Tensor Product Kernels: Independence and Beyond

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Motivation: 'Classical' Information Theory

- Kullback-Leibler divergence:

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

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Properties:

1. $I(\mathbb{P}) \geqslant 0$.
2. $I(\mathbb{P}) = 0 \Leftrightarrow \mathbb{P} = \otimes_{m=1}^{M}\mathbb{P}_m$.

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

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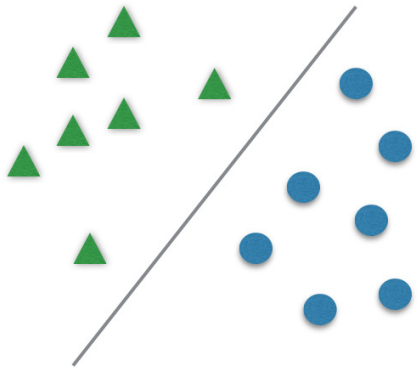

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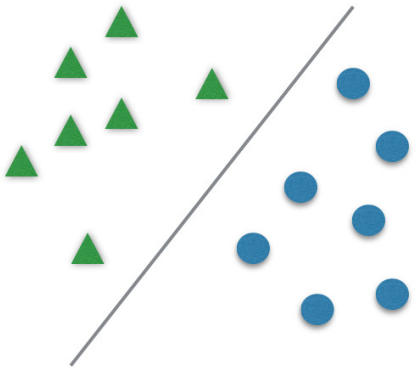

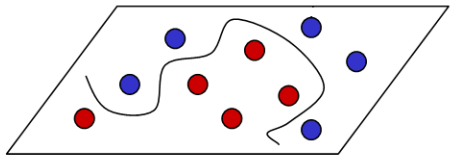

Input Space

Euclidean Space → Inner Product → Kernel

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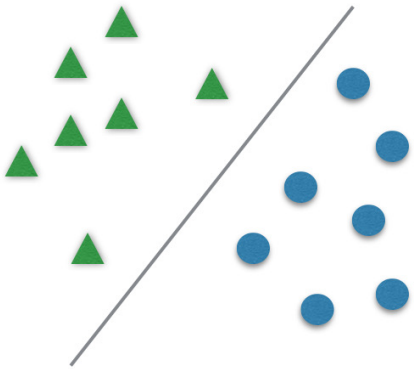

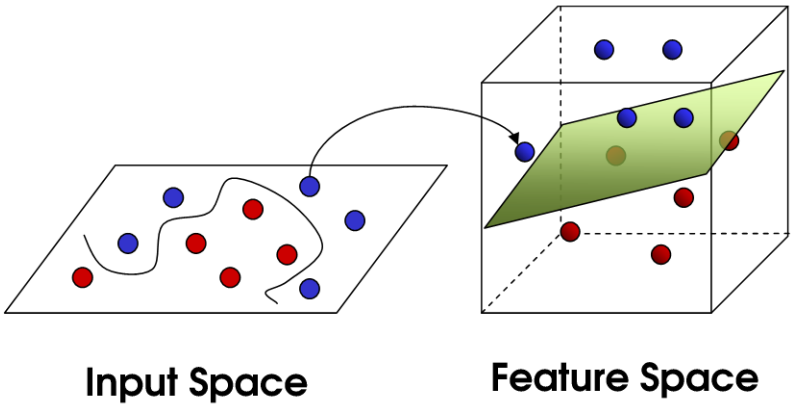

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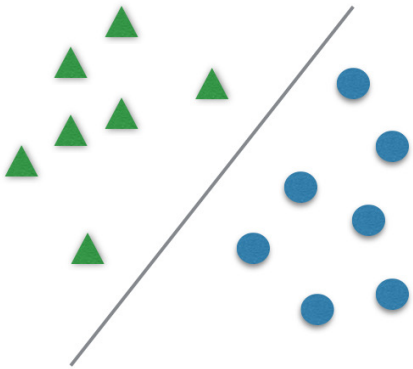
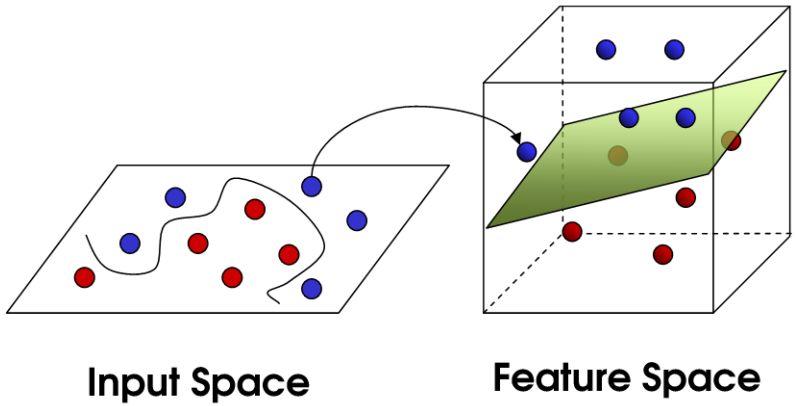


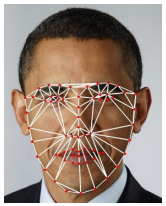


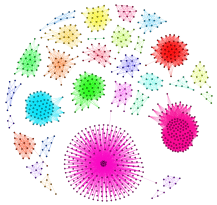
2. Representation of distributions (this talk):

$$\mathbb{P} \mapsto \mathbb{E}_{\mathbf{x}\sim\mathbb{P}}\varphi(\mathbf{x}).$$

$\varphi(\mathbf{x}) = \mathbf{x}$: mean, $\varphi(\mathbf{x}) = e^{i\langle\cdot,\mathbf{x}\rangle}$: characteristic function.

Diverse Set of Domains, Kernel Examples





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

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

$$k_e(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x}-\mathbf{y}\|_2}, \qquad k_C(\mathbf{x}, \mathbf{y}) = 1 + \frac{1}{\gamma \|\mathbf{x}-\mathbf{y}\|_2^2}.$$

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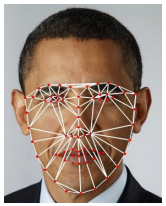

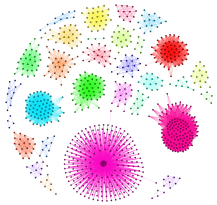

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  - r-spectrum kernel: # of common $\leqslant r$-substrings.

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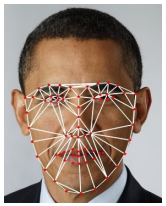

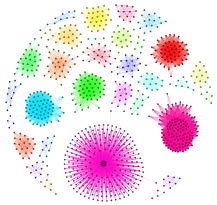

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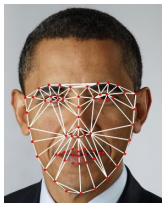

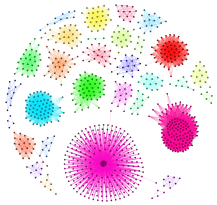

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- $\mathcal{X}$ = time-series: dynamic time-warping.
- $\mathcal{X}$ = trees, graphs, dynamical systems, sets, permutations, ...

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

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When is HSIC an independence measure? Conditions on k_m-s?

Ingredients

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Assumption

$\mathcal{X}_m$: kernel-enriched domains.

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

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

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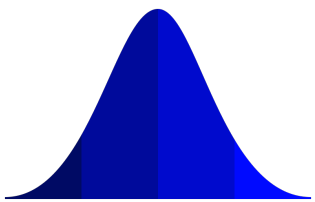

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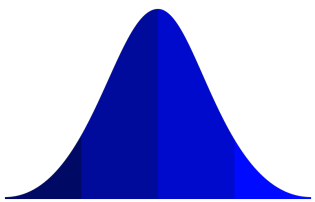

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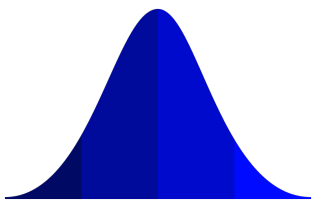

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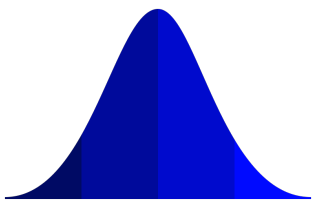

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Equivalent definitions. We represent distributions in an RKHS...

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Mean Embedding, MMD: Applications & Review

- Applications:
  - two-sample testing [Gretton et al., 2012], domain adaptation [Zhang et al., 2013], -generalization [Blanchard et al., 2017],
  - interpretable machine learning [Kim et al., 2016],
  - kernel belief propagation [Song et al., 2011], kernel Bayes' rule [Fukumizu et al., 2013], model criticism [Lloyd et al., 2014],
  - approximate Bayesian computation [Park et al., 2016], probabilistic programming [Schölkopf et al., 2015],
  - distribution classification [Muandet et al., 2011], distribution regression [Szabó et al., 2016], topological data analysis [Kusano et al., 2016].
- Review [Muandet et al., 2017].

Let us switch to HSIC.

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

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

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Applications:

- blind source separation [Gretton et al., 2005],
- feature selection [Song et al., 2012], post selection inference [Yamada et al., 2016],
- 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

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Wanted

- $\otimes_{m=1}^{M} k_m$ is $\mathcal{I}$-characteristic: conditions in terms of k_m-s?
- $\otimes_{m=1}^{M} k_m$ is characteristic: relation?

Characteristic Property: Description on $\mathbb{R}^d$

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

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

$(*)$: Bochner's theorem.

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$$\|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k} = \|c_{\mathbb{P}} - c_{\mathbb{Q}}\|_{L^2(\Lambda)}.$$

$(*)$: Bochner's theorem, $c_{\mathbb{P}}$: characteristic function of $\mathbb{P}$.

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$(*)$: Bochner's theorem, $c_{\mathbb{P}}$: characteristic function of $\mathbb{P}$.

Theorem ([Sriperumbudur et al., 2010])

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

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

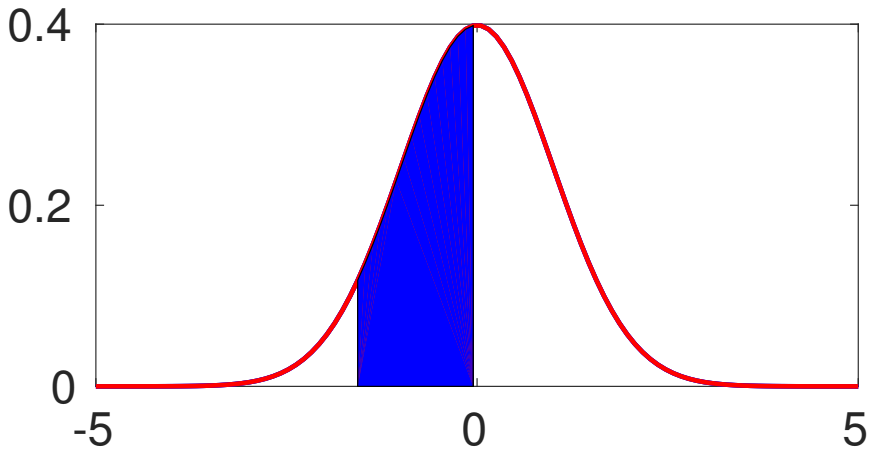
kernel name	k_0	$\widehat{k_0}(\omega)$	$supp(\widehat{k_0})$
Gaussian	$e^{-\frac{x^2}{2\sigma^2}}$	$\sigma e^{-\frac{\sigma^2\omega^2}{2}}$	$\mathbb{R}$
Laplacian	$e^{-\sigma\lvert x\rvert}$	$\sqrt{\frac{2}{\pi}}\frac{\sigma}{\sigma^2+\omega^2}$	$\mathbb{R}$
B_{2n+1}-spline	$*^{2n+2}\chi_{\left[-\frac{1}{2},\frac{1}{2}\right]}(x)$	$\frac{4^{n+1}}{\sqrt{2\pi}}\frac{\sin^{2n+2}\left(\frac{\omega}{2}\right)}{\omega^{2n+2}}$	$\mathbb{R}$
Sinc	$\frac{\sin(\sigma x)}{x}$	$\sqrt{\frac{\pi}{2}}\chi_{[-\sigma,\sigma]}(\omega)$	$[-\sigma,\sigma]$
Fejér	$\frac{1}{n+1}\frac{\sin^2\frac{(n+1)x}{2}}{\sin^2\left(\frac{x}{2}\right)}$	$\sqrt{2\pi}\sum_{j=-n}^{n}\left(1-\frac{\lvert j\rvert}{n+1}\right)\delta(\omega-j)$	$\{0,\pm1,\pm2,\ldots,\pm n\}$

Measures: Intuition

- Probability measures. Idea:

$$\int_{\mathcal{X}} p(x)\mathrm{d}x = 1, \ p \geqslant 0.$$

Usage: $\mathbb{P}(H) = \int_H p(x)\mathrm{d}x$.



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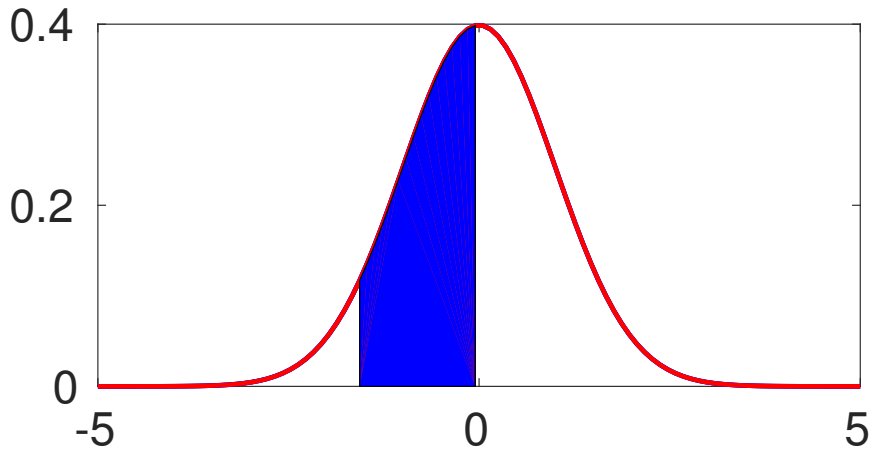

- Non-negative (finite) measures:

$$\int p(x)\mathrm{d}x < \infty, \ p \geqslant 0.$$

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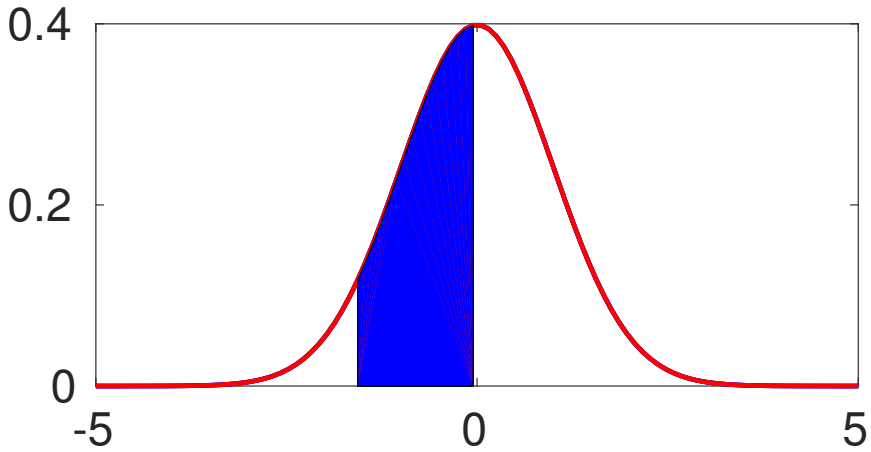

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$$\int_{\mathcal{X}} p(x)\mathrm{d}x \overset{NO}{=} 1,\ p \overset{NO}{\geqslant} 0, \qquad \sum_i p_i = 1,\ p_i \geqslant 0\ (\forall i).$$

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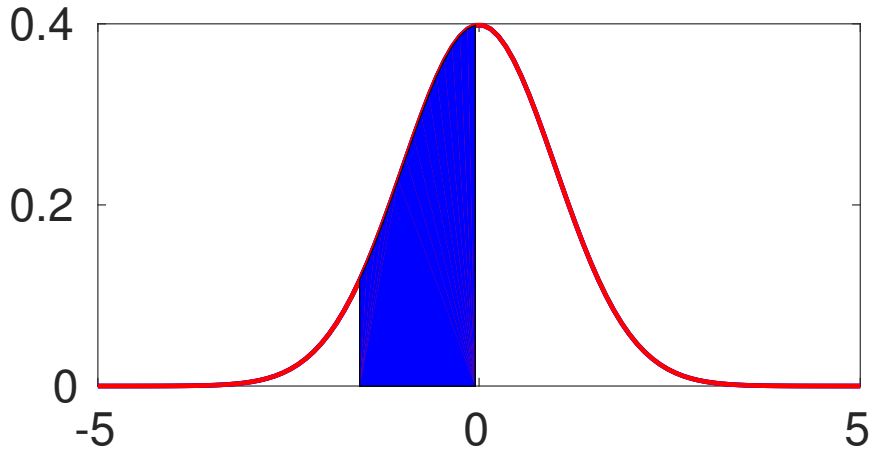

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Universality [Steinwart, 2001, Sriperumbudur et al., 2010]

k is called characteristic (recall!)/universal if

$$\mu_k : \underbrace{\mathcal{M}_1^+(\mathcal{X})}_{\text{probability measures on } \mathcal{X}} \mapsto \mathcal{H}_k, \qquad \mu_k : \underbrace{\mathcal{M}_b(\mathcal{X})}_{\text{bounded signed measures on } \mathcal{X}} \mapsto \mathcal{H}_k$$

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Challenge

Characteristic/$\mathcal{I}$-characteristic/universality of $\otimes_{m=1}^M k_m$ in terms of k_m-s!

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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Main Challenge

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

Idea: Characteristic Property as Ispd

- Characteristic property:

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

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

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- We saw: k is universal iff.

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$\mathcal{F}$-ispd Tensor Product Kernels

From now on: $\mathcal{X} = \times_{m=1}^{M} \mathcal{X}_m$. Let $\mathcal{F} \subseteq \mathcal{M}_b(\mathcal{X})$, $0 \in \mathcal{F}$.

Definition

$k = \otimes_{m=1}^{M} k_m$ is called $\mathcal{F}$-ispd if

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$$\mu_k(\mathbb{F}) = 0 \Rightarrow \mathbb{F} = 0 \quad (\mathbb{F} \in \mathcal{F}).$$

Examples

$\mathcal{F}$	$\mathcal{F}$-ispd k
$\mathcal{M}_b(\mathcal{X})$	universal
$[\mathcal{M}_b(\mathcal{X})]^0$	characteristic

$$\subseteq \qquad\qquad \subseteq \quad [\mathcal{M}_b(\mathcal{X})]^0 \subseteq \quad \mathcal{M}_b(\mathcal{X}) \,.$$

$$\Updownarrow$$

$$\Leftarrow \qquad\qquad \Leftarrow \quad \text{characteristic} \Leftarrow \quad \text{universal}.$$

$$\Downarrow$$

Examples

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$$\text{UI}$$

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$[\mathcal{M}_b(\mathcal{X})]^0$	characteristic
$\mathcal{I} := \{\mathbb{P} - \otimes_{m=1}^M \mathbb{P}_m\}$	$\mathcal{I}$-characteristic
$\left[\otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)\right]^0$	$\otimes$-characteristic

$$\subseteq \left[\otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)\right]^0 \subseteq \quad [\mathcal{M}_b(\mathcal{X})]^0 \subseteq \quad \mathcal{M}_b(\mathcal{X}).$$

$$\text{UI}$$

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$$\Leftarrow \otimes\text{-characteristic} \Leftarrow \quad \text{characteristic} \Leftarrow \quad \text{universal}.$$

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$\mathcal{F}$	$\mathcal{F}$-ispd k
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$[\mathcal{M}_b(\mathcal{X})]^0$	characteristic
$\mathcal{I} := \{\mathbb{P} - \otimes_{m=1}^M \mathbb{P}_m\}$	$\mathcal{I}$-characteristic
$\left[\otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)\right]^0$	$\otimes$-characteristic
$\otimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m)$	$\otimes_0$-characteristic

$$\otimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m) \subseteq \left[\otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)\right]^0 \subseteq [\mathcal{M}_b(\mathcal{X})]^0 \subseteq \mathcal{M}_b(\mathcal{X}).$$

$$\text{UI}$$

$$\mathcal{I}$$

$$\otimes_0\text{-characteristic} \Leftarrow \otimes\text{-characteristic} \Leftarrow \text{characteristic} \Leftarrow \text{universal}.$$

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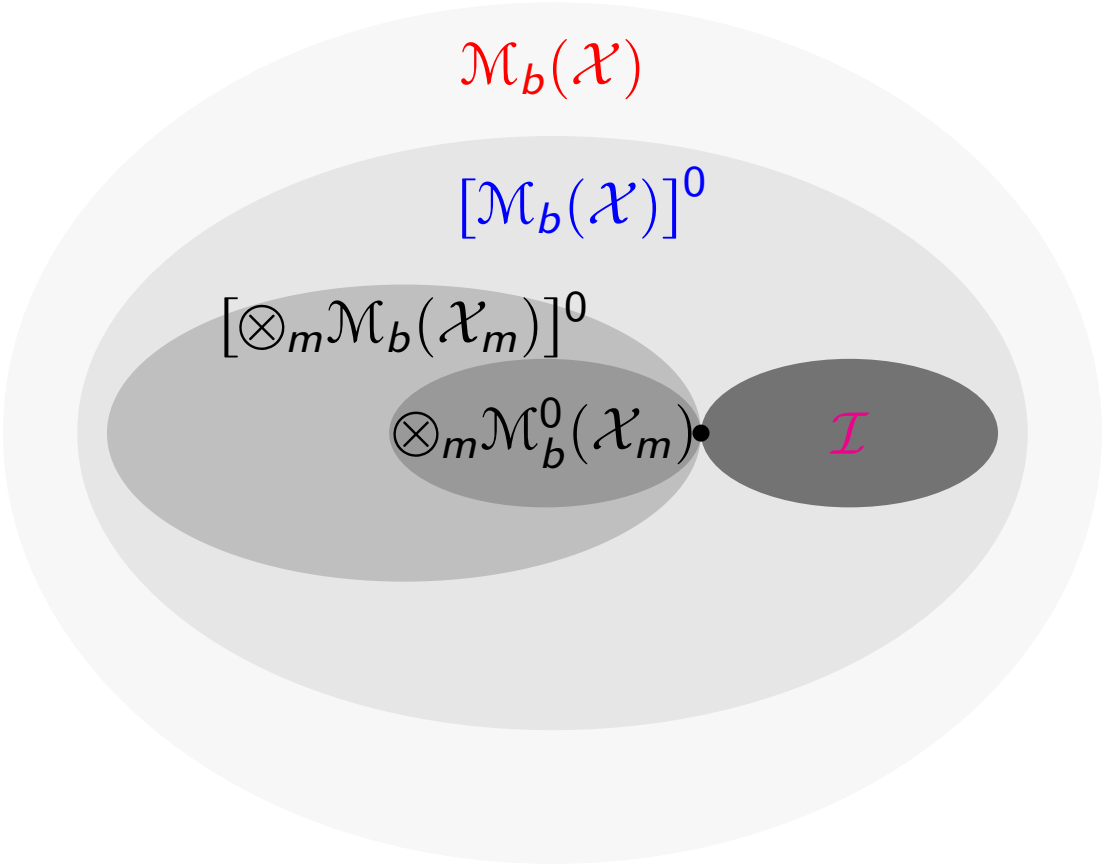
$\mathcal{M}_b(\mathcal{X})$
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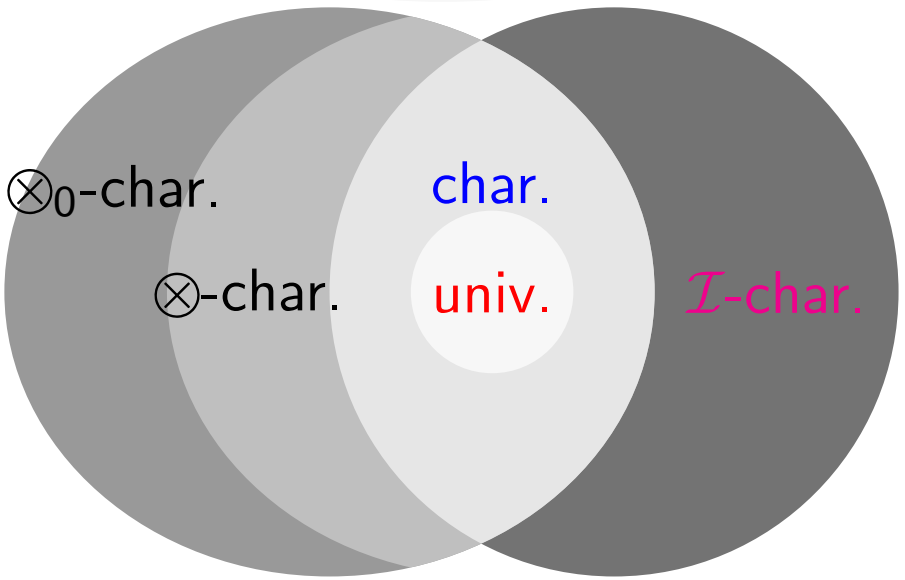
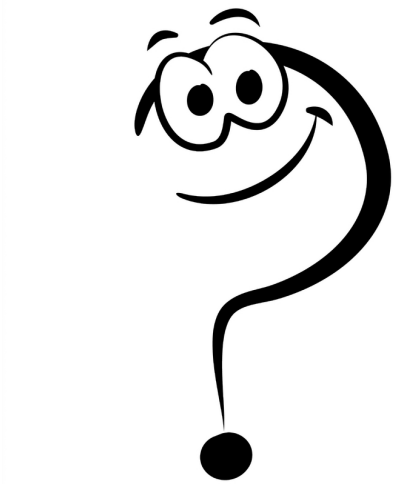
$[\otimes_m \mathcal{M}_b(\mathcal{X}_m)]^0$
$\otimes_m \mathcal{M}_b^0(\mathcal{X}_m)$
$\mathcal{I}$


$\otimes_0$-char.
char.
$\otimes$-char.
univ.
$\mathcal{I}$-char.

$\otimes_0$-char $\Longleftarrow$ $\otimes$-char $\Longleftarrow$ char $\Longleftarrow$ universal



char $\Downarrow$ $\mathcal{I}$-char

$(k_m)_{m=1}^M$ char $\overset{\text{[Sriperumbudur et al., 2011]}}{\underset{\text{[Sriperumbudur et al., 2011]}}{\rightleftarrows}}$ $(k_m)_{m=1}^M$ -universal

Results

Various Characteristic Properties of $\otimes_{m=1}^{M} k_m$

Proposition

(i) $\otimes_{m=1}^{M} k_m$: *characteristic* $\Rightarrow$ $\otimes$*-characteristic.*

(ii) $\otimes_{m=1}^{M} k_m$: $\otimes$*-characteristic* $\Rightarrow$ $\otimes_0$*-characteristic.*

(iii) $\otimes_{m=1}^{M} k_m$: $\otimes_0$*-characteristic* $\Leftrightarrow$ $(k_m)_{m=1}^{M}$ *are characteristic.*

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(iii) remains. Idea: with $k = \otimes_{m=1}^{M} k_m$, $\mathbb{F} = \otimes_{m=1}^{M} \mathbb{F}_m$,

$$\underbrace{\|\mu_k(\mathbb{F})\|_{\mathcal{H}_k}^2}_{>0} = \underbrace{\prod_{m=1}^{M}}_{\forall} \underbrace{\|\mu_{k_m}(\mathbb{F}_m)\|_{\mathcal{H}_{k_m}}^2}_{>0},$$

$\otimes_0$-characteristic $\not\Rightarrow$ even $\otimes$-characteristic

Reverse of (ii) does not hold.

Example

- $\mathcal{X}_m = \{1, 2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\{1, 2\})$, $k_m(x, x') = 2\delta_{x,x'} - 1$, $M = 2$.
- *$k_1 = k_2$: characteristic, but $k_1 \otimes k_2$ is not $\otimes$-characteristic.*
- *$k_1 \otimes k_2$ is $\mathcal{I}$-characteristic.*

Proof Idea: $k_1 \otimes k_2$: not $\otimes$-characteristic

Finite signed measures on $\mathcal{X}_m = \{1, 2\}$:

$$\mathbb{F}_1(\mathbf{a}) = a_1\delta_1 + a_2\delta_2, \qquad \mathbb{F}_2(\mathbf{b}) = b_1\delta_1 + b_2\delta_2.$$

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Goal: construct a witness $0 \neq \mathbb{F} = \mathbb{F}_1 \otimes \mathbb{F}_2 \in \otimes_{m=1}^{2} \mathcal{M}_b(\mathcal{X}_m)$ s.t.

$$0 = \mathbb{F}(\mathcal{X}_1 \times \mathcal{X}_2) = \mathbb{F}_1(\mathcal{X}_1)\mathbb{F}_2(\mathcal{X}_2),$$

$$0 = \int_{\mathcal{X}_1 \times \mathcal{X}_2} \int_{\mathcal{X}_1 \times \mathcal{X}_2} k_1(x_1, x_1')k_2(x_2, x_2')\, \mathrm{d}\mathbb{F}(x_1, x_2)\, \mathrm{d}\mathbb{F}(x_1', x_2').$$

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This gives

$$0 = (a_1 + a_2)(b_1 + b_2), \qquad 0 = (a_1 - a_2)^2(b_1 - b_2)^2.$$

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This gives

$$0 = (a_1 + a_2)(b_1 + b_2), \qquad 0 = (a_1 - a_2)^2(b_1 - b_2)^2.$$

$\Rightarrow$ Two symmetric solutions ($\mathbf{a} \neq \mathbf{0}$, $\mathbf{b} \neq \mathbf{0}$):

$$a_1 + a_2 = 0, \qquad b_1 = b_2.$$

$$a_1 = a_2, \qquad b_1 + b_2 = 0.$$

Towards $\mathcal{I}$-characteristicity

In the previous example:

$$k_1, k_2\text{: characteristic} \Rightarrow k_1 \otimes k_2\text{: } \mathcal{I}\text{-characteristic.}$$

In fact:

- this holds for any bounded kernel,
- +converse for any $M \geqslant 2$! Formally, ...

$\mathcal{I}$-characteristic Property

Proposition

(i) k_1, k_2: *characteristic* $\Rightarrow$ $k_1 \otimes k_2$: *$\mathcal{I}$-characteristic.*

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

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Proof idea:

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Proof idea:

(i) Induction: see later universality ($\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$).

(ii) If a k_m is not characteristic, witness can be constructed.

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

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&+ 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 \\
\hline
&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}
$$

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

$\mathbb{R}^d$ & Translation-invariance: All Notions Coincide

Proposition

Assume $k_m : \mathbb{R}^{d_m} \times \mathbb{R}^{d_m} \to \mathbb{R}$ are continuous, translation-invariant kernels. Then the followings are equivalent:

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

(ii) $\otimes_{m=1}^M k_m$*: $\otimes_0$-characteristic.*

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

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

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Proof idea: We already know

$$(v) \Rightarrow (iii) \Rightarrow (ii) \Leftrightarrow (i), \qquad (v) \Rightarrow (iv) \Rightarrow (i).$$

Remains: $(i) \Rightarrow (v)$.

$(k_m)_{m=1}^M$: characteristic $\Rightarrow \otimes_{m=1}^M k_m$: characteristic

- Since k_m is characteristic

$$k_m \xrightarrow{\text{Bochner thm}} \Lambda_m, \ supp(\Lambda_m) = \mathbb{R}^{d_m}.$$

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- Tensor kernel:

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- Tensor kernel:

$$\otimes_{m=1}^M k_m \xrightarrow{\text{Bochner thm}} \Lambda = \otimes_{m=1}^M \Lambda_m.$$

- $\text{supp}(\Lambda) = \times_{m=1}^M \underbrace{\text{supp}\left(\Lambda_m\right)}_{\mathbb{R}^{d_m}} = \mathbb{R}^d.$

Universality of $\otimes_{m=1}^{M} k_m$

We saw: for $M \geqslant 3$

$$(k_m)_{m=1}^{M} \text{ are characteristic } \not\Rightarrow \otimes_{m=1}^{M} k_m\text{: } \mathcal{I}\text{-characteristic.}$$

Proposition

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

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.

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

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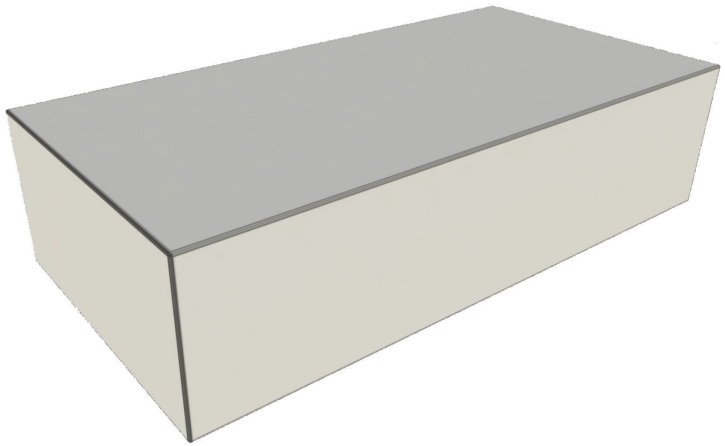
Enough:

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



Proof Idea

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

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

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$$0 = \int_{\mathcal{X}} \prod_{m=1}^{J} \chi_{B_m}(x_m) \otimes_{m=J+1}^{M} k_m(\cdot, x_m) \, \mathrm{d}\mathbb{F}(x), \ \forall B_m,$$

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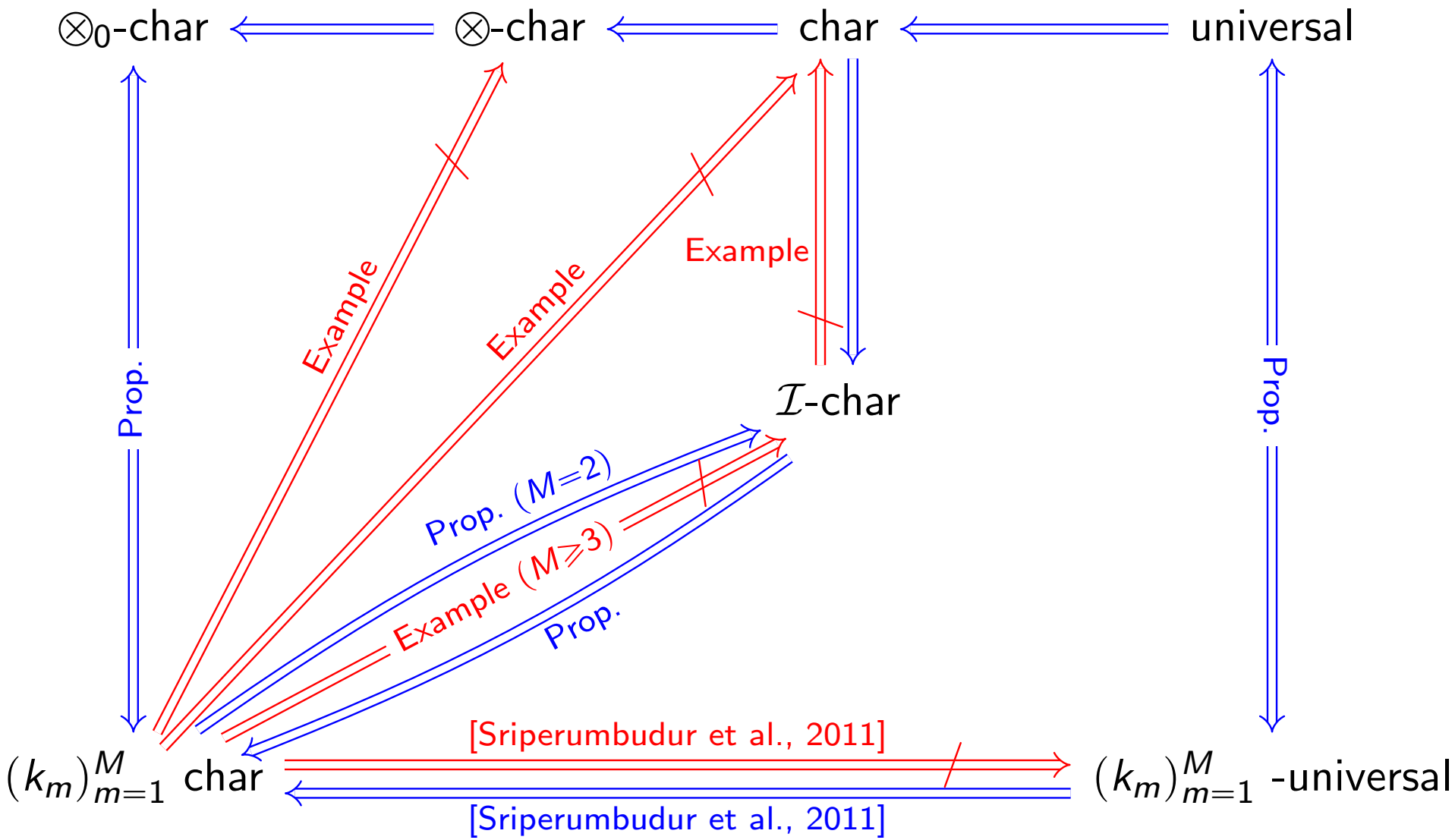
We proceed by induction ($J = 0, \ldots, M$).


$\otimes_0$-char
$\otimes$-char
char
universal
Prop.
Example
Example
Example
$\mathcal{I}$-char
Prop. (M=2)
Example ($M \geqslant 3$)
Prop.
Prop.
[Sriperumbudur et al., 2011]
$(k_m)_{m=1}^M$ char
$(k_m)_{m=1}^M$ -universal
[Sriperumbudur et al., 2011]

Summary

We studied the validness of HSIC.

- HSIC $\Rightarrow$ product structure:
  - Space: $\mathcal{X} = \times_{m=1}^{M} \mathcal{X}_m$.
  - Kernel: $k = \otimes_{m=1}^{M} k_m$.
- $\mathcal{F}$-ispd property $\Rightarrow$ complete answer in terms of k_m-s.

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- $\mathcal{F}$-ispd property $\Rightarrow$ complete answer in terms of k_m-s.
- ITE toolkit, preprint (maths $\rightarrow$ JMLR):

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

  http://arxiv.org/abs/1708.08157

Thank you for the attention!

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Blanchard, G., Deshmukh, A. A., Dogan, U., Lee, G., and Scott, C. (2017).
Domain generalization by marginal transfer learning.
Technical report.
https://arxiv.org/abs/1711.07910.


Blanchard, G., Lee, G., and Scott, C. (2011).
Generalizing from several related classification tasks to a new unlabeled sample.
In *Advances in Neural Information Processing Systems (NIPS)*, pages 2178–2186.


Fukumizu, K., Gretton, A., Sun, X., and Schölkopf, B. (2008).
Kernel measures of conditional dependence.
In *Neural Information Processing Systems (NIPS)*, pages 498–496.


Fukumizu, K., Song, L., and Gretton, A. (2013).
Kernel Bayes' rule: Bayesian inference with positive definite kernels.

Journal of Machine Learning Research, 14:3753–3783.


Gretton, A. (2015).
A simpler condition for consistency of a kernel independence test.
Technical report, University College London.
(`http://arxiv.org/abs/1501.06103`).


Gretton, A., Borgwardt, K. M., Rasch, M. J., Schölkopf, B., and Smola, A. (2012).
A kernel two-sample test.
Journal of Machine Learning Research, 13:723–773.


Gretton, A., Bousquet, O., Smola, A., and Schölkopf, B. (2005).
Measuring statistical dependence with Hilbert-Schmidt norms.
In *Algorithmic Learning Theory (ALT)*, pages 63–78.


Gretton, A., Fukumizu, K., Teo, C. H., Song, L., Schölkopf, B., and Smola, A. J. (2008).
A kernel statistical test of independence.

In *Neural Information Processing Systems (NIPS)*, pages 585–592.

Kim, B., Khanna, R., and Koyejo, O. O. (2016).
Examples are not enough, learn to criticize! criticism for interpretability.
In *Advances in Neural Information Processing Systems (NIPS)*, pages 2280–2288.

Kusano, G., Fukumizu, K., and Hiraoka, Y. (2016).
Persistence weighted Gaussian kernel for topological data analysis.
In *International Conference on Machine Learning (ICML)*, pages 2004–2013.

Lloyd, J. R., Duvenaud, D., Grosse, R., Tenenbaum, J. B., and Ghahramani, Z. (2014).
Automatic construction and natural-language description of nonparametric regression models.

In *AAAI Conference on Artificial Intelligence*, pages 1242–1250.


Lyons, R. (2013).
Distance covariance in metric spaces.
The Annals of Probability, 41:3284–3305.


Mooij, J. M., Peters, J., Janzing, D., Zscheischler, J., and Schölkopf, B. (2016).
Distinguishing cause from effect using observational data: Methods and benchmarks.
Journal of Machine Learning Research, 17:1–102.


Muandet, K., Fukumizu, K., Dinuzzo, F., and Schölkopf, B. (2011).
Learning from distributions via support measure machines.
In *Neural Information Processing Systems (NIPS)*, pages 10–18.


Muandet, K., Fukumizu, K., Sriperumbudur, B., and Schölkopf, B. (2017).

Kernel mean embedding of distributions: A review and beyond.
Foundations and Trends in Machine Learning, 10(1-2):1–141.


Park, M., Jitkrittum, W., and Sejdinovic, D. (2016).
K2-ABC: Approximate Bayesian computation with kernel embeddings.
In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 51, pages 51:398–407.


Pfister, N., Bühlmann, P., Schölkopf, B., and Peters, J. (2017).
Kernel-based tests for joint independence.
Journal of the Royal Statistical Society: Series B (Statistical Methodology).


Schölkopf, B., Muandet, K., Fukumizu, K., Harmeling, S., and Peters, J. (2015).
Computing functions of random variables via reproducing kernel Hilbert space representations.

Statistics and Computing, 25(4):755–766.


Sejdinovic, D., Sriperumbudur, B. K., Gretton, A., and Fukumizu, K. (2013).
Equivalence of distance-based and RKHS-based statistics in hypothesis testing.
Annals of Statistics, 41:2263–2291.


Song, L., Gretton, A., Bickson, D., Low, Y., and Guestrin, C. (2011).
Kernel belief propagation.
In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, pages 707–715.


Song, L., Smola, A., Gretton, A., Bedo, J., and Borgwardt, K. (2012).
Feature selection via dependence maximization.
Journal of Machine Learning Research, 13:1393–1434.


Sriperumbudur, B. K., Gretton, A., Fukumizu, K., Schölkopf, B., and Lanckriet, G. R. (2010).

Hilbert space embeddings and metrics on probability measures.

Journal of Machine Learning Research, 11:1517–1561.

Steinwart, I. (2001).
On the influence of the kernel on the consistency of support vector machines.
Journal of Machine Learning Research, 6(3):67–93.

Strobl, E. V., Visweswaran, S., and Zhang, K. (2017).
Approximate kernel-based conditional independence tests for fast non-parametric causal discovery.
Technical report.
`https://arxiv.org/abs/1702.03877`.

Szabó, Z., Sriperumbudur, B., Póczos, B., and Gretton, A. (2016).
Learning theory for distribution regression.
Journal of Machine Learning Research, 17(152):1–40.


Waegeman, W., Pahikkala, T., Airola, A., Salakoski, T., Stock, M., and Baets, B. D. (2012).
A kernel-based framework for learning graded relations from data.
IEEE Transactions on Fuzzy Systems, 20:1090–1101.


Yamada, M., Umezu, Y., Fukumizu, K., and Takeuchi, I. (2016).
Post selection inference with kernels.
Technical report.
(`https://arxiv.org/abs/1610.03725`).


Zhang, K., Schölkopf, B., Muandet, K., and Wang, Z. (2013).
Domain adaptation under target and conditional shift.
Journal of Machine Learning Research, 28(3):819–827.