Tensor Product Kernels for Independence

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Motivation: 'classical' information theory

- Kullback-Leibler divergence:

$$\mathrm{KL}\left(\mathbb{P},\mathbb{Q}\right)=\int_{\mathbb{R}^d} p(x)\log\left[\frac{p(x)}{q(x)}\right]\mathrm{d}x.$$

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

Kernels on $\mathbb{R}^d$: generalization of $\mathbf{x}^T\mathbf{y}$

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

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

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

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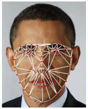
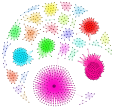
Kernels exist on various domains!





Some kernel-enriched domains: $(\mathcal{X}, k)$

- Strings
  [Watkins, 1999, Lodhi et al., 2002, Leslie et al., 2002, Kuang et al., 2004, Leslie and Kuang, 2004, Saigo et al., 2004, Cuturi and Vert, 2005],
- time series [Rüping, 2001, Cuturi et al., 2007, Cuturi, 2011, Király and Oberhauser, 2019],
- trees [Collins and Duffy, 2001, Kashima and Koyanagi, 2002],
- groups and specifically rankings [Cuturi et al., 2005, Jiao and Vert, 2016],
- sets [Haussler, 1999, Gärtner et al., 2002], probability distributions [Berlinet and Thomas-Agnan, 2004, Hein and Bousquet, 2005, Smola et al., 2007, Sriperumbudur et al., 2010],
- various generative models [Jaakkola and Haussler, 1999, Tsuda et al., 2002, Seeger, 2002, Jebara et al., 2004],
- fuzzy domains [Guevara et al., 2017], or
- graphs [Kondor and Lafferty, 2002, Gärtner et al., 2003, Kashima et al., 2003, Borgwardt and Kriegel, 2005, Shervashidze et al., 2009, Vishwanathan et al., 2010, Kondor and Pan, 2016, Bai et al., 2020, Borgwardt et al., 2020].

Kernel, RKHS: intuition

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

- Kernel:

$$k(a,b) = \langle \varphi(a), \varphi(b) \rangle_{\mathcal{H}}, \quad (\forall a, b \in \mathcal{X}).$$

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- Reproducing kernel of a $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$:

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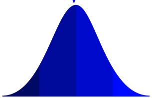

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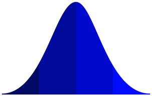

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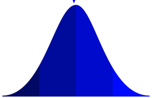

$$\xrightarrow{\text{spec.}} k(a,b) = \langle k(\cdot, a), k(\cdot, b) \rangle_{\mathcal{H}}. \quad \boxed{\mathcal{H}_k = \overline{\left\{\sum_{i=1}^n \alpha_i k(\cdot, x_i)\right\}}}.$$

Kernels: $+2$ definitions

- Def-1 (feature space):

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- Def-2 (reproducing kernel, constructive):

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- All these definitions are equivalent, $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$.
- We represent distributions in RKHSs: $\mu_{\mathbb{P}} \in \mathcal{H}_k$.

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Trick

φ: on any kernel-endowed domain!

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Mean embedding:

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Mean embedding → MMD, HSIC

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

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

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MMD, HSIC: easy to estimate!

Mean embedding, MMD, HSIC: a few applications

- two-sample testing [Baringhaus and Franz, 2004, Székely and Rizzo, 2004, Székely and Rizzo, 2005, Borgwardt et al., 2006, Harchaoui et al., 2007, Gretton et al., 2012, Jitkrittum et al., 2016], and its differential private variant [Raj et al., 2019]; independence [Gretton et al., 2008, Pfister et al., 2018, Jitkrittum et al., 2017a] and goodness-of-fit testing [Jitkrittum et al., 2017b, Balasubramanian et al., 2021], causal discovery [Mooij et al., 2016, Pfister et al., 2018],
- domain adaptation [Zhang et al., 2013], -generalization [Blanchard et al., 2017], change-point detection [Harchaoui and Cappé, 2007], post selection inference [Yamada et al., 2018],
- 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],
- topological data analysis [Kusano et al., 2016],
- 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],
- generative adversarial networks [Dziugaite et al., 2015, Li et al., 2015, Binkowski et al., 2018], understanding the dynamics of complex dynamical systems [Klus et al., 2018, Klus et al., 2019], ...

Central in applications: characteristic property

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

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

Injectivitity of $\mathbb{P} \mapsto \mu_k(\mathbb{P})$ on finite signed measures: universality [Steinwart, 2001].

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Wanted

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

Known: description of characteristic property on $\mathbb{R}^d$

For continuous bounded shift-invariant kernels on $\mathbb{R}^d$:

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

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Theorem ([Sriperumbudur et al., 2010])

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

Examples on $\mathbb{R}$; similarly $\mathbb{R}^d$

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	$e^{-\sigma\|x\|}$	$\sqrt{\frac{2}{\pi}}\frac{\sigma}{\sigma^2+\omega^2}$	$\mathbb{R}$
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	$\frac{\sin(\sigma x)}{x}$	$\sqrt{\frac{\pi}{2}}\chi_{[-\sigma,\sigma]}(\omega)$	$[-\sigma,\sigma]$
Fejér	$\frac{1}{n+1}\frac{\sin^2\frac{(n+1)x}{2}}{\sin^2\left(\frac{x}{2}\right)}$	$\sqrt{2\pi}\sum_{j=-n}^{n}\left(1-\frac{\|j\|}{n+1}\right)\delta(\omega-j)$	$\{0,\pm 1,\pm 2,\dots,\pm n\}$

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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- Distance covariance [Lyons, 2013, Sejdinovic et al., 2013]:

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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:

$$\mathbb{P}_1 - \mathbb{P}_2 \neq 0 \Rightarrow \mu_k(\mathbb{P}_1 - \mathbb{P}_2) \neq 0.$$

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- Observation [Sriperumbudur et al., 2010]: k is characteristic iff.

$$\forall \mathbb{F} \in \underbrace{\mathcal{M}_b(\mathcal{X})}_{\text{finite signed measures on } \mathcal{X}} \backslash\{0\} \;\&\; \mathbb{F}(\mathcal{X}) = 0 \Rightarrow \underbrace{\|\mu_k(\mathbb{F})\|^2_{\mathcal{H}_k}}_{\int_{\mathcal{X}}\int_{\mathcal{X}} k(x,x')\mathrm{d}\mathbb{F}(x)\mathrm{d}\mathbb{F}(x')} > 0.$$

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$$\forall \mathbb{F} \in \underbrace{\mathcal{M}_b(\mathcal{X})}_{\text{finite signed measures on } \mathcal{X}} \setminus \{0\} \ \& \ \mathbb{F}(\mathcal{X}) = 0 \Rightarrow \underbrace{\|\mu_k(\mathbb{F})\|^2_{\mathcal{H}_k}}_{\int_{\mathcal{X}}\int_{\mathcal{X}} k(x,x')\mathrm{d}\mathbb{F}(x)\mathrm{d}\mathbb{F}(x')} > 0.$$

- Witness construction:

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

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

- Characteristic property:

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- Witness construction:

$$\exists \underbrace{\mathbb{F} \in \mathcal{M}_b(\mathcal{X})}_{\mathbf{A}:=(a_{ij})} \backslash \{0\} \ \& \ \underbrace{\mathbb{F}(\mathcal{X}) = 0}_{eq_1(\mathbf{A})=0} \text{ for which } \underbrace{\|\mu_k(\mathbb{F})\|^2_{\mathcal{H}_k} = 0}_{eq_2(\mathbf{A})=0}.$$

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

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

Example

- $\mathcal{X}_m = \{1,2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\{1,2\})$, $k_m(x,x') = 2\delta_{x,x'} - 1$, $M = 3$.
- *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: $\mathbf{z} = (z_0, z_1, \ldots, z_5) \in [0, 1]^6$.

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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\\
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&+ 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\\
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&+ 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\\
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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

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

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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?

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.*

$$
\begin{aligned}
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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\end{aligned}
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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.*
- $\boxed{\not\Leftarrow}$ *[*$|\mathcal{X}_m| = 2$, $k_m(x,x') = 2\delta_{x,x'} - 1$*]*

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

Results: continued [Szabó and Sriperumbudur, 2018]

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

The followings are equivalent:

(i) $(k_m)_{m=1}^M$*-s are characteristic.*

(ii) $\otimes_{m=1}^M k_m$*: $\mathcal{I}$-characteristic.*

(iii) $\otimes_{m=1}^M k_m$*: characteristic.*

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We already know

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Remains: $(iii) \Leftarrow (i)$. Proof: Bochner theorem,

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Proposition (Universality)

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

The tricky direction: if $(k_m)_{m=1}^M$ are universal ...

Goal: injectivity of $\mu = \mu_{\otimes_{m=1}^M k_m}$ on $\mathcal{M}_b(\mathcal{X})$, i.e.

$$\mu(\mathbb{F}) = 0 \overset{?}{\Longrightarrow} \mathbb{F} = 0.$$

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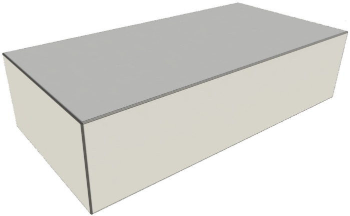
Enough:

$$\mathbb{F}\left(\times_{m=1}^M B_m\right) = 0, \quad \forall B_m.$$



Proof idea

$$0 = \mu(\mathbb{F}) = \int_{\mathcal{X}} \otimes_{m=1}^{M} k_m(\cdot, x_m) \mathrm{d}\mathbb{F}(x),$$

$$0 = \mathbb{F}\left(\times_{m=1}^{M} B_m\right) = \int_{\mathcal{X}} \times_{m=1}^{M} \mathcal{I}_{B_m}(x_m) \mathrm{d}\mathbb{F}(x), \ \forall B_m.$$

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We proceed by induction ($J = 0, \ldots, M$).

Summary

We studied the validness of HSIC.

- Space: $\mathcal{X} = \times_{m=1}^{M} \mathcal{X}_m$. Kernel: $k = \otimes_{m=1}^{M} k_m$.
- $\text{HSIC}_k(\mathbb{P}) = \text{MMD}_k\left(\mathbb{P}, \otimes_m \mathbb{P}_m\right) = \|\text{cross-cov. op.}\|_{\mathcal{H}_k}$.
- 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/`

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Thank you for the attention!

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