

Characterizing Independence with Tensor Product Kernels

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Motivation: 'Classical' Information Theory

- Kullback-Leibler divergence:

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

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

Euclidean Space \rightarrow Inner Product \rightarrow Kernel

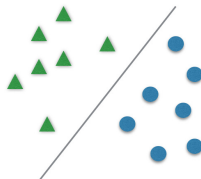
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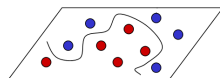
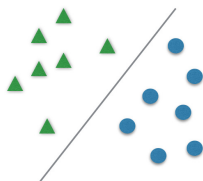
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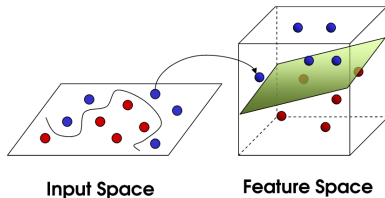
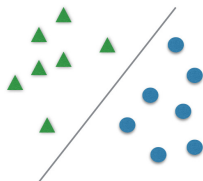


Input Space

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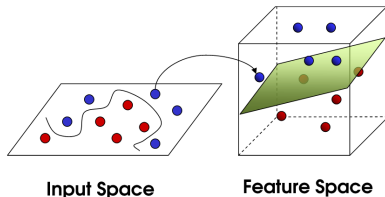
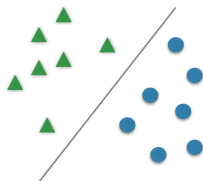
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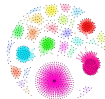


2 Representation of distributions:

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

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

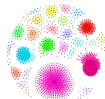
Diverse Set of Domains, Kernel Examples



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

$$\begin{aligned} k_p(\mathbf{x}, \mathbf{y}) &= (\langle \mathbf{x}, \mathbf{y} \rangle + \gamma)^p, & k_G(\mathbf{x}, \mathbf{y}) &= e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2^2}, \\ k_e(\mathbf{x}, \mathbf{y}) &= e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2}, & k_C(\mathbf{x}, \mathbf{y}) &= 1 + \frac{1}{\gamma \|\mathbf{x} - \mathbf{y}\|_2^2}. \end{aligned}$$

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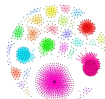


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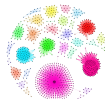


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- \mathcal{X} = time-series: dynamic time-warping.
- \mathcal{X} = trees, graphs, dynamical systems, sets, permutations, ...

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- Mean embedding:

$$\mu(\mathbb{P}) := \int_{\mathcal{X}} \varphi(x) \, d\mathbb{P}(x)$$

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$$\text{MMD}_k(\mathbb{P}, \mathbb{Q}) := \|\mu_k(\textcolor{red}{\mathbb{P}}) - \mu_k(\textcolor{blue}{\mathbb{Q}})\|_{\mathcal{H}_k}.$$

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

Ingredients

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- HSIC $\Rightarrow \mathcal{X} = \times_{m=1}^M \mathcal{X}_m$: product space.
- \mathcal{X}_m : different modalities \rightarrow images, texts, audio, ...



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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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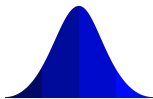
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$$k(\cdot, b) \in \mathcal{H},$$



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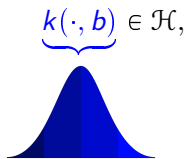
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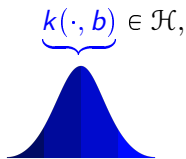
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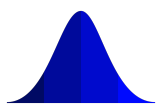
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Equivalent definitions. We represent distributions in an RKHS...

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- 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 $k = \bigotimes_{m=1}^M k_m$:

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Applications:

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

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Wanted

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

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

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

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

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Theorem ([Sriperumbudur et al., 2010])

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

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

| kernel name | k_0 | $\hat{k}_0(\omega)$ | $\text{supp}(\hat{k}_0)$ |
|--------------------|--|---|-------------------------------------|
| 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 | $*^{2n+2} \chi_{[-\frac{1}{2}, \frac{1}{2}]}(x)$ | $\frac{4^{n+1}}{\sqrt{2\pi}} \frac{\sin^{2n+2}(\frac{\omega}{2})}{\omega^{2n+2}}$ | \mathbb{R} |
| Sinc | $\frac{\sin(\sigma x)}{x}$ | $\sqrt{\frac{\pi}{2}} \chi_{[-\sigma, \sigma]}(\omega)$ | $[-\sigma, \sigma]$ |
| Fejér | $\frac{1}{n+1} \frac{\sin^2(\frac{(n+1)x}{2})}{\sin^2(\frac{x}{2})}$ | $\sqrt{2\pi} \sum_{j=-n}^n \left(1 - \frac{ j }{n+1}\right) \delta(\omega - j)$ | $\{0, \pm 1, \pm 2, \dots, \pm n\}$ |

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

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Challenge

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

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

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Extension to $M \geq 2$.

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Extension to $M \geq 2$.

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.

$$\|\mu_{\mathbb{F}}\|_{\mathcal{H}_k}^2 > 0, \quad \forall \underbrace{\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) \setminus \{0\}}_{\mathcal{F}_1} \quad \mathbb{F}(\mathcal{X}) = 0.$$

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- We saw: k is **universal** iff.

$$\|\mu_{\mathbb{F}}\|_{\mathcal{H}_k}^2 > 0, \quad \forall \underbrace{\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) \setminus \{0\}}_{\mathcal{F}_2}.$$

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

$$\begin{aligned} \|\mu_k(\mathbb{F})\|_{\mathcal{H}_k}^2 &> 0, \quad \forall \mathbb{F} \in \mathcal{F} \setminus \{0\}, \text{ equivalently} \\ \mu_k(\mathbb{F}) &= 0 \Rightarrow \mathbb{F} = 0 \quad (\mathbb{F} \in \mathcal{F}). \end{aligned}$$

Examples

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

$$\begin{array}{ccc}
 \subseteq & \subseteq & [\mathcal{M}_b(\mathcal{X})]^0 \subseteq \mathcal{M}_b(\mathcal{X}) . \\
 & & \text{UI} \\
 \Leftarrow & \Leftarrow & \text{characteristic} \Leftarrow \text{universal} . \\
 & & \Downarrow
 \end{array}$$

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| $[\bigotimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)]^0$ | \bigotimes -characteristic |

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

UI

\mathcal{I}

$$\Leftarrow \bigotimes\text{-characteristic} \Leftarrow \text{characteristic} \Leftarrow \text{universal} .$$



\mathcal{I} -characteristic

Examples

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| $[\bigotimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)]^0$ | \bigotimes -characteristic |
| $\bigotimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m)$ | \bigotimes_0 -characteristic |

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

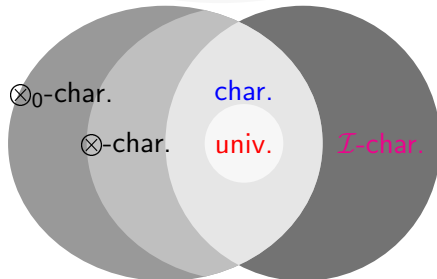
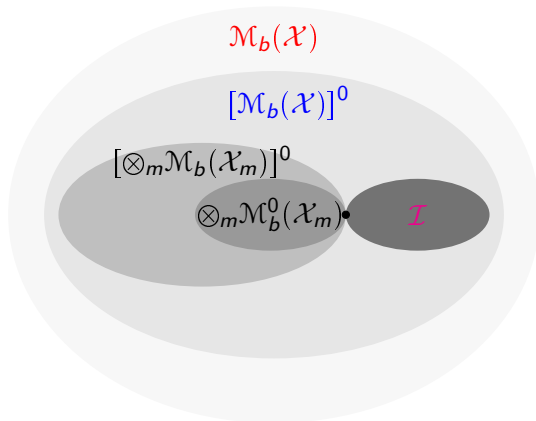
UI

\mathcal{I}

$$\bigotimes_0\text{-characteristic} \Leftarrow \bigotimes\text{-characteristic} \Leftarrow \text{characteristic} \Leftarrow \text{universal}.$$



\mathcal{I} -characteristic



$\otimes_0\text{-char}$ \longleftrightarrow $\otimes\text{-char}$ \longleftrightarrow char \longleftrightarrow universal



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

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

Results

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

Proposition

- (i) $\bigotimes_{m=1}^M k_m$: *characteristic* \Rightarrow \bigotimes -*characteristic*.
- (ii) $\bigotimes_{m=1}^M k_m$: \bigotimes -*characteristic* \Rightarrow \bigotimes_0 -*characteristic*.
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(iii) remains. Idea: with $k = \bigotimes_{m=1}^M k_m$, $\mathbb{F} = \bigotimes_{m=1}^M \mathbb{F}_m$,

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

\otimes_0 -characteristic \nRightarrow 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 $\mathcal{X}_m = \{1, 2\}$:

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

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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.

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

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

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This gives

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

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

$$\begin{aligned} a_1 + a_2 &= 0, & b_1 &= b_2. \\ a_1 &= a_2, & b_1 + b_2 &= 0. \end{aligned}$$

In the previous example:

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

In fact:

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

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

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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 $\Rightarrow \bigotimes_{m=1}^3 k_m$: \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.
 - $\bigotimes_{m=1}^3 k_m$: is **not** \mathcal{I} -characteristic. Witness:

$$\begin{array}{cccc} p_{1,1,1} = \frac{1}{5}, & p_{1,1,2} = \frac{1}{10}, & p_{1,2,1} = \frac{1}{10}, & p_{1,2,2} = \frac{1}{10}, \\ p_{2,1,1} = \frac{1}{5}, & p_{2,1,2} = \frac{1}{10}, & p_{2,2,1} = \frac{1}{10}, & p_{2,2,2} = \frac{1}{10}. \end{array}$$

Non- \mathcal{I} -characteristicity: Analytical Solution

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

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

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

Proposition

Assume $k_m : \mathbb{R}^{d_m} \times \mathbb{R}^{d_m} \rightarrow \mathbb{R}$ 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.
- (v) $\otimes_{m=1}^M k_m$: characteristic.

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Proof idea: We already know

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

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

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

- Since k_m is characteristic

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

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- Tensor kernel:

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

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

We saw: for $M \geq 3$

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

Proposition

$\bigotimes_{m=1}^M k_m$: *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.

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

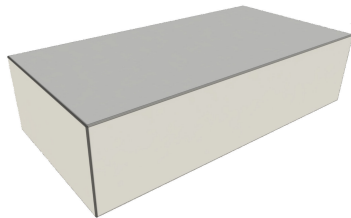
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$$\mu(\mathbb{F}) = 0 \stackrel{?}{\Rightarrow} \mathbb{F} = 0.$$

Enough:

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



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

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

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

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

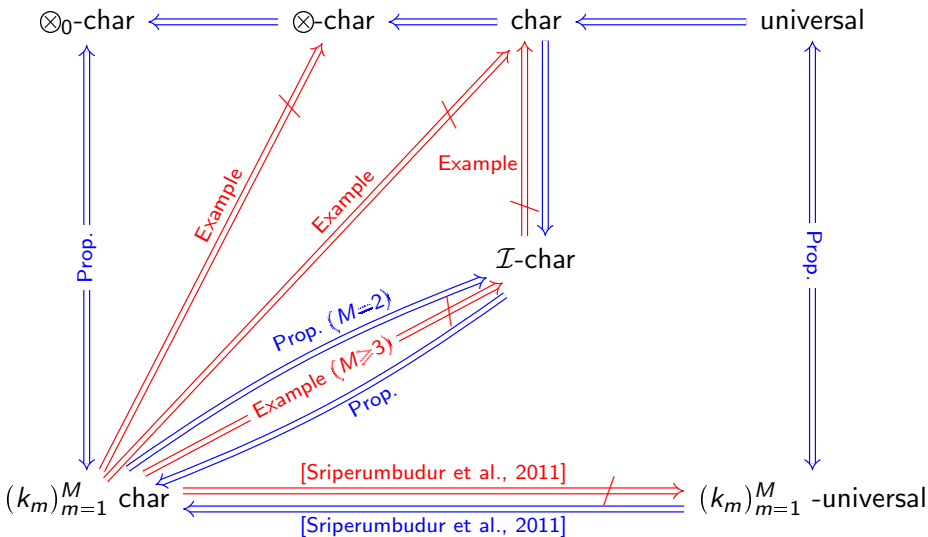
$$0 = \mathbb{F}\left(\times_{m=1}^M B_m\right) = \int_{\mathcal{X}} \times_{m=1}^M \chi_{B_m}(x_m) d\mathbb{F}(x), \quad \forall B_m.$$

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

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

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

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



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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- 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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