_{ij}\ell_{ij}},$$

$$\hat{c}_b = \frac{1}{n^3}\sum_{i,q,r=1}^{n} k_{iq}\ell_{ir},$$

$I_p^n = \{(i_1,\ldots,i_p) : i_j \in \{1,\ldots,n\}$ *without* replacement$\}$, $(n)_p = \left|I_p^n\right|$.

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{ij} \ell_{ij}, \qquad \hat{a}_u = \underbrace{\frac{1}{n(n-1)} \sum_{i \neq j} k_{ij} \ell_{ij}}_{\frac{1}{(n)_2} \sum_{(i,j) \in I_2^n} k_{ij} \ell_{ij}},$$

$$\hat{c}_b = \frac{1}{n^3} \sum_{i,q,r=1}^{n} k_{iq} \ell_{ir}, \qquad \hat{c}_u = \frac{1}{(n)_3} \sum_{(i,q,r) \in I_3^n} k_{iq} \ell_{ir},$$

$I_p^n = \{(i_1, \ldots, i_p) : i_j \in \{1, \ldots, n\}$ *without* replacement$\}$, $(n)_p = \left| I_p^n \right|$.

HSIC: unbiased estimator

Idea: get rid of the $i = j$-type terms. Let $k_{ij} := k(x_i, x_j)$, $\ell_{ij} := \ell(y_i, y_j)$.

$$\hat{a}_b = \frac{1}{n^2} \sum_{i,j=1}^{n} k_{ij}\ell_{ij}, \qquad \hat{a}_u = \underbrace{\frac{1}{n(n-1)} \sum_{i \neq j} k_{ij}\ell_{ij}}_{\frac{1}{(n)_2} \sum_{(i,j) \in I_2^n} k_{ij}\ell_{ij}},$$

$$\hat{c}_b = \frac{1}{n^3} \sum_{i,q,r=1}^{n} k_{iq}\ell_{ir}, \qquad \hat{c}_u = \frac{1}{(n)_3} \sum_{(i,q,r) \in I_3^n} k_{iq}\ell_{ir},$$

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HSIC: resulting unbiased estimator

After some linear algebra [Gretton et al., 2005a], $(M)_{++} := \sum_{i,j} M_{ij}$,

$$\widehat{\mathrm{HSIC}}^2_b(x,y) = \frac{1}{n^2}\left\langle \tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y \right\rangle_F,$$

$$\widehat{\mathrm{HSIC}}^2_u(x,y) = \frac{1}{n(n-3)}\left[\left\langle \tilde{\mathbf{G}}_x, \tilde{\mathbf{G}}_y \right\rangle_F - \frac{2}{n-2}(\tilde{\mathbf{G}}_x\tilde{\mathbf{G}}_y)_{++} + \frac{1}{(n-1)(n-2)}(\tilde{\mathbf{G}}_x)_{++}(\tilde{\mathbf{G}}_y)_{++}\right].$$

Estimation in practice: few ITE examples

(https://bitbucket.org/szzoli/ite/)
(https://bitbucket.org/szzoli/ite-in-python/)

KCCA estimation: Matlab

Goal: estimate KCCA,

```
>ds = [2;3;4]; Y = rand(sum(ds),5000);
>mult = 1;
>co = IKCCA_initialization(mult);
>KCCA = IKCCA_estimation(Y,ds,co);
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Alternative initialization:

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>co = IKCCA_initialization(mult,{'kappa',0.01,'eta',0.001});
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where κ: regularization constant, η: low-rank approximation.

KCCA & HSIC estimation: Matlab

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Note: HSIC similarly.

MMD estimation: Matlab

Using for example U-statistic:

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>X1 = randn(3,2000); X2 = randn(3,3000);
>mult = 1;
>co = DMMD_Ustat_initialization(mult);
>MMD = DMMD_Ustat_estimation(X1,X2,co);
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```

With low-rank approximation, and setting some parameters:

```
co2 = DMMD_Ustat_iChol_initialization(mult)
co3 = DMMD_Ustat_iChol_initialization(mult,{'sigma',0.2,
'eta',0.01})
```

HSIC estimation: Python

Import ITE (1x), generate observations:

```
>>> import ite
>>> from numpy.random import randn
>>> from numpy import array
>>> ds = array([2, 3, 4])
>>> t = 1000
>>> y = randn(t, sum(ds))
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Estimate HSIC:

```
>>> co = ite.cost.BIHSIC_IChol()
>>> hsic = co.estimation(y, ds)
```

HSIC estimation: Python

Alternative initialization-1:

```
>>> co2 = ite.cost.BIHSIC_IChol(eta=1e-3)
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Alternative-2:

```
>>> from ite.cost.x_kernel import Kernel
>>> k = Kernel({'name': 'RBF','sigma': 1})
>>> co3 = ite.cost.BIHSIC_IChol(kernel=k, eta=1e-3)
>>> hsic3 = co3.estimation(y, ds)
```

HSIC & KCCA estimation: Python

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Estimate MMD:

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>>> co = ite.cost.BDMMD_UStat_IChol()
>>> mmd = co.estimation(y1, y2)
```

MMD estimation: Python

Alternative initialization-1:

```
>>> co2 = ite.cost.BDMMD_UStat_IChol(eta=1e-2)
>>> mmd2 = co2.estimation(y1, y2)
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Towards unbiased estimators

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- Plugin methods: $i = j$, biased.
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Question

What is happening here? Concentration of the estimators?
$\rightarrow$ hypothesis testing: our statistics $:=$ these estimators

Unbiased estimators for $\mathbb{E}_{x,x'} k(x,x')$-type quantities – extensions of average

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- Goal: estimate

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- Assume (w.l.o.g.): h is symmetric,

$$h(x_1, \ldots, x_m) = h\left(x_{\pi(1)}, \ldots, x_{\pi(m)}\right) \quad \forall \pi \text{ permutation.}$$

Example: $k(x, x') = k(x', x)$.

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  Example: $k(x, x') = k(x', x)$.
- Otherwise: $h \leftarrow \frac{1}{m!} \sum_{\pi} h\left(x_{\pi(1)}, \ldots, x_{\pi(m)}\right)$.

U-statistic

- Estimator for $\mathbb{E}_{\mathbb{P}} h(X_1, \ldots, X_m)$:

$$U_n = U(x_1, \ldots, x_n) = \frac{1}{\binom{n}{m}} \sum_c h\left(x_{i_1}, \ldots, x_{i_m}\right),$$

$\sum_c$: m-tuples without replacement.

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- U_n: unbiased, i.e. $\mathbb{E}_{\mathbb{P}}(U_n) = \theta$.

V-statistic

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- Samples with replacement.

U-statistic: examples

- $\theta(\mathbb{P}) = \mathbb{E}_{X\sim\mathbb{P}} X$. Sample average:

$$h(x) = x, \qquad U(x_1, \ldots, x_n) = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

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F_n: empirical cdf.

Extension: if we have L independent samples $\rightarrow$ MMD: $L = 2$

- Given: $x_1^{(j)}, \ldots, x_{n_j}^{(j)} \overset{i.i.d.}{\sim} \mathbb{P}_j$ $(j = 1, \ldots, L)$, $n_j \geqslant m_j$.

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- Goal: estimate: $\theta = \mathbb{E}h\Big(\underbrace{X_1^{(1)}, \ldots, X_{m_1}^{(1)}}_{1^{st}\text{ block}}, \ldots, \underbrace{X_1^{(L)}, \ldots, X_{m_L}^{(L)}}_{\text{L}^{th}\text{ block}}\Big)$.

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- Assumption: symmetry for each block.
- L-sample U-statistic

$$U_{\mathbf{n}} = \frac{1}{\prod_{j=1}^{L}\binom{n_j}{m_j}} \sum_{c} h\left(X_1^{(1)}, \ldots, X_{m_1}^{(1)}, \ldots, X_1^{(L)}, \ldots, X_{m_L}^{(L)}\right).$$

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$$v_c := \mathrm{var}\, h_c\left(X_1,\ldots,X_c\right), v_0 = 0.$$

Results [Serfling, 1980]

U_n: minimum variance unbiased estimator. Notation:

- Asymptotics: depends on $\mathrm{var} \neq 0$ condition.

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In most applications

$c = 1$ or $c = 2$.

Asymptotics for $c = 1$

Assume: $\mathbb{E}_{\mathbb{P}} h^2 < \infty$, $c = 1$.

$$n^{\frac{1}{2}} (U_n - \theta) \xrightarrow{d} N\left(0, m^2 v_1\right),$$

i.e.

$$U_n \text{ is } AN\left(\theta, \frac{m^2 v_1}{n}\right),$$

AN := asymptotically normal.

Asymptotics for $c = 2$

Assume: $\mathbb{E}_{\mathbb{P}} h^2 < \infty$, $c = 2$.

$$n(U_n - \theta) \xrightarrow{d} \frac{m(m-1)}{2} Y, \qquad Y = \sum_{j=1}^{\infty} \lambda_j (\chi_j^2 - 1),$$

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- χ_j^2: i.i.d. $N^2(0,1)$ variables,
- λ_j: $\mathbb{R}$-eigenvalues of $T = T\left(\tilde{h}_2\right)$, $\tilde{h}_2 = h_2 - \theta$

$$(Tg)(x) = \int \tilde{h}_2(x,y) g(y) \mathrm{d}\mathbb{P}(y), \quad g \in L^2.$$

Exponential bound for U-statistic

Theorem (Hoeffding inequality)

Let $h(x_1, \ldots, x_m) \in [a, b]$*. If* $\sigma^2 = \mathrm{var}\, h$*, then for any* $t > 0$

$$\mathbb{P}(U_n - \theta \geqslant t) \leqslant e^{-\frac{2[n/m]t^2}{(b-a)^2}}.$$

U-statistic: local summary

- Minimum variance unbiased estimator.
- $c = 1$: asymptotically normal.
- $c = 2$: asymptotically ∞-sum of weighted χ^2.
- For bounded h: Hoeffding inequality.

Application

Hypothesis testing!

Hypothesis testing

What is a two-sample test?

- Given:
  - $X = \{x_i\}_{i=1}^m \overset{i.i.d.}{\sim} \mathbb{P}$, $Y = \{y_j\}_{j=1}^n \overset{i.i.d.}{\sim} \mathbb{Q}$.
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Discrepancy measure

Example: MMD

What is an independence test?

- Given: paired samples
  - $Z = \{(x_i, y_i)\}_{i=1}^n \overset{i.i.d.}{\sim} \mathbb{P}_{xy}$.
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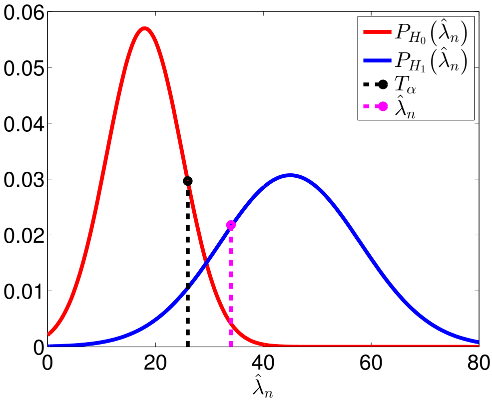
Discrepancy measure

Example: HSIC

Concepts in hypothesis testing

- Test statistic: $\hat{\lambda}_n = \hat{\lambda}_n(X, Y)$, random.
- Significance level: $\alpha = 0.01$.
- Under H_0: $P_{H_0}(\underbrace{\hat{\lambda}_n \leqslant T_\alpha}_{\text{correctly accepting } H_0}) = 1 - \alpha$.



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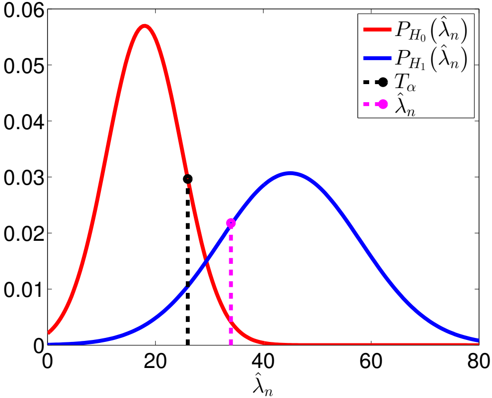
- Under H_1: $P_{H_1}(T_\alpha < \hat{\lambda}_n) = P(\text{correctly rejecting } H_0) =: \text{power}$.



Two-sample testing (aka homogeneity testing) – details.

Two-sample testing with MMD [Gretton et al., 2007, Gretton et al., 2012]

- Statistic: $\hat{\lambda}_n = \widehat{\mathrm{MMD}}_b^2$ or $\widehat{\mathrm{MMD}}_u^2$.

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- We need to control $\hat{\lambda}_n$.
- We will use U-statistic theory.

Finite-sample control

- Large deviation inequalities.
- $P\left(\left|\widehat{\mathrm{MMD}}(\mathbb{P},\mathbb{Q})-\mathrm{MMD}(\mathbb{P},\mathbb{Q})\right|\geqslant\epsilon\right)\leqslant f(\epsilon,m,n)\xrightarrow{m,n\to\infty}0.$

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- $\Rightarrow$ tests: consistent against fixed alternative.

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  - $\widehat{\mathrm{MMD}}_b^2$: bounded difference property, McDiarmid inequality.
  - $\widehat{\mathrm{MMD}}_u^2$: large deviation bound of U-statistics.

Needed: Asymptotic distribution of $\widehat{\mathrm{MMD}}_u^2$.

$$\widehat{\mathrm{MMD}}_u^2(\mathbb{P},\mathbb{Q}) = \frac{1}{m(m-1)}\sum_{i=1}^{m}\sum_{j\neq i}^{m} k(x_i,x_j) + \frac{1}{n(n-1)}\sum_{i=1}^{n}\sum_{j\neq i}^{n} k(y_i,y_j) - \frac{2}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n} k(x_i,y_j).$$

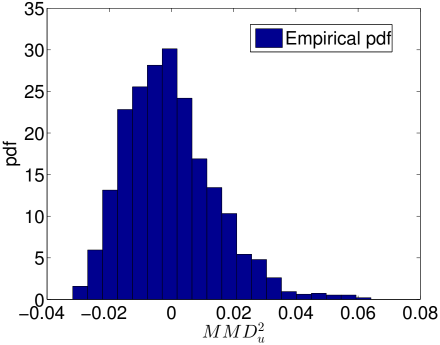
Two-sample test using MMD asymptotics: H_0 [$c = 2$!]

Under H_0 ($\mathbb{P} = \mathbb{Q}$): asymptotic distribution is

$$n\widehat{\mathrm{MMD}}_u^2(\mathbb{P}, \mathbb{P}) \sim \sum_{i=1}^{\infty} \lambda_i (z_i^2 - 2),$$

where $z_i \sim N(0, 2)$ i.i.d.,

$$\int_{\mathcal{X}} \tilde{k}(x, x') v_i(x) \mathrm{d}\mathbb{P}(x) = \lambda_i v_i(x'), \ \tilde{k}(x, x') = \langle \varphi_x - \mu_{\mathbb{P}}, \varphi_{x'} - \mu_{\mathbb{P}} \rangle_{\mathcal{H}_k}.$$



In practice

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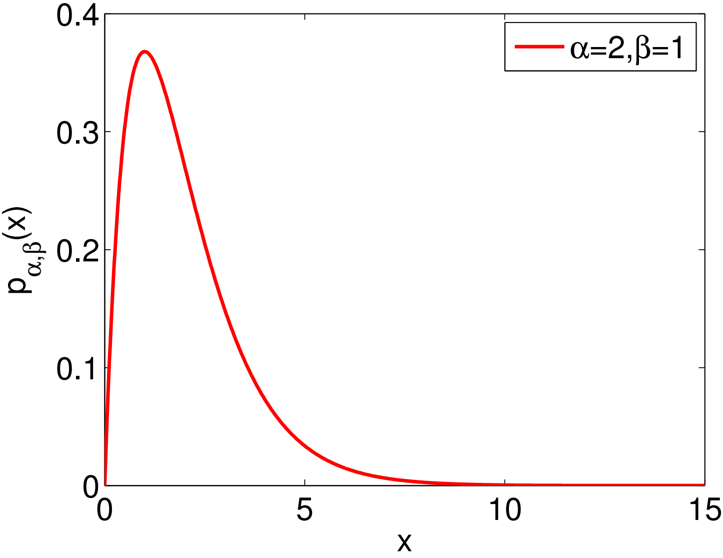
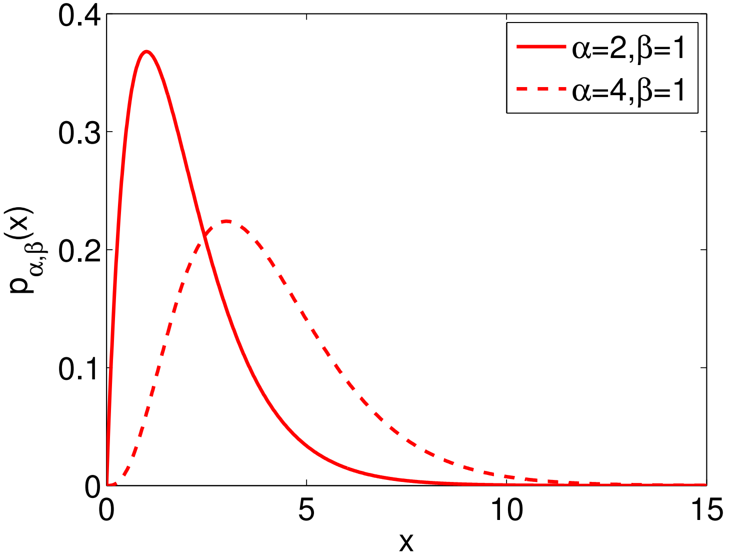
- two-parameter gamma distribution [Johnson et al., 1994]:

$$p_{\alpha,\beta}(x) = \frac{x^{\alpha-1}e^{-\frac{x}{\beta}}}{\beta^{\alpha}\Gamma(\alpha)} \quad (x > 0, \alpha\text{: shape} > 0, \beta\text{: scale} > 0).$$


0.4
0.3
0.2
0.1
0
0
5
10
15
x
$p_{\alpha,\beta}(x)$
α=2,β=1

Gamma distribution: demo



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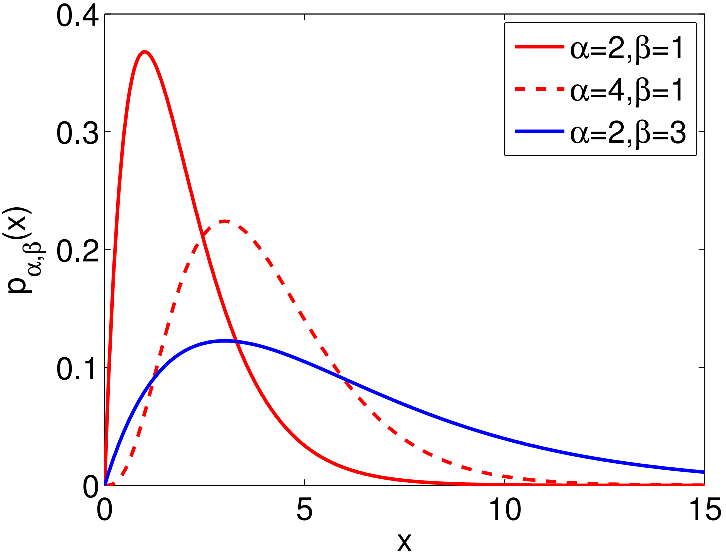

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- Thus, $\widehat{\mathbb{E}T}$ and $\widehat{\mathrm{var}(T)} \rightarrow \hat{\alpha}, \hat{\beta}$.
- Consistency of the test is lost.

Which null approximation to use?

Rules-of-thumb:

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Rules-of-thumb:

- Small sample size: permutation test.
- Medium sample size: gamma approximation, truncated expansion [Gretton et al., 2009],
- Large sample size:
  - online techniques [Gretton et al., 2012], or
  - recent linear methods (next time).

Independence testing: HSIC

Independence testing

Theorem ([Gretton et al., 2008, Pfister et al., 2017])

Under H_0

$$n\widehat{\mathrm{HSIC}}_b^2 \xrightarrow{d} \sum_{i=1}^{\infty} \lambda_i z_i^2, \quad z_i \sim N(0,1).$$

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- For U-statistic: $\sum_i \lambda_i (z_i^2 - 1)$.
- In practice: permutation-test/gamma-approximation.

Related work

Two-sample problem: truncated expansion

[Gretton et al., 2009]: $n = m$, $z_i = (x_i, y_i)$. Estimator:

$$\widehat{\mathrm{MMD}}^2_{u'}(\mathbb{P}, \mathbb{Q}) = \frac{1}{n(n-1)} \sum_{i \neq j} h(z_i, z_j),$$

$$h(z, z') = k(x, x') + k(y, y') - k(x, y') - k(x', y).$$

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$\widehat{\mathrm{MMD}}^2_{u'}$: unbiased.

Two-sample problem: truncated expansion – continued

Theorem

Assuming $\sum_{i=1}^{\infty} \lambda_i^{\frac{1}{2}} < \infty$, *the empirical null converges as* $n \to \infty$

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Note:

$$\hat{\lambda}_{i,n} := \frac{\lambda_i\left(\tilde{\mathbf{G}}_x\right)}{n} \quad (i = 1, \ldots, n), \quad \tilde{\mathbf{G}}_x \in \mathbb{R}^{n \times n}.$$

Online variant [Gretton et al., 2012]

$$\widehat{\mathrm{MMD}}^2_{u'}(\mathbb{P},\mathbb{Q}) = \frac{1}{n(n-1)}\sum_{i\neq j} h(z_i,z_j),$$

has a natural online approximation, $n_2 := [n/2]$

$$\widehat{\mathrm{MMD}}^2_{l}(\mathbb{P},\mathbb{Q}) = \frac{1}{n_2}\sum_{i=1}^{n_2} h((x_{2i-1},y_{2i-1}),(x_{2i},y_{2i})).$$

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- Unbiased.
- Linear-time: streaming data.
- In practice: high variance.

Online variant – continued

By the average the CLT kicks in:

Theorem

Assuming $\mathbb{E}h^2 \in (0, \infty)$, $\widehat{\mathrm{MMD}}_l^2$ *is asymptotically normal*

$$\sqrt{n}\left[\widehat{\mathrm{MMD}}_l^2(\mathbb{P},\mathbb{Q}) - \mathrm{MMD}^2(\mathbb{P},\mathbb{Q})\right] \xrightarrow{d} N\left(0,\sigma^2\right),$$

where $\sigma^2 = 2\left[\mathbb{E}_{z,z'}h^2\left(z,z'\right) - \mathbb{E}^2_{z,z'}h\left(z,z'\right)\right]$.

Block version [Zaremba et al., 2013]

Idea:

- partition the data to blocks of size B,
- on each block: compute $\widehat{\mathrm{MMD}}_l^2$,
- average the results.

Block version – continued

Properties:

- Statistic: asymptotically normal (H_0, H_1).
- For consistency: increase B_m s.t. $\frac{m}{B_m} \to \infty$.
- Reduced variance.

Three-variable interaction test

- Goal (interaction):

$$([x_1; x_2] \perp x_3) \vee ([x_1; x_3] \perp x_2) \vee ([x_2; x_3] \perp x_1).$$

Example: $\mathbb{P} = \mathbb{P}_{12} \otimes \mathbb{P}_3$.

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  Example: $\mathbb{P} = \mathbb{P}_{12} \otimes \mathbb{P}_3$.
- Applications:
  - structure learning of graphical models,
  - discovering V-structures.

Three-variable interaction test – continued

Analogy

Independence $\Leftrightarrow \mathbb{P} = \mathbb{P}_1 \otimes \mathbb{P}_2 \Leftrightarrow \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2 = 0$.

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- Lancaster 3-variable interaction [Lancaster, 1969]:

$$L(\mathbb{P}) = \mathbb{P} - \mathbb{P}_{1,2} \otimes \mathbb{P}_3 - \mathbb{P}_{2,3} \otimes \mathbb{P}_1 - \mathbb{P}_{1,3} \otimes \mathbb{P}_2 + 2\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3.$$

is a signed measure,

$$\text{interaction} \Rightarrow L(\mathbb{P}) = 0.$$

Analogy

Independence $\Leftrightarrow \mathbb{P} = \mathbb{P}_1 \otimes \mathbb{P}_2 \Leftrightarrow \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2 = 0.$

- Lancaster 3-variable interaction [Lancaster, 1969]:

  $$L(\mathbb{P}) = \mathbb{P} - \mathbb{P}_{1,2} \otimes \mathbb{P}_3 - \mathbb{P}_{2,3} \otimes \mathbb{P}_1 - \mathbb{P}_{1,3} \otimes \mathbb{P}_2 + 2\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3.$$

  is a signed measure,

  $$\text{interaction} \Rightarrow L(\mathbb{P}) = 0.$$

- $x_i \in (\mathcal{X}_i, k_i)$ are kernel endowed domains.

Three-variable interaction test – continued

- Interaction index [Sejdinovic et al., 2013a]:

$$I = \left\| \mu_{L(\mathbb{P})} \right\|^2_{\mathcal{H}_{k_1} \otimes \mathcal{H}_{k_2} \otimes \mathcal{H}_{k_3}}.$$

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- Null approximation: permutation-test.

Time-series tests: independence

- Goal: test independence of stationary processes.
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  - Idea: shift-approach = preserves 'time structure' [Chwialkowski and Gretton, 2014].

- Permutation approach (i.i.d): ± 1.

Time-series tests: two-sample, independence, interaction

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- Implementation [Chwialkowski et al., 2014]: based on wild bootstrap [Leucht and H.Neumann, 2013].

3-variable interaction:

- Lancaster interaction + wild bootstrap [Rubenstein et al., 2016].

Goodness-of-fit test

- Given:
  - $\{x_i\}_{i=1}^n \overset{i.i.d.}{\sim} q$,
  - p: target distribution.

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- Goal:

$$H_0 : p = q,$$
$$H_1 : p \neq q.$$

Goodness-of-fit test: continued

- Idea [Chwialkowski et al., 2016, Liu et al., 2016]: Stein operator

$$(S_p f)(x) = \sum_{i=1}^{d} \left[\frac{\partial \log p(x)}{\partial x_i} f_i(x) + \frac{\partial f_i(x)}{\partial x_i} \right], \quad f \in \mathcal{H} := \otimes_{i=1}^{d} \mathcal{H}_k,$$

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- For c_0-universal k: $T_p(q) = 0 \Leftrightarrow p = q$.
- Enough: p up to multiplicative constant ($\nabla \log p$).
- Null approximation: wild bootstrap (including non-i.i.d.).

Quadratic-time methods

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Next step

Linear-time tests, with high-power!

Questions

- Lancaster-interaction measure: reason of the last term?
- Stein operator: why does it work?
- Stein operator: how to estimate it?

Lancaster interaction

Interaction measure:

$$L(\mathbb{P}) = \mathbb{P} - \mathbb{P}_{1,2} \otimes \mathbb{P}_3 - \mathbb{P}_{2,3} \otimes \mathbb{P}_1 - \mathbb{P}_{1,3} \otimes \mathbb{P}_2 + 2\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3.$$

Assume for example:

$$\mathbb{P} = \mathbb{P}_1 \otimes \mathbb{P}_{2,3} \quad \Rightarrow \quad \mathbb{P}_{1,2} = \mathbb{P}_1 \otimes \mathbb{P}_2, \quad \mathbb{P}_{1,3} = \mathbb{P}_1 \otimes \mathbb{P}_3,$$

$$x_1 \perp [x_2; x_3], \qquad x_1 \perp x_2, \qquad x_1 \perp x_3,$$

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and L simplifies to

$$L(\mathbb{P}) = \mathbb{P} - \underbrace{\mathbb{P}_{1,2} \otimes \mathbb{P}_3}_{\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3} - \mathbb{P}_{2,3} \otimes \mathbb{P}_1 - \underbrace{\mathbb{P}_{1,3} \otimes \mathbb{P}_2}_{\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3} + 2\mathbb{P}_1 \otimes \mathbb{P}_2 \otimes \mathbb{P}_3 = 0.$$

Stein operator ($d = 1$ for simplicity): why?

Let $f \in \mathcal{H}_k$.

$$(S_p f)(x) = [\log p(x)]' f(x) + f'(x)$$

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Assumption: $\lim_{|x|\to\infty} p(x)f(x) = 0$.

Stein operator: computation

Test statistics:

$$T_p(q) = \sup_{\|f\|_{\mathcal{H}_k} \leqslant 1} \mathbb{E}_{x\sim q}(S_p f)(x).$$

We rewrite $(S_p f)(x)$ by the reproducing property:

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Stein operator: computation finished

Until now: with $g = \mathbb{E}_{x\sim q}\xi_p(\cdot, x)$, $\xi_p(\cdot, x) = [\log p(x)]' k(\cdot, x) + k'(\cdot, x)$

$$[T_p(q)]^2 = \|g\|^2_{\mathcal{H}_k} = \left\langle \mathbb{E}_{x\sim q}\xi_p(\cdot, x), \mathbb{E}_{x'\sim q}\xi_p(\cdot, x') \right\rangle_{\mathcal{H}_k}$$

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\left\langle \xi_p(\cdot,x), \xi_p(\cdot,x')\right\rangle_{\mathcal{H}_k} &= \big\langle [\log p(x)]' k(\cdot,x) + k'(\cdot,x), \\
&\qquad [\log p(x')]' k(\cdot,x') + k'(\cdot,x')\big\rangle_{\mathcal{H}_k} =: h_p(x,x'), \\
h_p(x,y) &= [\log p(x)]'[\log p(y)]' k(x,y) + [\log p(x)]' k'_y(x,y) + \\
&\qquad [\log p(y)]' k'_x(x,y) + k''_{xy}(x,y).
\end{aligned}
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$\Rightarrow$ Quadratic-time estimator (U-statistic):

$$[\widehat{T_p(q)}]^2 = \frac{1}{n(n-1)} \sum_{i\neq j} h_p(x_i,x_j).$$

Hypothesis testing: linear-time methods

Outline

- Nyström method, random Fourier features.
- Analytic representations $\rightarrow$ linear-time two-sample testing.
- High-power linear-time techniques:
  - two-sample testing,
  - independence testing.
  - goodness-of-fit testing.

Three schemes

Exemplified in independence testing [Zhang et al., 2017]:

- block-HSIC: analog of block-MMD.

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- block-HSIC: analog of block-MMD.
- 2 low-rank schemes:
  - Nyström method [Williams and Seeger, 2001, Drineas and Mahoney, 2005].
  - random Fourier features: [Rahimi and Recht, 2007, Sutherland and Schneider, 2015, Sriperumbudur and Szabó, 2015].

HSIC recall

$$\begin{aligned} C_{xy}^{c} &= \mathbb{E}_{xy}\Big[\big(\varphi(x)-\mu_x\big)\otimes\big(\psi(y)-\mu_y\big)\Big] \\ &= \mathbb{E}_{xy}\left[\varphi(x)\otimes\psi(y)\right]-\mu_x\otimes\mu_y, \\ \mathrm{HSIC}(x,y) &= \left\|C_{xy}^{c}\right\|_{HS}. \end{aligned}$$

Nyström method

Idea

Approximate $\mathbf{G} \in \mathbb{R}^{n \times n}$ with a (random) subset of size $r \ll n$.

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- Without centering:

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Implementation for x and y, separately

On x:

$$\hat{\mathbf{G}}_x \approx \Phi_x^u (\Phi_x^u)^T$$

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Nyström-based HSIC estimator

Population quantity:

$$\mathrm{HSIC}^2(x,y) = \left\| \mathbb{E}_{xy}\left[\varphi(x)\otimes\psi(y)\right] - \mu_x \otimes \mu_y \right\|_{HS}^2$$
$$= \left\| \mathbb{E}_{xy}\left[\left(\varphi(x)-\mu_x\right)\otimes\left(\psi(y)-\mu_y\right)\right]\right\|_{HS}^2.$$

Estimator:

$$\widehat{\mathrm{HSIC}^2_{b,N}}(x,y) = \left\| \frac{1}{n}\sum_{i=1}^{n} \Phi^u_{x,i}\left(\Phi^u_{y,i}\right)^T - \left(\frac{1}{n}\sum_{i=1}^{n}\Phi^u_{x,i}\right)\left(\frac{1}{n}\sum_{i=1}^{n}\Phi^u_{y,i}\right)^T \right\|_F^2$$

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Nyström-based HSIC estimator – conclusion

$$\mathrm{HSIC}^2(x, y) = \left\| C_{xy}^c \right\|_{HS}^2,$$

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In short

C_{xy}^c changed to $\frac{1}{n}\left(\Phi_x^c\right)^T \Phi_y^c$, with Frobenius norm.

Nyström technique: notes

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- GP [Snelson and Ghahramani, 2006, Titsias, 2009]:
  - subset $\to$ optimized subset of size r,
  - inducing points.

Random Fourier features

Characteristic functions: quick summary [Sasvári, 2013]

$\mathbb{P} \mapsto \phi_{\mathbb{P}}$:

$$\phi_{\mathbb{P}}(\mathbf{t}) := \mathbb{E}_{\mathbf{x}\sim\mathbb{P}}\left[e^{i\langle\mathbf{t},\mathbf{x}\rangle}\right] = \int_{\mathbb{R}^d} e^{i\langle\mathbf{t},\mathbf{x}\rangle}\mathrm{d}\mathbb{P}(\mathbf{x}), \quad \mathbf{t} \in \mathbb{R}^d.$$

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Recall

Bochner's theorem & $\mathbf{G} \succcurlyeq 0$ definition of kernels!

Characteristic functions: continued

Operations, closedness:

- Sum of independent variables:

$$\phi_{\sum_{i=1}^{n}\mathbf{x}_i}(\mathbf{t}) = \prod_{i=1}^{n}\phi_{\mathbf{x}_i}(\mathbf{t}), \quad \forall \mathbf{t} \in \mathbb{R}^d.$$

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$$\phi_{\sum_{i=1}^{n}\mathbf{x}_i}(\mathbf{t}) = \prod_{i=1}^{n}\phi_{\mathbf{x}_i}(\mathbf{t}), \quad \forall \mathbf{t} \in \mathbb{R}^d.$$

- Affine transformation ($\mathbf{A} \in \mathbb{R}^{d_1 \times d_2}$):

$$\phi_{\mathbf{Ax}+\mathbf{b}}(\mathbf{t}) = e^{i\langle \mathbf{t},\mathbf{b}\rangle}\phi_{\mathbf{x}}\left(\mathbf{A}^T\mathbf{t}\right), \quad \forall \mathbf{t} \in \mathbb{R}^d.$$

Characteristic functions: continued

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Recall

Distance covariance!

Characteristic functions: continued

Moment condition on $\mathbb{P}$ $\Rightarrow$ differentiability of $\phi_{\mathbb{P}}$.

Assume that exists:

$$M_{\mathbf{a}} = \mathbb{E}_{\mathbf{x}\sim\mathbb{P}}\left[\mathbf{x}^{\mathbf{a}}\right] \quad \mathbf{a} \in \mathbb{N}^d, \ \left(\mathbf{x}^{\mathbf{a}} := \prod_{i=1}^{d} x_i^{a_i}\right).$$

Then $\exists \partial^{\mathbf{a}}\phi_{\mathbb{P}}$ and

$$\partial^{\mathbf{a}}\phi_{\mathbb{P}}(\mathbf{t}) = i^{|\mathbf{a}|}\int_{\mathbb{R}^d} \mathbf{x}^{\mathbf{a}} e^{i\langle \mathbf{t},\mathbf{x}\rangle} \mathrm{d}\mathbb{P}(x), \ \forall \mathbf{t} \in \mathbb{R}^d,$$

$$\partial^{\mathbf{a}}\phi_{\mathbb{P}}(\mathbf{0}) = i^{|\mathbf{a}|} M_{\mathbf{a}}, \ |\mathbf{a}| = \sum_{i=1}^{d} a_i,$$

and $\partial^{\mathbf{a}}\phi_{\mathbb{P}}$ is uniformly continuous.

RFF idea

- k: continuous bounded & shift-invariant on $\mathbb{R}^d$ $[k(\mathbf{x},\mathbf{y}) = k_0(\mathbf{x}-\mathbf{y})]$. By Bochner:

$$k(\mathbf{x},\mathbf{y}) = \int_{\mathbb{R}^d} \underbrace{e^{i\boldsymbol{\omega}^T(\mathbf{x}-\mathbf{y})}}_{\cos(\boldsymbol{\omega}^T(\mathbf{x}-\mathbf{y}))+i\sin(\boldsymbol{\omega}^T(\mathbf{x}-\mathbf{y}))} \mathrm{d}\Lambda(\boldsymbol{\omega})$$

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- RFF trick [Rahimi and Recht, 2007] (MC): $\boldsymbol{\omega}_{1:m} := (\boldsymbol{\omega}_j)_{j=1}^m \overset{i.i.d.}{\sim} \Lambda$,

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Recall (characteristic kernels)

We saw many $k \to \Lambda$ examples!

Questions

- Why is RFF useful?
- Does it converge ($k - \hat{k} \approx 0$)? Rates?

Why is RFF useful?

Kernel approximation:

$$\hat{k}(\mathbf{x}, \mathbf{y}) = \frac{1}{m} \sum_{j=1}^{m} \cos\left(\omega_j^T (\mathbf{x} - \mathbf{y})\right).$$

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Key

We got (random) explicit feature maps!

RFF application in independence testing

Previous slide $\Rightarrow$

$$\left(\Phi_x^u\right)^T := \left[\hat{\phi}(x_1); \ldots; \hat{\phi}(x_n)\right], \left(\Phi_y^u\right)^T := \left[\hat{\phi}(y_1); \ldots; \hat{\phi}(y_n)\right],$$

$$\mathbf{G}_x \approx \Phi_x^u \left(\Phi_x^u\right)^T, \qquad \mathbf{G}_y \approx \Phi_y^u \left(\Phi_y^u\right)^T,$$

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and hence

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$$= \ldots = \left\| \frac{1}{n} \left(\Phi_x^c\right)^T \Phi_y^c \right\|_F^2.$$

Briefly

We simply 'overloaded' the features with the RFF ones.

Some further RFF-accelerated measures

- KCCA [Lopez-Paz et al., 2014].
- MMD [Sutherland and Schneider, 2015, Zhao and Meng, 2015, Lopez-Paz, 2016].

RFF: in kernel ridge regression

- Given: $\{(x_i, y_i)\}_{i=1}^{\ell}$.
- Task: find $f \in \mathcal{H}_k$ s.t. $f(x_i) \approx y_i$,

$$J(f) = \frac{1}{\ell}\sum_{i=1}^{\ell}[f(x_i) - y_i]^2 + \lambda \|f\|_{\mathcal{H}_k}^2 \to \min_{f \in \mathcal{H}_k} \quad (\lambda > 0).$$

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- Analytical solution, $\mathcal{O}(\ell^3)$ – expensive:

$$f(x) = [k(x_1, x), \ldots, k(x_\ell, x)](\mathbf{G} + \lambda \ell I)^{-1}[y_1; \ldots; y_\ell],$$
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- **Idea**: $\hat{\mathbf{G}}$, matrix-inversion lemma, fast primal solvers → RFF.

Approximation quality

- Hoeffding inequality + union bound [Rahimi and Recht, 2007, Sutherland and Schneider, 2015]:

$$\left\| k - \hat{k} \right\|_{L^\infty(\mathcal{S})} = \mathcal{O}_p\left(|\mathcal{S}| \frac{\sqrt{\log(m)}}{\sqrt{m}} \right).$$

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- RFF in ridge regression [Rudi and Rosasco, 2017], kernel PCA [Sriperumbudur and Sterge, 2018, Ullah et al., 2018], classification with 0-1 loss [Sun et al., 2018], Lipschitz losses [Li et al., 2018].

Optimal $\|k - \hat{k}\|_{L^\infty(\mathcal{S})}$: proof idea

- Empirical process form $[\mathbb{P}g := \int g \mathrm{d}\mathbb{P};\ g(\boldsymbol{\omega}) = \cos\left(\boldsymbol{\omega}^T(\mathbf{x} - \mathbf{y})\right)]$:

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- $\mathcal{G}$ is 'nice' (uniformly bounded, separable Carathéodory) $\Rightarrow$

$$\mathbb{E}_{\boldsymbol{\omega}_{1:m}} \|\Lambda - \Lambda_m\|_{\mathcal{G}} \lesssim \mathbb{E}_{\boldsymbol{\omega}_{1:m}} \underbrace{\mathcal{R}\left(\mathcal{G}, \boldsymbol{\omega}_{1:m}\right)}_{\mathbb{E}_\epsilon \sup_{g\in\mathcal{G}}\left|\frac{1}{m}\sum_{j=1}^m \epsilon_j g(\omega_j)\right|}.$$

Proof idea – continued

- Using Dudley's entropy bound:

$$\mathcal{R}\left(\mathcal{G}, \omega_{1:m}\right) \lesssim \frac{1}{\sqrt{m}} \int_0^{|\mathcal{G}|_{L^2(\Lambda_m)}} \sqrt{\log \mathcal{N}\left(\mathcal{G}, L^2(\Lambda_m), r\right)} \mathrm{d}r.$$

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- $\mathcal{G}$ is smoothly parameterized by a compact set $\Rightarrow$

$$\mathcal{N}\left(\mathcal{G}, L^2(\Lambda_m), r\right) \leqslant \left(\frac{4|\mathcal{S}|A}{r} + 1\right)^d, \qquad A(\omega_{1:m}) = \sqrt{\frac{1}{m}\sum_{j=1}^m \|\omega_j\|_2^2}.$$

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- Putting together [$|\mathcal{G}|_{L^2(\Lambda_m)} \leqslant 2$, Jensen inequality] we get ...

Theorem (Finite-sample, asymptotically optimal uniform bound for RFF)

Let k be continuous, bounded, shift-invariant, and $\sigma^2 := \int \|\boldsymbol{\omega}\|^2 \,\mathrm{d}\Lambda(\boldsymbol{\omega}) < \infty$. Then for $\forall \tau > 0$ and compact set $\mathcal{S} \subset \mathbb{R}^d$

$$\Lambda^m \left(\|\hat{k} - k\|_{L^\infty(\mathcal{S})} \geqslant \frac{h(d, |\mathcal{S}|, \sigma) + \sqrt{2\tau}}{\sqrt{m}} \right) \leqslant e^{-\tau},$$

$$h(d, |\mathcal{S}|, \sigma) := 32\sqrt{2d \log(2|\mathcal{S}| + 1)} + 16\sqrt{\frac{2d}{\log(2|\mathcal{S}| + 1)}} + 32\sqrt{2d \log(\sigma + 1)}.$$

Empirical process theory: motivation

The object of interest:

$$\sup_{f \in \mathcal{F}} |\mathbb{P}f - \mathbb{P}_n f|.$$

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$$= \sup_{f\in\mathcal{F}} |\mathbb{P}f - \mathbb{P}_n f|, \quad \mathcal{F} = \left\{\chi_{(\infty,x)} : x \in \mathbb{R}^d\right\}.$$

Ref: [van der Vaart and Wellner, 1996, van der Vaart, 1998, van de Geer, 2009].

Notes on RFF: L^p bounds, kernel derivatives

- One can also get:
  - $L^p(\mathcal{S})$ results ($\Leftarrow$ uniform bound, type of L^p).
  - bounds for $\partial k^{\mathbf{p},\mathbf{q}}$ [Szabó and Sriperumbudur, 2019].

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- Kernel derivatives: $\frac{\partial^{\mathbf{p},\mathbf{q}} f(\mathbf{x},\mathbf{y})}{\partial^{\mathbf{p}}\mathbf{x}\partial^{\mathbf{q}}\mathbf{y}}$,
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  - nonlinear variable selection [Rosasco et al., 2010, Rosasco et al., 2013],
  - infinite-dimensional exponential family fitting [Sriperumbudur et al., 2017].

Let us look at the examples!

Nonlinear variable selection

- Objective function, $\lambda > 0$:

$$J(f) = \frac{1}{n}\sum_{i=1}^{n}\left[f(x_i) - y_i\right]^2 + \lambda \sum_{j=1}^{d} \|\partial_j f\| \rightarrow \min_{f \in \mathcal{H}_k},$$

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- Intuition:
  - if f does not depend on variable j, then $\partial_j f = 0$.

Infinite-dimensional exponential family ($\mathbb{R}^d$)

- Exponential family:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) \propto e^{\langle \boldsymbol{\theta}, T(\mathbf{x}) \rangle},$$

where $\boldsymbol{\theta}$: natural parameter, $T(\mathbf{x})$: sufficient statistics.

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Fitting idea (score matching, Fischer divergence):

$$J(p_*, p_f) := \int p_*(\mathbf{x}) \left\| \frac{\partial \log p_*(\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial \log p_f(\mathbf{x})}{\partial \mathbf{x}} \right\|_2^2 \mathrm{d}\mathbf{x} \to \min_{f \in \mathcal{H}_k}.$$

Notes on RFF: operator-valued extension

- Standard setup: $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

$$\mathcal{H}_k = \{f : \mathcal{X} \to \mathbb{R} \mid \ldots\}.$$

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Y: (separable) Hilbert. Example: $Y = \mathbb{R}^d$, $\mathcal{L}(Y) = \mathbb{R}^{d \times d}$.

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- RFF idea
  - works [Brault et al., 2016]; $(\mathbb{R}^d, +) \to \text{LCA} : \checkmark$
  - open question: 'optimal' rates.

Nyström method, RFF: the end.

Linear-time two-sample testing: analytic representations.

Linear-time 2-sample test [Chwialkowski et al., 2015]

- Recall:

$$\text{MMD}(\mathbb{P},\mathbb{Q}) = \left\|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\right\|_{\mathcal{H}_k}.$$

Linear-time 2-sample test [Chwialkowski et al., 2015]

- Recall:

$$\textcolor{blue}{\mathrm{MMD}}(\mathbb{P},\mathbb{Q}) = \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}.$$

- Idea: change the norm

$$\textcolor{red}{\rho}(\mathbb{P},\mathbb{Q}) := \textcolor{red}{\rho}\left(\mathbb{P},\mathbb{Q};\{\mathbf{v}_j\}_{j=1}^J\right) := \sqrt{\frac{1}{J}\sum_{j=1}^J[\mu_{\mathbb{P}}(\mathbf{v}_j) - \mu_{\mathbb{Q}}(\mathbf{v}_j)]^2}$$

with random $\{\mathbf{v}_j\}_{j=1}^J$ test locations.

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Is ρ a random metric? How do we estimate it? Distribution under H_0?

What is a random metric?

In short

It is a metric almost surely (assumptions: next slide).

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$\mathcal{V} = \{\mathbf{v}_j\}_{j=1}^J \subset \mathbb{R}^d$: reason of randomness.

Result

Theorem

If $\mathcal{X} \subset \mathbb{R}^d$ is connected open, and k is

- *bounded:* $\sup_{\mathbf{x},\mathbf{x}'} k(\mathbf{x},\mathbf{x}') \leqslant B_k < \infty$,

Result

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then

$$\rho(\mathbb{P},\mathbb{Q}) := \sqrt{\frac{1}{J}\sum_{j=1}^{J}[\mu_{\mathbb{P}}(\mathbf{v}_j) - \mu_{\mathbb{Q}}(\mathbf{v}_j)]^2}$$

is a metric a.s. w.r.t. $\{\mathbf{v}_j\}_{j=1}^{J}$.

Why do analytic features work? – proof idea

- μ is injective and maps to analytic functions:
  - k: bounded, analytic $\Rightarrow$ elements of $\mathcal{H}_k$: analytic.
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- μ: characteristic $\Rightarrow$ for $\mathbb{P} \neq \mathbb{Q}$, $f := \mu_{\mathbb{P}} - \mu_{\mathbb{Q}} \neq 0$.
- f: analytic, thus

$$\rho(\mathbb{P},\mathbb{Q}) = \sqrt{\sum_{j=1}^{J} \left[\mu_{\mathbb{P}}(\mathbf{v}_j) - \mu_{\mathbb{Q}}(\mathbf{v}_j)\right]^2}$$

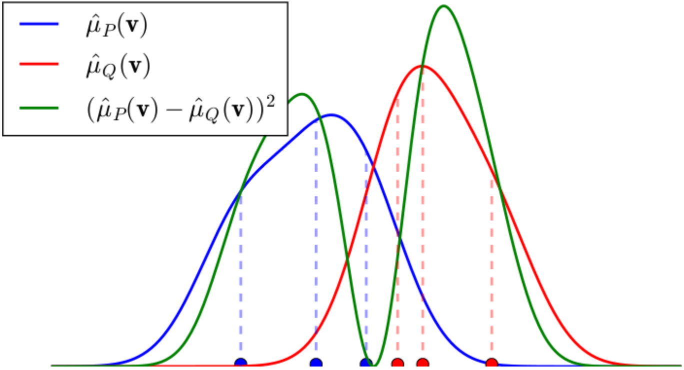
is a metric, a.s. w.r.t. ($\mathbf{v}_j \overset{i.i.d.}{\sim}$) $m \ll \lambda$. Reason: for an analytic $f \neq 0$, $m\{\mathbf{v} : f(\mathbf{v}) = 0\} = 0$.

Estimation

Compute

$$\widehat{\rho^2}(\mathbb{P},\mathbb{Q}) = \frac{1}{J}\sum_{j=1}^{J}[\hat{\mu}_{\mathbb{P}}(\mathbf{v}_j) - \hat{\mu}_{\mathbb{Q}}(\mathbf{v}_j)]^2,$$

where $\hat{\mu}_{\mathbb{P}}(\mathbf{v}) = \frac{1}{n}\sum_{i=1}^{n} k(\mathbf{x}_i,\mathbf{v})$. Example using $k(\mathbf{x},\mathbf{v}) = e^{-\frac{\|\mathbf{x}-\mathbf{v}\|^2}{2\sigma^2}}$:



Estimation – continued

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- Good news: estimation is linear in n!
- Bad news: intractable null distr. $= \sqrt{n}\widehat{\rho^2}(\mathbb{P},\mathbb{P}) \xrightarrow{d}$ sum of J correlated χ^2.

Normalized version gives tractable (asymptotic) null

- Modified test statistic:

$$\hat{\lambda}_n = n\bar{\mathbf{z}}_n^T \boldsymbol{\Sigma}_n^{-1} \bar{\mathbf{z}}_n,$$

  where $\boldsymbol{\Sigma}_n = cov\left(\{\mathbf{z}_i\}_{i=1}^n\right)$.
- Under H_0:
  - $\hat{\lambda}_n \xrightarrow{d} \chi^2(J)$. $\Rightarrow$ Easy to get the $(1-\alpha)$-quantile!

Notes

- Characteristic functions – 'poor' choice:

$$\rho_2(\mathbb{P},\mathbb{Q}) := \sqrt{\frac{1}{J}\sum_{j=1}^{J}[\phi_{\mathbb{P}}(\mathbf{v}_j) - \phi_{\mathbb{Q}}(\mathbf{v}_j)]^2}.$$

  [Chwialkowski et al., 2015, Prop. 1]: It fails to distinguish a large class of distributions.

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- [Moulines et al., 2007]:

$$\rho_3(\mathbb{P},\mathbb{Q}) := \frac{n_x n_y}{n}\left\|C^{-\frac{1}{2}}(\mu_{\mathbb{Q}} - \mu_{\mathbb{P}})\right\|_{\mathcal{H}_k},$$

$$C = \frac{n_x}{n_x+n_y}C_{xx} + \frac{n_y}{n_x+n_y}C_{yy} : \text{ pooled covariance operator.}$$

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  Computational cost: high (cubic).

Notes – continued

- Until now: spatial domain.
- Smoothed characteristic functions:

$$\psi_{\mathbb{P}}(\mathbf{t}) = \int_{\mathbb{R}^d} \phi_{\mathbb{P}}(\boldsymbol{\omega})\ell(\mathbf{t}-\boldsymbol{\omega})\mathrm{d}\boldsymbol{\omega}, \quad \mathbf{t}\in\mathbb{R}^d,$$

$$\rho_4(\mathbb{P},\mathbb{Q}) := \sqrt{\frac{1}{J}\sum_{j=1}^{J}[\psi_{\mathbb{P}}(\mathbf{v}_j)-\psi_{\mathbb{Q}}(\mathbf{v}_j)]^2}.$$

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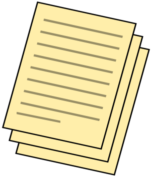
- Notes:
  - For analytic smoothing kernels (ℓ), it works.
  - It is more sensitive to differences in the frequency domain.

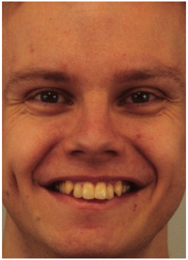
Linear-time high-power two-sample testing

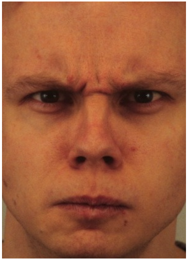
Example-1: NLP

- Given: two categories of documents (Bayesian inference, neuroscience).
- Task:
    - test their distinguishability,
    - most discriminative words $\rightarrow$ interpretability.



Example-2: computer vision





- Given: two sets of faces (happy, angry).
- Task:
    - check if they are different,
    - determine the most discriminative features/regions.

One-page summary [Jitkrittum et al., 2016a]

- We get a nonparametric t-test.
- It gives a reason why H_0 is rejected.
- It is
  - adaptive → high test power.
  - fast (linear time).

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Code:

- https://github.com/wittawatj/interpretable-test

Idea

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- Instead: choose $\theta = \{\mathcal{V}, \sigma\}$ to

  maximize lower bound on the test power.

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Theorem (Lower bound on power, for large n)

Test power $\geqslant L(\lambda_n)$; L: explicit function, monotonically increasing.

- Here,
  - $\lambda_n = n\boldsymbol{\mu}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}$: population version of $\hat{\lambda}_n = n\bar{\mathbf{z}}_n^T\boldsymbol{\Sigma}_n^{-1}\bar{\mathbf{z}}_n$.
  - $\boldsymbol{\mu} = \mathbb{E}_{\mathbf{xy}}[\mathbf{z}_1]$, $\boldsymbol{\Sigma} = \mathbb{E}_{\mathbf{xy}}\left[(\mathbf{z}_1 - \boldsymbol{\mu})(\mathbf{z}_1 - \boldsymbol{\mu})^T\right]$.

Convergence of the λ_n estimator

But λ_n is unknown. $\Rightarrow$ Split (X, Y) into (X_{tr}, Y_{tr}) and (X_{te}, Y_{te}).

- Locations, kernel parameter: $\hat{\theta} = \arg\max_{\theta} \hat{\lambda}^{tr}_{\frac{n}{2}}(\theta)$.

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- Test statistic: $\hat{\lambda}^{te}_{\frac{n}{2}}(\hat{\theta})$.

Convergence of the λ_n estimator

Theorem (Guarantee on objective approximation, $\gamma_n \to 0$)

$$\sup_{\mathcal{V},\mathcal{K}} \left| \bar{\mathbf{z}}_n^T (\boldsymbol{\Sigma}_n + \gamma_n)^{-1} \bar{\mathbf{z}}_n - \boldsymbol{\mu}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} \right| = \mathcal{O}\left(n^{-\frac{1}{4}}\right).$$

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Examples:

$$\mathcal{K} = \left\{ k_\sigma(\mathbf{x}, \mathbf{y}) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}} : \sigma > 0 \right\},$$

$$\mathcal{K} = \left\{ k_{\mathbf{A}}(\mathbf{x}, \mathbf{y}) = e^{-(\mathbf{x}-\mathbf{y})^T \mathbf{A} (\mathbf{x}-\mathbf{y})} : \mathbf{A} \succ 0 \right\}.$$

Proof idea

- Lower bound on the test power:
  - $|\hat{\lambda}_n - \lambda_n| \lesssim \|\bar{\mathbf{z}}_n - \boldsymbol{\mu}\|_2 + \|\boldsymbol{\Sigma}_n - \boldsymbol{\Sigma}\|_F$.
  - Bound the r.h.s. by Hoeffding inequality $\Rightarrow P(|\hat{\lambda}_n - \lambda_n| \geqslant t)$.
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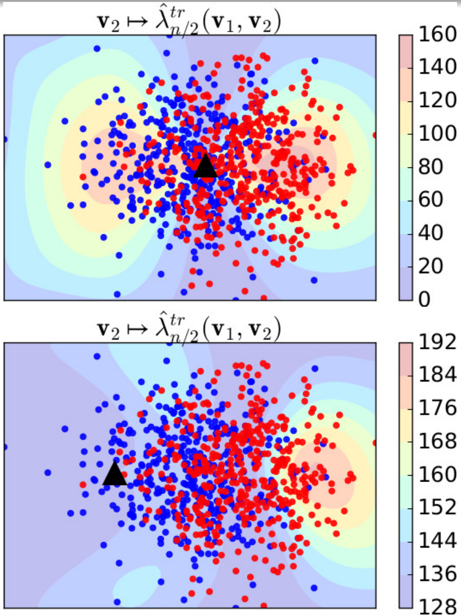
  - By reparameterization: $P(\hat{\lambda}_n \geqslant T_\alpha)$ bound.
- Uniformly $\hat{\lambda}_n \approx \lambda_n$:
  - Reduction to bounding $\sup_{\mathcal{V},\mathcal{S}} \left\|\bar{\mathbf{z}}_n - \boldsymbol{\mu}\right\|_2$, $\sup_{\mathcal{V},\mathcal{S}} \left\|\boldsymbol{\Sigma}_n - \boldsymbol{\Sigma}\right\|_F$.
  - Empirical processes, Dudley entropy bound.

Non-convexity, informative features

- 2D problem:

$$\mathbb{P} := \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \mathbb{Q} := \mathcal{N}(\mathbf{e}_1, \mathbf{I}).$$

- $\mathcal{V} = \{\mathbf{v}_1, \mathbf{v}_2\}$. Fix $\mathbf{v}_1$ to the triangle.
- $\mathbf{v}_2 \mapsto \hat{\lambda}_n(\{\mathbf{v}_1, \mathbf{v}_2\})$: contour plot.



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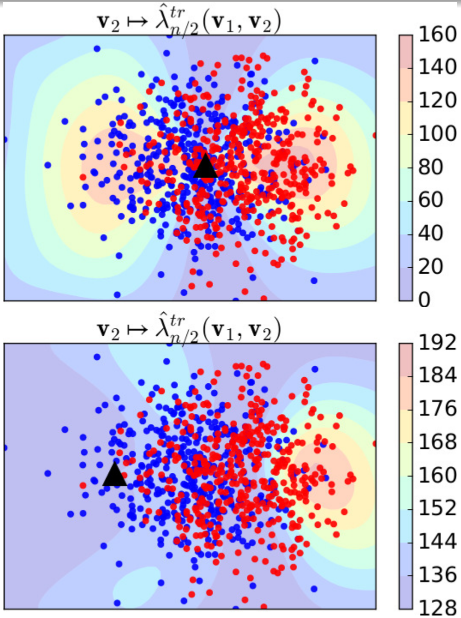


- Nearby locations: do not increase discrimininability.
- Non-convexity: reveals multiple ways to capture the difference.

Computational complexity

- Optimization & testing: linear in n.
- Testing: $\mathcal{O}\left(ndJ + nJ^2 + J^3\right)$.
- Optimization: $\mathcal{O}\left(ndJ^2 + J^3\right)$ per gradient ascent.

Number of locations (J)

- Small J:
  - often enough to detect the difference of $\mathbb{P}$ & $\mathbb{Q}$.
  - few distinguishing regions to reject H_0.
  - faster test.

Number of locations (J)

- Very large J:
    - test power need not increase monotonically in J (more locations $\Rightarrow$ statistic can gain in variance).
    - defeats the purpose of a linear-time test.

Numerical demos

Parameter settings

- Gaussian kernel (σ). $\alpha = 0.01$. $J = 1$. Repeat 500 trials.
- Report

$$P(\text{reject } H_0) \approx \frac{\#\text{times } \hat{\lambda}_n > T_\alpha \text{ holds}}{\#\text{trials}}.$$

- Compare 4 methods
  - **ME-full**: Optimize $\mathcal{V}$ and Gaussian bandwidth σ.
  - **ME-grid**: Optimize σ. Random $\mathcal{V}$ [Chwialkowski et al., 2015].
  - **MMD-quad**: Test with quadratic-time MMD [Gretton et al., 2012].
  - **MMD-lin**: Test with linear-time MMD [Gretton et al., 2012].
- Optimize kernels to power in MMD-lin, MMD-quad.

NLP: discrimination of document categories

- 5903 NIPS papers (1988-2015).
- Keyword-based category assignment into 4 groups:
  - Bayesian inference, Deep learning, Learning theory, Neuroscience
- $d = 2000$ nouns. TF-IDF representation.

Problem	n^{te}	**ME-full**	ME-grid	MMD-quad	MMD-lin
1. Bayes-Bayes	215	.012	.018	.022	.008
2. Bayes-Deep	216	.954	.034	.906	.262
3. Bayes-Learn	138	.990	.774	1.00	.238
4. Bayes-Neuro	394	1.00	.300	.952	.972
5. Learn-Deep	149	.956	.052	.876	.500
6. Learn-Neuro	146	.960	.572	1.00	.538

- Performance of ME-full $[\mathcal{O}(n)]$ is comparable to MMD-quad $[\mathcal{O}(n^2)]$.

NLP: most/least discriminative words

- Aggregating over trials; example: 'Bayes-Neuro'.
- Most discriminative words:

  spike, markov, cortex, dropout, recurr, iii, gibb.

  - learned test locations: highly interpretable,
  - 'markov', 'gibb' ($\Leftarrow$ Gibbs): Bayesian inference,
  - 'spike', 'cortex': key terms in neuroscience.

NLP: most/least discriminative words

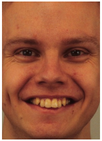
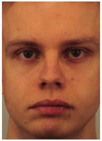
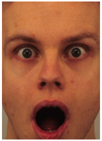
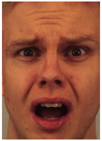
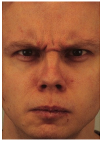
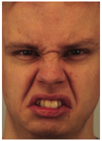
- Aggregating over trials; example: 'Bayes-Neuro'.

- Least dicriminative ones:

  circumfer, bra, dominiqu, rhino, mitra, kid, impostor.

Distinguish positive/negative emotions

- Karolinska Directed Emotional Faces (KDEF) [Lundqvist et al., 1998].
- 70 actors = 35 females and 35 males.
- $d = 48 \times 34 = 1632$. Grayscale. Pixel features.

$+$:    $-$:   

happy neutral surprised afraid angry disgusted

Problem	n^{te}	**ME-full**	ME-grid	MMD-quad	MMD-lin
$\pm$ vs. $\pm$	201	.010	.012	.018	.008
$+$ vs. $-$	201	.998	.656	1.00	.578

- Learned test location (averaged) = 

Linear-time high-power two-sample testing: finished

Linear-time high-power independence testing

Example: dependency testing of media annotations

- We are given paired samples. Task: test independence.
- Examples:
  - (song, year of release) pairs

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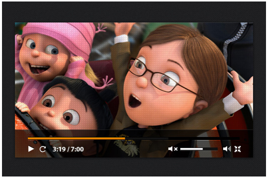

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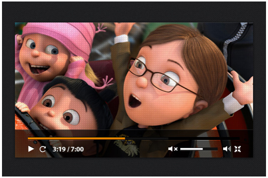

- $\{(x_i, y_i)\}_{i=1}^n \xrightarrow{?} H_0 : \mathbb{P}_{xy} = \mathbb{P}_x\mathbb{P}_y, \; H_1 : \mathbb{P}_{xy} \neq \mathbb{P}_x\mathbb{P}_y.$

2-sample test → independence test

Until now:

- adaptive linear-time 2-sample test (automatic parameter tuning).

2-sample test → independence test

2-sample test:

$$\mathrm{MMD}(\mathbb{P},\mathbb{Q}) = \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}, \quad \rho(\mathbb{P},\mathbb{Q}) = \sqrt{\frac{1}{J}\sum_{j=1}^{J}[\mu_{\mathbb{P}}(\mathbf{v}_j) - \mu_{\mathbb{Q}}(\mathbf{v}_j)]^2},$$

2-sample test $\to$ independence test

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Independence test [Jitkrittum et al., 2016b]:

$$\text{HSIC}(x,y) = \|\mu_{xy} - \mu_x \otimes \mu_y\|_{\mathcal{H}_k \otimes \mathcal{H}_\ell}, \quad \text{FSIC}(\mathbf{x},\mathbf{y}) = \sqrt{\frac{1}{J}\sum_{j=1}^{J} u^2(\mathbf{v}_j, \mathbf{w}_j)}$$

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with $u(\mathbf{v},\mathbf{w}) = \mu_{xy}(\mathbf{v},\mathbf{w}) - \mu_x(\mathbf{v})\mu_y(\mathbf{w})$ witness function.

FSIC: covariance view

$(\mathbf{v}, \mathbf{w})$: fixed. By rewriting

$$
\begin{aligned}
u(\mathbf{v}, \mathbf{w}) &= \mu_{\mathbf{xy}}(\mathbf{v}, \mathbf{w}) - \mu_{\mathbf{x}}(\mathbf{v})\mu_{\mathbf{y}}(\mathbf{w}) \\
&= \mathbb{E}_{\mathbf{xy}}[k(\mathbf{x}, \mathbf{v})\ell(\mathbf{y}, \mathbf{w})] - \mathbb{E}_{\mathbf{x}}[k(\mathbf{x}, \mathbf{v})]\mathbb{E}_{\mathbf{y}}[\ell(\mathbf{y}, \mathbf{w})] \\
&= cov_{\mathbf{xy}}\left(k(\mathbf{x}, \mathbf{v}), \ell(\mathbf{y}, \mathbf{w})\right).
\end{aligned}
$$

$\Rightarrow$ We picked the $(\mathbf{v}, \mathbf{w})^{th}$ entry of

$$
\begin{aligned}
C_{\mathbf{xy}}^c &= \mathbb{E}_{xy}\left[\varphi(\mathbf{x}) \otimes \psi(\mathbf{y})\right] - \mu_{\mathbf{x}} \otimes \mu_{\mathbf{y}}, \\
\mathrm{HSIC} &= \left\| C_{\mathbf{xy}}^c \right\|_{HS}.
\end{aligned}
$$

FSIC is an independence measure

Theorem

If $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ *are bounded, characteristic, analytic kernels [*$\mathcal{X} \subseteq \mathbb{R}^{d_x}$, $\mathcal{Y} \subseteq \mathbb{R}^{d_y}$*: connected open], then almost surely*

$$\mathrm{FSIC}(\mathbf{x}, \mathbf{y}) = 0 \Leftrightarrow \mathbf{x} \perp \mathbf{y}.$$

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Consequence

FSIC can be applied in ISA, feature selection, outlier-robust image registration, ...

Empirical estimator for FSIC

$$\mathrm{FSIC}^2(\mathbf{x},\mathbf{y}) = \frac{1}{J}\sum_{j=1}^{J} u^2(\mathbf{v}_j,\mathbf{w}_j), \quad u(\mathbf{v},\mathbf{w}) = \mu_{xy}(\mathbf{v},\mathbf{w}) - \mu_x(\mathbf{v})\mu_y(\mathbf{w}),$$

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$$= \frac{1}{J}\|\mathbf{u}\|_2^2,$$

where we use the unbiased estimators [2nd = '$\mu_x(\mathbf{v})\mu_y(\mathbf{w})$ - diag']:

$$\widehat{\mu_{xy}}(\mathbf{v},\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} k(\mathbf{x}_i,\mathbf{v})\ell(\mathbf{y}_i,\mathbf{w}),$$

$$\widehat{\mu_x\mu_y}(\mathbf{v},\mathbf{w}) = \frac{1}{n(n-1)}\sum_{i\neq j} k(\mathbf{x}_i,\mathbf{v})\ell(\mathbf{y}_j,\mathbf{w}).$$

Asymptotic distribution of $\hat{\mathbf{u}}$

For fixed $(\mathbf{v}, \mathbf{w})$:

$$\hat{u}(\mathbf{v}, \mathbf{w}) = \frac{2}{n(n-1)} \sum_{i<j} h_{\mathbf{v},\mathbf{w}}\left((\mathbf{x}_i, \mathbf{y}_i), (\mathbf{x}_j, \mathbf{y}_j)\right),$$

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thus $\xrightarrow{\text{theory of U-statistics}}$

Theorem (Asymptotic normality)

For any fixed locations $\mathcal{V} = \{(\mathbf{v}_j, \mathbf{w}_j)\}_{j=1}^J$, $\hat{\mathbf{u}} := [\hat{u}(\mathbf{v}_j, \mathbf{w}_j)]_{j=1}^J$

$$\sqrt{n}\,(\hat{\mathbf{u}} - \mathbf{u}) \xrightarrow{d} N(\mathbf{0}, \mathbf{\Sigma}),$$

$$\Sigma_{ij} = cov_{\mathbf{xy}}\left(\hat{u}(\mathbf{v}_i, \mathbf{w}_i), \hat{u}(\mathbf{v}_j, \mathbf{w}_j)\right).$$

NFSIC = FSIC + whitening

- $n\widehat{\mathrm{FSIC}}^2(x,y) = n\frac{\|\mathbf{u}\|_2^2}{J}$: asymptotically sum of correlated χ^2-s.

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Theorem

- *Under H_0: with $\gamma_n \to 0$*

$$\hat{\lambda}_n = n\hat{\mathbf{u}}^T \left(\hat{\boldsymbol{\Sigma}}_n + \gamma_n \mathbf{I}_J\right)^{-1} \hat{\mathbf{u}} \xrightarrow{d} \chi^2(J).$$

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- *Under H_1: we get a consistent test (i.e., power $\to 1$).*

NFSIC can be estimated easily

Test statistic:

$$\hat{\lambda}_n = n\hat{\mathbf{u}}^T \left(\hat{\mathbf{\Sigma}}_n + \gamma_n \mathbf{I}_J\right)^{-1} \hat{\mathbf{u}}.$$

Estimator: no $n \times n$ Gram matrix

- $\mathbf{K} := [k(\mathbf{v}_i, \mathbf{x}_j)] \in \mathbb{R}^{J\times n}$, $\mathbf{L} := [\ell(\mathbf{w}_i, \mathbf{y}_j)] \in \mathbb{R}^{J\times n}$,
- $\hat{\mathbf{\Sigma}}_n = \frac{\mathbf{\Gamma}\mathbf{\Gamma}^T}{n}$, $\mathbf{\Gamma} = (\mathbf{K}\mathbf{H}_n) \circ (\mathbf{L}\mathbf{H}_n) - \hat{\mathbf{u}}\mathbf{1}_n^T$, $\hat{\mathbf{u}} := \frac{(\mathbf{K}\circ\mathbf{L})\mathbf{1}_n}{n-1} - \frac{(\mathbf{K}\mathbf{1}_n)\circ(\mathbf{L}\mathbf{1}_n)}{n(n-1)}$.

Computational time:

$$\mathcal{O}\left(J^3 + J^2 n + (d_x + d_y) J n\right).$$

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Code with demos:

https://github.com/wittawatj/fsic-test

Choosing the locations & kernel parameters

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$$\textit{test power} \geqslant L(\lambda_n),$$

L: monotonically increasing.

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- In practice: data-splitting (a la 2-sample testing).

HSIC versus FSIC

Question

Which one to choose?

- HSIC $= \|u\|_{\mathcal{H}_k \otimes \mathcal{H}_\ell}$.
- FSIC $= \|u\|_{L^2(\mathcal{V})}$, $\mathcal{V} = \{(\mathbf{v}_j, \mathbf{w}_j)\}_{j=1}^J$.

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- $\mathrm{FSIC} = \|u\|_{L^2(\mathcal{V})}$, $\mathcal{V} = \{(\mathbf{v}_j, \mathbf{w}_j)\}_{j=1}^J$.
  - When $p_{xy} - p_x p_y$ is local, with many peaks.

Demo settings

- k, ℓ: Gaussian. $J = 10$.
- Report: rejection rate of H_0.
- Compare 6 methods:

Method	Description	Tuning	Test size	Complexity
NFSIC-opt	Studied	Gradient descent	$n/2$	$\mathcal{O}(n)$
NFSIC-med	No tuning	Random locations	n	$\mathcal{O}(n)$
QHSIC	Full HSIC	Median heuristic	n	$\mathcal{O}(n^2)$
NyHSIC	Nyström + HSIC	Median heuristic	n	$\mathcal{O}(n)$
FHSIC	RFF + HSIC	Median heuristic	n	$\mathcal{O}(n)$
RDC	RFF + CCA	Median heuristic	n	$\mathcal{O}(n \log n)$

Demo-1: million song data

(Song, year of release) $=:$ $(\mathbf{x}, y)$.

- Western commercial tracks from 1922 to 2011 [Bertin-Mahieux et al., 2011].
- $\mathbf{x} \in \mathbb{R}^{90=d_x}$: audio features.
- Left: break $(\mathbf{x}, y)$ pairs, i.e. H_0 holds; right: H_1 is true.

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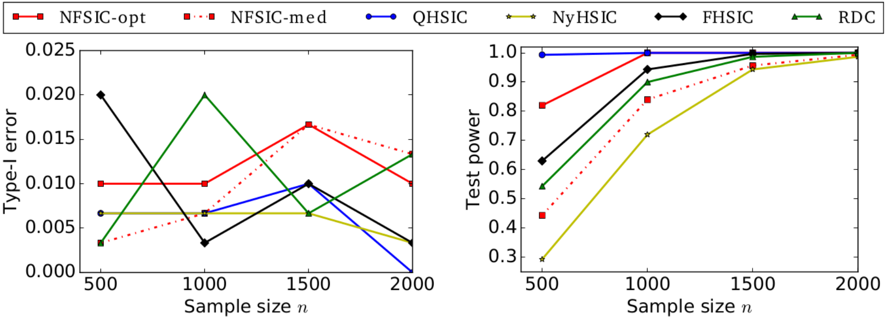

Demo-2: videos and captions

(Youtube video, caption) $=:$ $(\mathbf{x}, \mathbf{y})$.

- VideoStory46K [Habibian et al., 2014]
- $\mathbf{x} \in \mathbb{R}^{2000=d_x}$: Fisher vector encoding of motion boundary histograms [Wang and Schmid, 2013].
- $\mathbf{y} \in \mathbb{R}^{1878=d_y}$: bag of words. TF.
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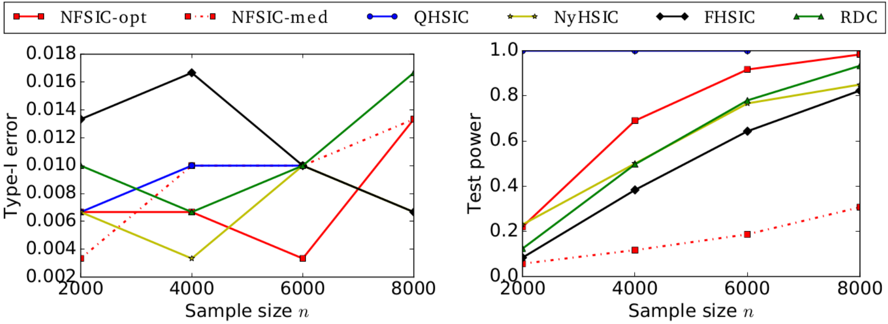
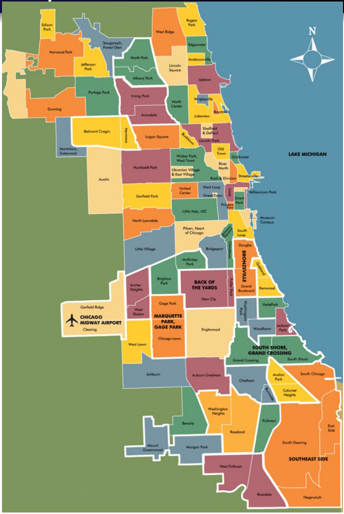


Linear-time goodness-of-fit testing: Stein operator & analytical kernels [Jitkrittum et al., 2017]

Given:

- Density/model: p.



Given:

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- Samples: $X = \{x_i\}_{i=1}^n \sim q$ (unknown).

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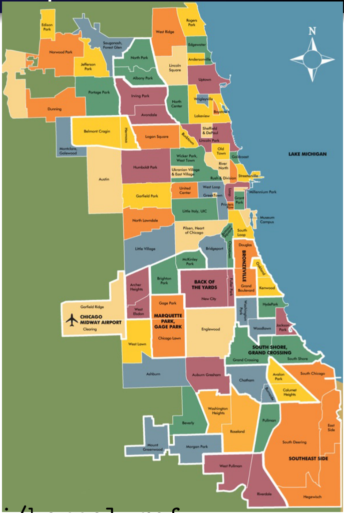

Given:

- Density/model: p.
- Samples: $X = \{x_i\}_{i=1}^n \sim q$ (unknown).

Problem: using p, X test

$$H_0 : p = q, \text{ vs}$$
$$H_1 : p \neq q.$$

Quick summary:

- Best paper award (NIPS-2017, 3/3240).
- Demo: criminal data analysis.
- Code: `https://github.com/wittawatj/kernel-gof`

Summary

- Dependency measures, distances: KCCA, HSIC, MMD.
- Mean embedding, cross-covariance operator.

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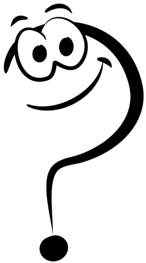
- Dependency measures, distances: KCCA, HSIC, MMD.
- Mean embedding, cross-covariance operator.
- Applications:
  - ISA, distribution regression, image registration, feature selection,
  - hypothesis testing.
- Hypothesis testing:
  - quadratic methods,
  - scaling: block-variants, Nyström, RFF,
  - linear-time adaptive nonparametric tests.

Thank you for the attention!



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