Independence via Cross-Covariance Operators

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Motivation: 'classical' information theory

- Kullback-Leibler divergence:

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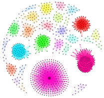
Alternatives: Rényi, Tsallis, L^2 divergence... Typically: $\mathcal{X} = \mathbb{R}^d$.

From $\mathbb{R}^d$ to diverse set of domains, kernel examples





- $\mathcal{X} = \mathbb{R}^d$, $\gamma > 0$:

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}$$

$$k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + \gamma)^p, \qquad k_G(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x}-\mathbf{y}\|_2^2},$$

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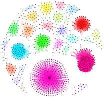

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  - r-spectrum kernel: # of common $\leqslant r$-substrings.

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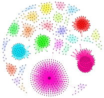

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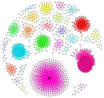

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- $\mathcal{X}$ = graphs, sets, permutations, ...

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Trick

φ: on any kernel-endowed domain!

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'KL divergence & mutual information' on kernel-endowed domains.

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- Maximum mean discrepancy:

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

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- Hilbert-Schmidt independence criterion, $k = \otimes_{m=1}^{M} k_m$:

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$$\begin{aligned}\mathrm{HSIC}_k(\mathbb{P}) &= \mathrm{MMD}_k\left(\mathbb{P}, \otimes_{m=1}^{M} \mathbb{P}_m\right), \\ &= \Big\| \underbrace{\mu_{\otimes_{m=1}^{M} k_m}(\mathbb{P}) - \otimes_{m=1}^{M} \mu_{k_m}(\mathbb{P}_m)}_{\text{cross-covariance operator}} \Big\|_{\otimes_{m=1}^{M} \mathcal{H}_{k_m}}.\end{aligned}$$

MMD, HSIC: easy to estimate!

RKHS intuition ($\mathcal{X} := \mathcal{X}_m$, $k := k_m$)

Given: $\mathcal{X}$ set. $\mathcal{H}$(ilbert space).

- Kernel:

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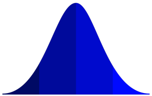
$$\underbrace{k(\cdot, b)} \in \mathcal{H}, \qquad \underbrace{f(b) = \langle f, k(\cdot, b) \rangle_{\mathcal{H}}}_{\text{reproducing property}}.$$



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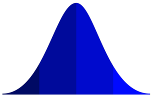

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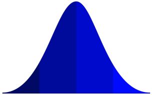

$$\xrightarrow{\text{spec.}} k(a,b) = \langle k(\cdot,a), k(\cdot,b) \rangle_{\mathcal{H}}. \quad \mathcal{H}_k = \overline{\left\{\sum_{i=1}^n \alpha_i k(\cdot,x_i)\right\}}.$$

Mean embedding, MMD: Applications & Review

- Applications:
  - two-sample testing [Borgwardt et al., 2006, Gretton et al., 2012],
  - domain adaptation [Zhang et al., 2013], -generalization [Blanchard et al., 2017],
  - kernel Bayesian inference [Song et al., 2011, Fukumizu et al., 2013]
  - approximate Bayesian computation [Park et al., 2016], probabilistic programming [Schölkopf et al., 2015],
  - model criticism [Lloyd et al., 2014, Kim et al., 2016], goodness-of-fit [Balasubramanian et al., 2017],
  - distribution classification [Muandet et al., 2011, Lopez-Paz et al., 2015], [Zaheer et al., 2017], distribution regression [Szabó et al., 2016], [Law et al., 2018],
  - topological data analysis [Kusano et al., 2016].
- Review [Muandet et al., 2017].

Switching to HSIC ...

MMD $\xrightarrow{\text{spec.}}$ HSIC

MMD with $k = \otimes_{m=1}^{M} k_m$:

$$k(x, x') := \prod_{m=1}^{M} k_m(x_m, x'_m),$$

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Applications:

- blind source separation [Gretton et al., 2005],
- feature selection [Song et al., 2012], post selection inference [Yamada et al., 2018],
- independence testing [Gretton et al., 2008], causal inference [Mooij et al., 2016, Pfister et al., 2017, Strobl et al., 2017].

Central in applications: Characteristic Property

- MMD: k is called characteristic [Fukumizu et al., 2008] if

$$\mathrm{MMD}_k(\mathbb{P}, \mathbb{Q}) = 0 \Leftrightarrow \mathbb{P} = \mathbb{Q}.$$

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Wanted

- Characteristic properties of $\otimes_{m=1}^{M} k_m$ in terms of k_m-s?

Well-known: cont., bounded, shift-invariant kernels on $\mathbb{R}^d$

By Bochner's theorem:

$$k(\mathbf{x}, \mathbf{x}') = k_0(\mathbf{x} - \mathbf{x}') = \int_{\mathbb{R}^d} e^{-i\langle \mathbf{x}-\mathbf{x}', \boldsymbol{\omega}\rangle} \mathrm{d}\Lambda(\boldsymbol{\omega})$$

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Theorem ([Sriperumbudur et al., 2010])

k is characteristic iff. $\mathrm{supp}(\Lambda) = \mathbb{R}^d$.

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Example on $\mathbb{R}$:

kernel name	k_0	$\widehat{k_0}(\omega)$	$supp\left(\widehat{k_0}\right)$
Gaussian	$e^{-\frac{x^2}{2\sigma^2}}$	$\sigma e^{-\frac{\sigma^2\omega^2}{2}}$	$\mathbb{R}$
Laplacian	$e^{-\sigma\lvert x\rvert}$	$\sqrt{\frac{2}{\pi}}\frac{\sigma}{\sigma^2+\omega^2}$	$\mathbb{R}$
Sinc	$\frac{\sin(\sigma x)}{x}$	$\sqrt{\frac{\pi}{2}}\chi_{[-\sigma,\sigma]}(\omega)$	$[-\sigma,\sigma]$

Well-known: $M = 2$

- [Blanchard et al., 2011, Gretton, 2015]:

  k_1&k_2: universal $\Rightarrow$ $k_1 \otimes k_2$: universal ($\Rightarrow$ $\mathcal{I}$-characteristic).

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Goal

Extension to $M \geqslant 2$.

Discrete case: 'easy', e.g. k_1, k_2: char $\not\Rightarrow$ $k_1 \otimes k_2$: char.

- Characteristic property:

$$\mathbb{P}_1 - \mathbb{P}_2 \neq 0 \Rightarrow \mu_{\mathbb{P}_1 - \mathbb{P}_2} \neq 0.$$

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$$\forall \mathbb{F} \in \underbrace{\mathcal{M}_b(\mathcal{X})}_{\text{finite signed measures on } \mathcal{X}} \backslash \{0\} \;\&\; \mathbb{F}(\mathcal{X}) = 0 \Rightarrow \|\mu_{\mathbb{F}}\|^2_{\mathcal{H}_k} > 0.$$

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- Witness construction:

$$\exists \mathbb{F} \in \mathcal{M}_b(\mathcal{X})\backslash\{0\} \;\&\; \mathbb{F}(\mathcal{X}) = 0 \text{ for which } \|\mu_{\mathbb{F}}\|^2_{\mathcal{H}_k} = 0.$$

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Example: $\mathcal{X}_m = \{1, 2\}$, $k_m(x, x') = 2\delta_{x,x'} - 1$ (solvable for $\mathbf{A} \neq \mathbf{0}$).

Example

- $\mathcal{X}_m = \{1,2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\{1,2\})$, $k_m(x,x') = 2\delta_{x,x'} - 1$, $M = 3$.
- *Then*
  - $(k_m)_{m=1}^3$: *characteristic.*
  - $\otimes_{m=1}^3 k_m$: *is not $\mathcal{I}$-characteristic. Witness:*

$$p_{1,1,1} = \frac{1}{5}, \quad p_{1,1,2} = \frac{1}{10}, \quad p_{1,2,1} = \frac{1}{10}, \quad p_{1,2,2} = \frac{1}{10},$$
$$p_{2,1,1} = \frac{1}{5}, \quad p_{2,1,2} = \frac{1}{10}, \quad p_{2,2,1} = \frac{1}{10}, \quad p_{2,2,2} = \frac{1}{10}.$$

Non-$\mathcal{I}$-characteristicity: analytical solution

Parameter: $\mathbf{z} = (z_0, z_1, \ldots, z_5) \in [0, 1]^6$.

Non-$\mathcal{I}$-characteristicity: analytical solution

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$$
-\frac{\begin{aligned} & z_2 + z_1 + z_4 + z_5 - 3z_2z_1 - 4z_2z_4 - 4z_1z_4 - z_2z_3 - 2z_2z_0 - 2z_1z_3 - 3z_2z_5 \\ & - 2z_4z_3 - z_1z_0 - 3z_1z_5 - 2z_4z_0 - 4z_4z_5 - z_3z_0 - z_3z_5 - z_0z_5 + 2z_2z_1^2 + 2z_2^2z_1 \\ & + 4z_2z_4^2 + 2z_2^2z_4 + 4z_1z_4^2 + 2z_1^2z_4 + 2z_2^2z_0 + 2z_1^2z_3 + 2z_2z_5^2 + 2z_2^2z_5 + 2z_4^2z_3 \\ & + 2z_1z_5^2 + 2z_1^2z_5 + 2z_4^2z_0 + 2z_4z_5^2 + 4z_4^2z_5 - z_2^2 - z_1^2 - 3z_4^2 + 2z_4^3 - z_5^2 \\ & + 6z_2z_1z_4 + 2z_2z_1z_3 + 2z_2z_4z_3 + 2z_2z_1z_0 + 4z_2z_1z_5 + 4z_2z_4z_0 + 4z_1z_4z_3 \\ & + 6z_2z_4z_5 + 2z_1z_4z_0 + 6z_1z_4z_5 + 2z_2z_3z_0 + 2z_2z_3z_5 + 2z_1z_3z_0 + 2z_2z_0z_5 \\ & + 2z_1z_3z_5 + 2z_4z_3z_0 + 2z_4z_3z_5 + 2z_1z_0z_5 + 2z_4z_0z_5 \end{aligned}}{\begin{aligned} & 2z_2z_1 - z_1 - 2z_4 - z_3 - z_0 - 2z_5 - z_2 + 2z_2z_4 + 2z_1z_4 + 2z_2z_0 + 2z_1z_3 + 2z_2z_5 \\ & + 2z_4z_3 + 2z_1z_5 + 2z_4z_0 + 4z_4z_5 + 2z_3z_0 + 2z_3z_5 + 2z_0z_5 + 2z_4^2 + 2z_5^2 \end{aligned}}.
$$

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We chose: $\mathbf{z} = \left(\frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}\right)$.

Non-$\mathcal{I}$-characteristicity: analytical solution

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We chose: $\mathbf{z} = \left(\frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}\right)$. Universality: helps?

k_1, k_2: universal, k_3: char $\not\Rightarrow$ $\otimes_{m=1}^3 k_m$: $\mathcal{I}$-characteristic

Example

- $\mathcal{X}_m = \{1,2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\{1,2\})$, $M = 3$.
- $k_1(x,x') = k_2(x,x') = \delta_{x,x'}$: *universal.*
- $k_3(x,x') = 2\delta_{x,x'} - 1$: *characteristic.*
- *Different constraints & $P(\mathbf{z})$ solution; same witness: useful.*

$$p_{1,1,1} = \frac{1}{5}, \quad p_{1,1,2} = \frac{1}{10}, \quad p_{1,2,1} = \frac{1}{10}, \quad p_{1,2,2} = \frac{1}{10},$$
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Results [Szabó and Sriperumbudur, 2018]

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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Proposition ($\mathcal{I}$-characteristic property)

- k_1, k_2: *characteristic* $\Rightarrow$ $k_1 \otimes k_2$: $\mathcal{I}$*-characteristic.*
- $\Leftarrow$: *for* $\forall M \geqslant 2$.
- k_1, k_2, k_3: *characteristic* $\not\Rightarrow$ $\otimes_{m=1}^{3} k_m$: $\mathcal{I}$*-characteristic [Ex].*
- k_1, k_2: *universal*, k_3: *char* $\not\Rightarrow$ $\otimes_{m=1}^{3} k_m$: $\mathcal{I}$*-characteristic [Ex].*

Results: continued [Szabó and Sriperumbudur, 2018]

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

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

Results: continued [Szabó and Sriperumbudur, 2018]

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

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

Proposition (Universality)

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

Summary

We studied the validness of HSIC.

- HSIC $\Rightarrow$ product structure:
  - Space: $\mathcal{X} = \times_{m=1}^{M} \mathcal{X}_m$. Kernel: $k = \otimes_{m=1}^{M} k_m$.
  - $=$MMD$(\mathbb{P}, \otimes_m \mathbb{P}_m) = \|$cross-cov. op.$\|_{\mathcal{H}_k}$.
- Complete answer in terms of k_m-s.

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- Complete answer in terms of k_m-s.
- ITE toolkit, JMLR:

https://bitbucket.org/szzoli/ite/

Z. Szabó, B. K. Sriperumbudur. Characteristic and Universal Tensor Product Kernels. JMLR 18(233):1-29, 2018.

Thank you for the attention!

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