

Kernel Cumulant Embedding

Zoltán Szabó @ Department of Statistics, LSE

Joint work with:

- Patric Bonnier, Harald Oberhauser
- @ Mathematical Institute, University of Oxford.



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- Moments $\mu(\gamma) := \left(\mu^{(i)}(\gamma) \right)_{i \in \mathbb{N}}$:

$$\mu^{(i)}(\gamma) := \mathbb{E} \left(X^i \right) \in \mathbb{R},$$

$$\mu^{(0)}(\gamma) := 1.$$

Moments and cumulants [McCullagh, 2018] on $\mathbb{R} \ni X \sim \gamma$

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- Cumulants $\kappa(\gamma) = (\kappa^{(i)}(\gamma))_{i \in \mathbb{N}}$: from the **moment-generating function**

$$\sum_{i \in \mathbb{N}} \kappa^{(i)}(\gamma) \frac{\theta^i}{i!} = \log \left(\sum_{i \in \mathbb{N}} \mu^{(i)}(\gamma) \frac{\theta^i}{i!} \right).$$

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$$\kappa^{(1)}(\gamma) = \mathbb{E}(X)$$

mean

$$\kappa^{(2)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^2$$

variance

$$\kappa^{(3)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^3$$

3rd central moment

$$\kappa^{(4)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^4 - 3 [\mathbb{E}(X - \mathbb{E}X)^2]^2$$

$$\kappa^{(5)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^5 - 10\mathbb{E}(X - \mathbb{E}X)^3\mathbb{E}(X - \mathbb{E}X)^2$$

Unzipping cumulants on \mathbb{R} : (known) combinatorial description [Speed, 1983, Speed, 1984]

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where $X, X' \sim \gamma$, independent.

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$\{\{1, 2, 3\}\}, \{\{1, 2\}, \{3\}\},$
 $\{\{1, 3\}, \{2\}\}, \{\{2, 3\}, \{1\}\},$
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...

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Question

What are the **weights** in front of the moments?

Unzipping cumulants on \mathbb{R} : the weights

m	elements of $\pi \in P(m)$	$ \pi $	c_π
1	{1}	1	1
2	{1,2}	1	1
	{1},{2}	2	-1
3	{1,2,3}	1	1
	{1,2}, {3}	2	-1
	{1,3}, {2}	2	-1
	{2,3}, {1}	2	-1
	{1}, {2}, {3}	3	2

with $P(m) :=$ all partitions of $[m]$, $c_\pi = (-1)^{|\pi|-1}(|\pi| - 1)!$

Motivation, i.e. one reason why one likes cumulants

Moment and cumulants on \mathbb{R}^d

Change $\mathbb{E}(X^i) \in \mathbb{R}$ to $\mathbb{E}[X_1^{i_1} \cdots X_d^{i_d}] \in \mathbb{R}$ ($\mathbf{i} \in \mathbb{N}^d$). log, $P(m)$: \checkmark

Known theorem [Billingsley, 2012]

Let γ be a probability measure on a bounded subset of \mathbb{R}^d with cumulants $\kappa(\gamma)$ and let $(X_1, \dots, X_d) \sim \gamma$. Then

- 1 $\gamma \mapsto \kappa(\gamma)$ is injective.
- 2 X_1, \dots, X_d are independent $\Leftrightarrow \kappa^{\mathbf{i}}(\gamma) = 0$ for all $\mathbf{i} \in \mathbb{N}_+^d$.

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Motivation

- 1 Various data types, nonlinear features: kernels.
- 2 Linear: not even characteristic (see MMD and HSIC).
- 3 Computable estimators.

Lifting

$$(X_1, \dots, X_d) \in \times_{j=1}^d \mathcal{X}_j \rightarrow (\Phi_1(X_1), \dots, \Phi_d(X_d)) \in \times_{j=1}^d \mathcal{H}_{k_j}.$$

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Ingredients:

① Moments: swap out $\mathbb{E} [X_1^{i_1} \dots X_d^{i_d}] \in \mathbb{R}$ to

$$\mathbb{E} \left[[\Phi_1(X_1)]^{\otimes i_1} \otimes \dots \otimes [\Phi_d(X_d)]^{\otimes i_d} \right] \in \mathcal{H}_{k_1}^{\otimes i_1} \otimes \dots \otimes \mathcal{H}_{k_d}^{\otimes i_d}.$$

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- 2 From moments to cumulants:
 - log on tensor algebras, or
 - combinatorial description of cumulants (\leftarrow a bit simpler, but \Leftrightarrow).

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- 2 From moments to cumulants:
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 - combinatorial description of cumulants (\leftarrow a bit simpler, but \Leftrightarrow).
- 3 Computation: by the 'expected kernel trick' (V-statistics).

Kernel (generalization of $\mathbf{a}^\top \mathbf{b}$), RKHS

[Aronszajn, 1950, Steinwart and Christmann, 2008]

- Def-1 (feature space):

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

- Def-2 (reproducing kernel):

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

- Def-3 (Gram matrix): $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \in \mathbb{R}^{n \times n} \succeq \mathbf{0}$.

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Notes

- $k \xleftrightarrow{1:1} \mathcal{H}_k = \overline{\text{Span}(k(\cdot, x) : x \in \mathcal{X})}$: Fourier analysis, approximation with polynomials, splines, ...
- Examples: $k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^p$, $k_G(\mathbf{x}, \mathbf{y}) = e^{-c\|\mathbf{x}-\mathbf{y}\|_2^2}$.
- 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, Balanca and Herbin, 2012, Fellmann et al., 2023], **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].

Mean embedding

- Mean embedding (integral; [Berlinet and Thomas-Agnan, 2004, Smola et al., 2007]):

$$\mu_k(\gamma) := \int_{\mathcal{X}} \underbrace{k(\cdot, x)}_{\Phi(x) \in \mathcal{H}_k} d\gamma(x) \in \mathcal{H}_k.$$

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$$\text{MMD}_k(\gamma, \eta) := \|\mu_k(\gamma) - \mu_k(\eta)\|_{\mathcal{H}_k}.$$

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- Hilbert-Schmidt independence criterion [Gretton et al., 2005] ($d=2$), [Quadrianto et al., 2009, Sejdinovic et al., 2013a] ($d \geq 3$), $k := \otimes_{j=1}^d k_j$:

$$\text{HSIC}_k(\gamma) := \text{MMD}_k(\gamma, \otimes_{j=1}^d \gamma | x_j)$$

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$$\begin{aligned} \text{HSIC}_k(\gamma) &:= \text{MMD}_k\left(\gamma, \otimes_{j=1}^d \gamma|_{\mathcal{X}_j}\right), \\ &= \left\| \underbrace{\mu_{\otimes_{j=1}^d k_j}(\gamma) - \otimes_{j=1}^d \mu_{k_j}(\gamma|_{\mathcal{X}_j})}_{\text{cross-covariance operator}} \right\|_{\mathcal{H}_k}. \end{aligned}$$

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Notes before clarification of what $\otimes_{j=1}^d k_j$ and $\otimes_{j=1}^d \mu_{k_j}(\gamma|_{\mathcal{X}_j})$ are.

- M MD:

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- \Leftrightarrow **energy distance** [Baringhaus and Franz, 2004, Székely and Rizzo, 2004, Székely and Rizzo, 2005], a.k.a. N-distance [Zinger et al., 1992, Klebanov, 2005].

† [Sejdinovic et al., 2013b].

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- HSIC ($d = 2$) $\overset{\dagger}{\Leftrightarrow}$ distance covariance

[Székely et al., 2007, Székely and Rizzo, 2009, Lyons, 2013].

\dagger [Sejdinovic et al., 2013b].

Interaction measures: $d = 3$, $(X_1, X_2, X_3) \in \mathcal{X}_1 \times \mathcal{X}_2 \times \mathcal{X}_3$

$(X_1, X_2, X_3) \sim \gamma$, Lancaster interaction measure [Lancaster, 1969]

$$L(\gamma) := \gamma - \gamma|_{\mathcal{X}_1\mathcal{X}_2} \otimes \gamma|_{\mathcal{X}_3} - \gamma|_{\mathcal{X}_2\mathcal{X}_3} \otimes \gamma|_{\mathcal{X}_1} - \gamma|_{\mathcal{X}_1\mathcal{X}_3} \otimes \gamma|_{\mathcal{X}_2} \\ + 2\gamma|_{\mathcal{X}_1} \otimes \gamma|_{\mathcal{X}_2} \otimes \gamma|_{\mathcal{X}_3}.$$

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In case of **some factorization** (\neq):

$$(X_1, X_2) \perp\!\!\!\perp X_3 \vee (X_1, X_3) \perp\!\!\!\perp X_2 \vee (X_2, X_3) \perp\!\!\!\perp X_1 \Rightarrow L(\gamma) = 0.$$

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Idea [Sejdicinovic et al., 2013a], acceleration [Kalinke and Szabó, 2023]

$$\left\| \mu_{k_{X_1} \otimes k_{X_2} \otimes k_{X_3}}(L(\gamma)) \right\|_{\mathcal{H}_{k_{X_1}} \otimes \mathcal{H}_{k_{X_2}} \otimes \mathcal{H}_{k_{X_3}}}^2 \stackrel{?}{>} 0 \Rightarrow \text{no factorization.}$$

Interaction measures: $d \geq 2$, $X = (X_j)_{j=1}^d \in \times_{j=1}^d \mathcal{X}_j$

- Partition measure: $\pi \in P(d)$, $b = |\pi|$,

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- Weights: $c_\pi = (-1)^{|\pi|-1} (|\pi| - 1)!$.
- Streitberg interaction [Streitberg, 1990], $X \sim \gamma$:

$$S(\gamma) = \sum_{\pi \in P(d)} c_\pi \gamma_\pi$$

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- One could **kernelize** it (analogously to Lancaster interaction):

$$\left\| \mu_{\otimes_{j=1}^d k_j}(S(\gamma)) \right\|_{\otimes_{j=1}^d \mathcal{H}_{k_j}}^2.$$

We now return to the meaning of

$$\otimes_{j=1}^d k_j \text{ and } \otimes_{j=1}^d \mu_{k_j}(\gamma|_{\mathcal{X}_j}).$$

Tensor product: $\otimes_{j=1}^d \mathbf{a}_j$

- If $\mathbf{a} \in \mathbb{R}^{n_1}$, $\mathbf{b} \in \mathbb{R}^{n_2}$:

$$\mathbb{R} \ni \mathbf{v}^\top (\mathbf{a}\mathbf{b}^\top) \mathbf{w} = (\mathbf{v}^\top \mathbf{a}) (\mathbf{b}^\top \mathbf{w}) = \langle \mathbf{a}, \mathbf{v} \rangle_{\mathbb{R}^{n_1}} \langle \mathbf{b}, \mathbf{w} \rangle_{\mathbb{R}^{n_2}},$$

$\mathbf{a} \otimes \mathbf{b} := \mathbf{a}\mathbf{b}^\top$ is an $\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \rightarrow \mathbb{R}$ bilinear form.

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- For $a \in \mathcal{H}_1$, $b \in \mathcal{H}_2$ Hilbert spaces, i.e. for $d = 2$:

$$(a \otimes b)(v, w) := \langle a, v \rangle_{\mathcal{H}_1} \langle b, w \rangle_{\mathcal{H}_2}.$$

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- If $\mathbf{a} \in \mathbb{R}^{n_1}$, $\mathbf{b} \in \mathbb{R}^{n_2}$:

$$\mathbb{R} \ni \mathbf{v}^\top (\mathbf{a}\mathbf{b}^\top) \mathbf{w} = (\mathbf{v}^\top \mathbf{a}) (\mathbf{b}^\top \mathbf{w}) = \langle \mathbf{a}, \mathbf{v} \rangle_{\mathbb{R}^{n_1}} \langle \mathbf{b}, \mathbf{w} \rangle_{\mathbb{R}^{n_2}},$$

$\mathbf{a} \otimes \mathbf{b} := \mathbf{a}\mathbf{b}^\top$ is an $\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \rightarrow \mathbb{R}$ bilinear form.

- For $\mathbf{a} \in \mathcal{H}_1$, $\mathbf{b} \in \mathcal{H}_2$ Hilbert spaces, i.e. for $d = 2$:

$$(\mathbf{a} \otimes \mathbf{b})(\mathbf{v}, \mathbf{w}) := \langle \mathbf{a}, \mathbf{v} \rangle_{\mathcal{H}_1} \langle \mathbf{b}, \mathbf{w} \rangle_{\mathcal{H}_2}.$$

- For $d \geq 2$ and $\mathbf{a}_j \in \mathcal{H}_j$,

$$\left(\otimes_{j=1}^d \mathbf{a}_j \right) (\mathbf{b}_1, \dots, \mathbf{b}_d) := \prod_{j=1}^d \langle \mathbf{a}_j, \mathbf{b}_j \rangle_{\mathcal{H}_j}.$$

Tensor product: $\otimes_{j=1}^d \mathcal{H}_j$

$$\otimes_{j=1}^d \mathcal{H}_j := \overline{\text{Span}(\otimes_{j=1}^d a_j : a_j \in \mathcal{H}_j)}.$$

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$\xrightarrow{\text{spec.}}$ The tensor product of RKHSs is an RKHS

[Berlinet and Thomas-Agnan, 2004]

$$\mathcal{H}_k = \otimes_{j=1}^d \mathcal{H}_{k_j},$$

$$k(x, x') := (\otimes_{j=1}^d k_j)(x, x') := \prod_{j=1}^d \underbrace{k_j(x_j, x'_j)}_{\text{coordinate-wise similarity}}.$$

Validness:

- $\text{MMD}_k(\gamma, \eta) = 0 \Leftrightarrow \gamma = \eta$: k is **characteristic**
[Fukumizu et al., 2008, Sriperumbudur et al., 2010].

Validness of MMD & HSIC, their estimation

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- $\text{HSIC}_k(\gamma) = 0 \Leftrightarrow \gamma = \otimes_{j=1}^d \gamma|_{\mathcal{X}_j}$ \leftarrow [Szabó and Sriperumbudur, 2018]
 k_j -s are **universal** [Steinwart, 2001, Micchelli et al., 2006].

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Properties:

- 1 Injectivity of μ_k on **probability** / **finite signed** measures, so
universal \Rightarrow **characteristic**.
- 2 Easy-to-estimate: expected kernel trick

$$\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} = \int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) d\gamma(x) d\eta(y).$$

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, Schrab et al., 2022, Hagrass et al., 2022, Zhang et al., 2022], and its **differential private** variant [Raj et al., 2019]; **independence** [Gretton et al., 2008, Pfister et al., 2018, Jitkrittum et al., 2017a, Albert et al., 2022] and **goodness-of-fit testing** [Jitkrittum et al., 2017b, Balasubramanian et al., 2021, Baum et al., 2022], **causal discovery** [Mooij et al., 2016, Pfister et al., 2018, Chakraborty and Zhang, 2019, Schölkopf et al., 2021], **learning fair representations** [Deka and Sutherland, 2023],
- **feature selection** [Camps-Valls et al., 2010, Song et al., 2012, Wang et al., 2022] $\xrightarrow{\text{app.}}$ **biomarker detection** [Climente-González et al., 2019], **wind power prediction** [Bouche et al., 2023], **clustering** [Song et al., 2007, Climente-González et al., 2019],
- **domain adaptation** [Zhang et al., 2013], **-generalization** [Blanchard et al., 2021], **change-point detection** [Harchaoui and Cappé, 2007, Kalinke et al., 2023], **post selection inference** [Yamada et al., 2018], **sensitivity analysis** [da Veiga, 2021, Fellmann et al., 2023],
- **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], **Bayesian optimization** [Buathong et al., 2020],
- **topological data analysis** [Kusano et al., 2016], **learning on distributions** [Sutherland, 2016]: **classification** [Muandet et al., 2011, Lopez-Paz et al., 2015, Zaheer et al., 2017], **regression** [Szabó et al., 2016, Sutherland et al., 2016, Law et al., 2018, Fang et al., 2020, Mücke, 2021],
- **generative adversarial networks** [Dziugaite et al., 2015, Li et al., 2015, Sutherland et al., 2017, Binkowski et al., 2018], understanding the **dynamics of complex dynamical systems** [Klus et al., 2019, Klus et al., 2020],
- **functional data analysis** [Wynne and Nagy, 2021, Wynne and Duncan, 2022], ...

- From now:

- $X = (X_j)_{j=1}^d \in \times_{j=1}^d \mathcal{X}_j$, $X \sim \gamma$,
- kernels $k_j : \mathcal{X}_j \times \mathcal{X}_j \rightarrow \mathbb{R}$, $j \in [d]$,
- lifting $\Phi(X) = (\Phi_j(X_j))_{j=1}^d$ with $\Phi_j(x_j) := k_j(\cdot, x_j)$,
- RKHS $\mathcal{H}^{\otimes i} := \mathcal{H}_{k_1}^{\otimes i_1} \otimes \cdots \otimes \mathcal{H}_{k_d}^{\otimes i_d}$ with kernel $k^{\otimes i} := k_1^{\otimes i_1} \otimes \cdots \otimes k_d^{\otimes i_d}$, and feature

$$\Phi^{\otimes i}(X) := [\Phi_1(X_1)]^{\otimes i_1} \otimes \cdots \otimes [\Phi_d(X_d)]^{\otimes i_d}.$$

Kernelized moments – towards kernelized cumulants

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$$\Phi^{\otimes \mathbf{i}}(X) := [\Phi_1(X_1)]^{\otimes i_1} \otimes \cdots \otimes [\Phi_d(X_d)]^{\otimes i_d}.$$

- Moment sequence:

$$\mu(\gamma) = \left(\mu^{\mathbf{i}}(\gamma) \right)_{\mathbf{i} \in \mathbb{N}^d}, \quad \mu^{\mathbf{i}}(\gamma) := \mathbb{E} \left[\Phi^{\otimes \mathbf{i}}(X) \right] \in \mathcal{H}^{\otimes \mathbf{i}}.$$

Kernelized cumulants: examples first, analogous to \mathbb{R}

- $d = 1, m \in [3]: X \sim \gamma,$

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- $d = 1, m \in [3]$: $X, X' \sim \gamma$, independent,

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$$\begin{aligned} \kappa_k^{(3)}(\gamma) &= \mathbb{E}[\Phi^{\otimes 3}(X)] - \mathbb{E}[\Phi(X) \otimes \Phi(X) \otimes \Phi(X')] \\ &\quad - \mathbb{E}[\Phi(X) \otimes \Phi(X') \otimes \Phi(X)] - \mathbb{E}[\Phi(X') \otimes \Phi(X) \otimes \Phi(X)] \\ &\quad + 2\mathbb{E}^{\otimes 3}[\Phi(X)]. \end{aligned}$$

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- $d = 2, m = 2$: $(X_1, X_2) \sim \gamma$,

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$$\kappa_{k_1, k_2}^{(0,2)}(\gamma) = \mathbb{E}[\Phi_2^{\otimes 2}(X_2)] - \mathbb{E}^{\otimes 2}[\Phi_2(X_2)].$$

Wanted: repetition and partitioning. **Weights**: as before (c_π).

Kernelized cumulants: $X \sim \gamma$ prob. measure on $\times_{j=1}^d \mathcal{X}_j$

- Repetition (diagonal measure): $\mathbf{i} \in \mathbb{N}^d$,

$$\gamma^{\mathbf{i}} := \text{Law}(\underbrace{X_1, \dots, X_1}_{i_1 \text{ times}}, \underbrace{X_2, \dots, X_2}_{i_2 \text{ times}}, \dots, \underbrace{X_d, \dots, X_d}_{i_d \text{ times}}).$$

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⇒ expected kernel trick is applicable

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Theorem

- Assume:
 - γ, η : probability measures on $\times_{j=1}^d \mathcal{X}_j$,
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- Then, $\gamma = \eta \Leftrightarrow \kappa_{k_1, \dots, k_d}(\gamma) = \kappa_{k_1, \dots, k_d}(\eta)$, and

$$\begin{aligned} d^i(\gamma, \eta) &:= \|\kappa_{k_1, \dots, k_d}^i(\gamma) - \kappa_{k_1, \dots, k_d}^i(\eta)\|_{\mathcal{H}^{\otimes i}}^2 \\ &= \sum_{\pi, \tau \in P(m)} c_\pi c_\tau \left[\mathbb{E}_{\gamma_\pi^i \otimes \gamma_\tau^i} k^{\otimes i}((X_1, \dots, X_m), (Y_1, \dots, Y_m)) \right. \\ &\quad \left. + \mathbb{E}_{\eta_\pi^i \otimes \eta_\tau^i} k^{\otimes i}((X_1, \dots, X_m), (Y_1, \dots, Y_m)) \right. \\ &\quad \left. - 2\mathbb{E}_{\gamma_\pi^i \otimes \eta_\tau^i} k^{\otimes i}((X_1, \dots, X_m), (Y_1, \dots, Y_m)) \right]. \end{aligned}$$

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$$\|\kappa_{k_1, \dots, k_d}^{\mathbf{i}}(\gamma)\|_{\mathcal{H}^{\otimes \mathbf{i}}}^2 = \sum_{\pi, \tau \in P(m)} c_{\pi} c_{\tau} \mathbb{E}_{\gamma_{\pi}^{\mathbf{i}} \otimes \gamma_{\tau}^{\mathbf{i}}} k^{\otimes \mathbf{i}}((X_j)_{j=1}^m, (Y_j)_{j=1}^m),$$

where $m = \deg(\mathbf{i})$.

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where $m = \deg(\mathbf{i})$.

Estimation in both cases

$\mathbb{E} k^{\otimes \mathbf{i}}((X_1, \dots, X_m), (Y_1, \dots, Y_m)) \Rightarrow V\text{-statistics } \checkmark$

Distance between kernel variance embeddings

- By our theorem: if $\gamma = \eta$, then $d^{(2)}(\gamma, \eta) = 0$.
- V-statistic estimator of $d^{(2)}(\gamma, \eta)$:

$$\frac{1}{N^2} \text{Tr}[(\mathbf{K}_x \mathbf{J}_N)^2] + \frac{1}{M^2} \text{Tr}[(\mathbf{K}_y \mathbf{J}_M)^2] - \frac{2}{NM} \text{Tr}[\mathbf{K}_{xy} \mathbf{J}_M \mathbf{K}_{xy}^\top \mathbf{J}_N],$$

with $(x_n)_{n=1}^N \stackrel{\text{i.i.d.}}{\sim} \gamma$, $(y_m)_{m=1}^M \stackrel{\text{i.i.d.}}{\sim} \eta$, $\mathbf{K}_x = [k(x_i, x_j)]_{i,j=1}^N$,
 $\mathbf{K}_y = [k(y_i, y_j)]_{i,j=1}^M$, $\mathbf{K}_{x,y} = [k(x_i, y_j)]_{i,j=1}^{N,M}$, $\mathbf{J}_n = \mathbf{I}_n - \mathbf{H}_n = \mathbf{I}_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top$.

Distance between kernel variance/skewness embeddings

- By our theorem: if $\gamma = \eta$, then $d^{(2)}(\gamma, \eta) = 0$.
- V-statistic estimator of $d^{(2)}(\gamma, \eta)$:

$$\frac{1}{N^2} \text{Tr}[(\mathbf{K}_x \mathbf{J}_N)^2] + \frac{1}{M^2} \text{Tr}[(\mathbf{K}_y \mathbf{J}_M)^2] - \frac{2}{NM} \text{Tr}[\mathbf{K}_{xy} \mathbf{J}_M \mathbf{K}_{xy}^\top \mathbf{J}_N],$$

with $(x_n)_{n=1}^N \stackrel{\text{i.i.d.}}{\sim} \gamma$, $(y_m)_{m=1}^M \stackrel{\text{i.i.d.}}{\sim} \eta$, $\mathbf{K}_x = [k(x_i, x_j)]_{i,j=1}^N$,
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Time complexity

Quadratic as MMD.

- $d^{(3)}(\gamma, \eta)$: similarly; quadratic time.

Cross-skewness independence criterion (CSIC)

- By our theorem: if $\gamma = \gamma|_{\mathcal{X}_1} \otimes \gamma|_{\mathcal{X}_2}$, then $\kappa_{k,\ell}^{(2,1)}(\gamma) = 0$ and $\kappa_{k,\ell}^{(1,2)}(\gamma) = 0$.
- V-statistic estimator of $\|\kappa_{k,\ell}^{(1,2)}(\gamma)\|_{\mathcal{H}_k^{\otimes 1} \otimes \mathcal{H}_\ell^{\otimes 2}}^2$:

$$\begin{aligned} & \frac{1}{N^2} \left\langle \mathbf{K} \circ \mathbf{K} \circ \mathbf{L} - 4\mathbf{K} \circ \mathbf{KH} \circ \mathbf{L} - 2\mathbf{K} \circ \mathbf{K} \circ \mathbf{LH} + 4\mathbf{KH} \circ \mathbf{K} \circ \mathbf{LH} \right. \\ & \quad + 2\mathbf{K} \circ \mathbf{L} \left\langle \frac{\mathbf{K}}{N^2} \right\rangle + 2\mathbf{KH} \circ \mathbf{HK} \circ \mathbf{L} + 4\mathbf{K} \circ \mathbf{HK} \circ \mathbf{LH} + \mathbf{K} \circ \mathbf{K} \left\langle \frac{\mathbf{L}}{N^2} \right\rangle \\ & \quad \left. - 8\mathbf{K} \circ \mathbf{LH} \left\langle \frac{\mathbf{K}}{N^2} \right\rangle - 4\mathbf{K} \circ \mathbf{HK} \left\langle \frac{\mathbf{L}}{N^2} \right\rangle + 4 \left\langle \frac{\mathbf{K}}{N^2} \right\rangle^2 \mathbf{L} \right\rangle, \end{aligned}$$

with kernels $k : \mathcal{X}_1^2 \rightarrow \mathbb{R}$, $\ell : \mathcal{X}_2^2 \rightarrow \mathbb{R}$, $\mathbf{K} := \mathbf{K}_x$, $\mathbf{L} := \mathbf{L}_y$, $\langle \mathbf{A} \rangle := \sum_{i,j} A_{i,j}$.

- Time complexity: quadratic.

Numerical illustrations ($\alpha = 0.05$): improved power

① Seoul bicycle rental data [E et al., 2020]:

- features: temperature, humidity, wind speed, visibility, rainfall, snowfall, ...



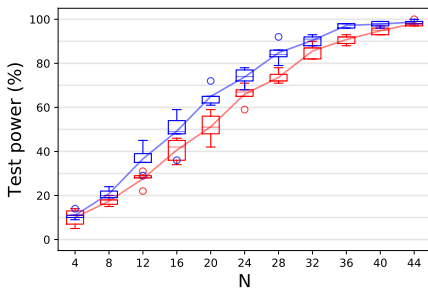
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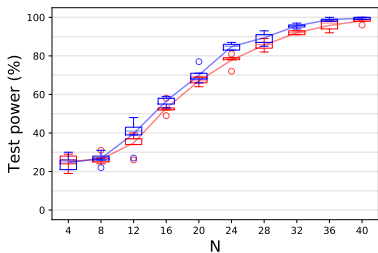
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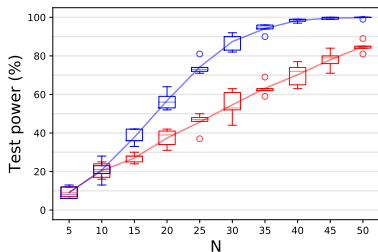
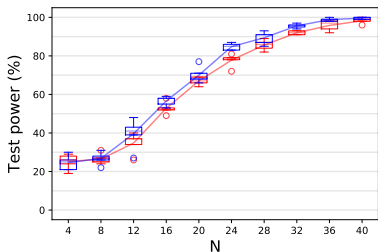
- independence test (HSIC, CSIC); (blockage, fire, flood, ...) vs slowness of traffic; $d_1 = 16$, $d_2 = 1$; l.h.s.



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- independence test (HSIC, CSIC); (blockage, fire, flood, ...) vs slowness of traffic; $d_1 = 16$, $d_2 = 1$; l.h.s.,
- two-sample test (MMD, $d^{(3)}$): slow vs fast moving traffic, $d = 16$; r.h.s.



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- Bell numbers
- Characteristic kernels
- Universal kernels:
 - equivalent definitions, Hahn-Banach theorem
 - properties, examples
- Moments and cumulants on \mathbb{R}^d
- Estimator for $d^{(3)}(\gamma, \eta)$
- Bochner integral
- Mean embedding: expected kernel trick

Bell numbers

- $B(m) :=$ number of elements in $P(m)$.
- $B_0 = B_1 = 1, B_2 = 2, B_3 = 5, B_4 = 15, B_5 = 52, B_6 = 203, B_7 = 877, B_8 = 4140, \dots$

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- Recursion:

$$B_{m+1} = |P(m+1)| = \sum_{k=0}^m \binom{m}{k} B_k.$$

Bell numbers – continued

- Easy computation by the Bell triangle (like Pascal triangle for $\binom{n}{k}$)

1					
1	2				
2	3	5			
5	7	10	15		
15	20	27	37	52	
52	...				

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- Asymptotics [de Bruijn, 1981, Lovász, 1993]:

$$\frac{\ln B_m}{m} = \ln m - \ln \ln m - 1 + \frac{\ln \ln m}{\ln m} + \frac{1}{\ln m} + \frac{1}{2} \left(\frac{\ln \ln m}{\ln m} \right)^2 + \mathcal{O} \left(\frac{\ln \ln m}{\ln^2 m} \right)$$

as $m \rightarrow \infty$.

Description of characteristic kernels 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 [Sriperumbudur et al., 2010]

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

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

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For $x \in \mathbb{R}^d$: $k_0(x) = \prod_{j=1}^d k_0(x_j)$, $\widehat{k}_0(\omega) = \prod_{j=1}^d \widehat{k}_0(\omega_j)$.

Universal kernel

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

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

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

Denseness in $C(\mathcal{X}) \Leftrightarrow$ injectivity of μ_k on $\mathcal{M}_b(\mathcal{X})$

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Properties of universal kernels

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- The normalized kernel (like 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 $C^\infty \ni f : (-r, r) \rightarrow \mathbb{R}$

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

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

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

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

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

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

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

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

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

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

Moments and cumulants on $\mathbb{R}^d \ni X \sim \gamma, \mathbf{i} \in \mathbb{N}^d$

	$d = 1$	$d \geq 1$
moment sequence	$\mu(\gamma) := \left(\mu^{(i)}(\gamma) \right)_{i \in \mathbb{N}}$	$\mu(\gamma) := \left(\mu^{\mathbf{i}}(\gamma) \right)_{\mathbf{i} \in \mathbb{N}^d}$
moments	$\mu^{(i)}(\gamma) := \mathbb{E}(X^i) \in \mathbb{R}$	$\mu^{\mathbf{i}}(\gamma) := \mathbb{E} \left[X_1^{i_1} \cdots X_d^{i_d} \right] \in \mathbb{R}$

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m -th moment	$\mu^{(m)}(\gamma)$	$\mu^m(\gamma) := (\mu^{\mathbf{i}}(\gamma))_{\deg(\mathbf{i})=m}$

where $\deg(\mathbf{i}) := i_1 + \cdots + i_d, \mu^0(\gamma) = 1$

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and cumulants $\kappa(\gamma) = (\kappa^{\mathbf{i}}(\gamma))_{\mathbf{i} \in \mathbb{N}^d}$

$$\sum_{\mathbf{i} \in \mathbb{N}^d} \kappa^{\mathbf{i}}(\gamma) \frac{\boldsymbol{\theta}^{\mathbf{i}}}{\mathbf{i}!} = \log \left(\sum_{\mathbf{i} \in \mathbb{N}^d} \mu^{\mathbf{i}}(\gamma) \frac{\boldsymbol{\theta}^{\mathbf{i}}}{\mathbf{i}!} \right), \quad \boldsymbol{\theta} \in \mathbb{R}^d,$$

where $\deg(\mathbf{i}) := i_1 + \cdots + i_d$, $\mu^0(\gamma) = 1$, $\mathbf{i}! = i_1! \cdots i_d!$, $\boldsymbol{\theta}^{\mathbf{i}} = \theta_1^{i_1} \cdots \theta_d^{i_d}$.

Estimator for $d^{(3)}(\gamma, \eta) = \|\kappa_k^{(3)}(\gamma) - \kappa_k^{(3)}(\eta)\|_{\mathcal{H}_k^{\otimes 3}}^2$, $N = M$

$$d^{(3)}(\gamma, \eta) = \|\kappa_k^{(3)}(\gamma)\|_{\mathcal{H}_k^{\otimes 3}}^2 + \|\kappa_k^{(3)}(\eta)\|_{\mathcal{H}_k^{\otimes 3}}^2 - 2\langle \kappa_k^{(3)}(\gamma), \kappa_k^{(3)}(\eta) \rangle_{\mathcal{H}_k^{\otimes 3}}$$

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$$\begin{aligned} \langle \kappa_k^{(3)}(\gamma), \kappa_k^{(3)}(\eta) \rangle_{\mathcal{H}_k^{\otimes 3}} &\approx \frac{1}{N^2} \left\langle \mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{K}_{xy} - 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \right. \\ &\quad - 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} + 6\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \circ \mathbf{H}\mathbf{K}_{xy} \\ &\quad + 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle + 2\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \\ &\quad + 2\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \circ \mathbf{K}_{xy}\mathbf{H} - 6\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle \\ &\quad \left. - 6\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle + 4 \left\langle \frac{\mathbf{K}}{N^2} \right\rangle^2 \mathbf{K}_{xy} \right\rangle. \end{aligned}$$

Note: Matrix multiplication takes precedence over the Hadamard one.

Estimator for $d^{(3)}(\gamma, \eta)$ – continued

$$\begin{aligned}\|\kappa_k^{(3)}(\gamma)\|_{\mathcal{H}_k^{\otimes 3}}^2 &\approx \frac{1}{N^2} \left\langle \mathbf{K}_x \circ \mathbf{K}_x \circ \mathbf{K}_x - 6\mathbf{K}_x \circ \mathbf{K}_x \mathbf{H} \circ \mathbf{K}_x \right. \\ &\quad + 4\mathbf{K}_x \mathbf{H} \circ \mathbf{K}_x \circ \mathbf{K}_x \mathbf{H} + 3\mathbf{K}_x \circ \mathbf{K}_x \left\langle \frac{\mathbf{K}_x}{N^2} \right\rangle \\ &\quad + 6\mathbf{K}_x \mathbf{H} \circ \mathbf{H} \mathbf{K}_x \circ \mathbf{K}_x - 12\mathbf{K}_x \circ \mathbf{H} \mathbf{K}_x \left\langle \frac{\mathbf{K}_x}{N^2} \right\rangle \\ &\quad \left. + 4 \left\langle \frac{\mathbf{K}_x}{N^2} \right\rangle^2 \mathbf{K}_x \right\rangle.\end{aligned}$$

$\|\kappa_k^{(3)}(\eta)\|_{\mathcal{H}_k^{\otimes 3}}^2$: similarly (change \mathbf{K}_x to \mathbf{K}_y).

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

- Given:
 - $(\mathcal{X}, \mathcal{A}, \gamma)$: σ -finite measure space,
 - $f : (\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{H}$ -valued function (note: Banach-valued f ✓).

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

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 - $(\mathcal{X}, \mathcal{A}, \gamma)$: σ -finite measure space,
 - $f : (\mathcal{X}, \mathcal{A}) \rightarrow \mathcal{H}$ -valued function (note: Banach-valued f ✓).
- For $f = \sum_{i=1}^n c_i \chi_{A_i}$ ($A_i \in \mathcal{A}$, $c_i \in \mathcal{H}$) **step functions**

$$\int_{\mathcal{X}} f d\gamma := \sum_{i=1}^n c_i \gamma(A_i) \in \mathcal{H}.$$

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

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- f **measurable function** is Bochner γ -integrable if
 - $\exists (f_n)_{n \in \mathbb{N}}$ step functions: $\lim_{n \rightarrow \infty} \int_{\mathcal{X}} \|f - f_n\|_{\mathcal{H}} d\gamma = 0$.
 - In this case $\lim_{n \rightarrow \infty} \int_{\mathcal{X}} f_n d\gamma$ exists, $=: \int_{\mathcal{X}} f d\gamma$.

Bochner integral: properties

- $f : \mathcal{X} \rightarrow \mathcal{H}$ is Bochner integrable $\Leftrightarrow \int_{\mathcal{X}} \|f\|_{\mathcal{H}} d\gamma < \infty$.

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Bochner integral: properties

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- In this case $\|\int_{\mathcal{X}} f d\gamma\|_{\mathcal{H}} \leq \int_{\mathcal{X}} \|f\|_{\mathcal{H}} d\gamma$. ('Jensen inequality')
- In our context: $\mathcal{H} = \mathcal{H}_k$,

$$\mu_k(\gamma) \text{ exists iff. } \int_{\mathcal{X}} \underbrace{\|k(\cdot, x)\|_{\mathcal{H}_k}}_{\sqrt{k(x,x)}} d\gamma(x) < \infty.$$

Specifically: for bounded kernel $(\sup_{x,x' \in \mathcal{X}} k(x,x') < \infty)$ ✓.

Bochner integral: properties – continued

- If
 - $S : B \rightarrow B_2$: **bounded linear** operator,
 - $f : X \rightarrow B$: **Bochner integrable**, then $S \circ f : X \rightarrow B_2$ is Bochner integrable and

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

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In short

$\left| \int f d\gamma \right| \leq \int |f| d\gamma$ and $c \int f d\gamma = \int c f d\gamma$ generalize nicely.

Contents

, mean embedding and friends

Mean embedding: expected kernel trick

$$\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} \stackrel{(a)}{=} \langle \mu_k(\gamma), \int_{\mathcal{X}} k(\cdot, y) d\eta(y) \rangle_{\mathcal{H}_k}$$

(a): μ_k definition

Mean embedding: expected kernel trick

$$\begin{aligned}\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} &\stackrel{(a)}{=} \langle \mu_k(\gamma), \int_{\mathcal{X}} k(\cdot, y) d\eta(y) \rangle_{\mathcal{H}_k} \\ &\stackrel{(b)}{=} \int_{\mathcal{X}} \langle \mu_k(\gamma), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y)\end{aligned}$$

(a): μ_k definition, (b): $S(\int_{\mathcal{X}} f d\mu) = \int_{\mathcal{X}} S f d\mu$, $S(z) = \langle \mu_k(\gamma), z \rangle_{\mathcal{H}_k}$ [\Leftarrow Hille's theorem]

Mean embedding: expected kernel trick

$$\begin{aligned}\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} &\stackrel{(a)}{=} \langle \mu_k(\gamma), \int_{\mathcal{X}} k(\cdot, y) d\eta(y) \rangle_{\mathcal{H}_k} \\ &\stackrel{(b)}{=} \int_{\mathcal{X}} \langle \mu_k(\gamma), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y) \\ &\stackrel{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) d\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y)\end{aligned}$$

(a): μ_k definition, (b): $S(\int_{\mathcal{X}} f d\mu) = \int_{\mathcal{X}} S f d\mu$, $S(z) = \langle \mu_k(\gamma), z \rangle_{\mathcal{H}_k}$ [\Leftarrow Hille's theorem], (c): μ_k definition

Mean embedding: expected kernel trick





$$\begin{aligned}\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} &\stackrel{(a)}{=} \langle \mu_k(\gamma), \int_{\mathcal{X}} k(\cdot, y) d\eta(y) \rangle_{\mathcal{H}_k} \\ &\stackrel{(b)}{=} \int_{\mathcal{X}} \langle \mu_k(\gamma), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y) \\ &\stackrel{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) d\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y) \\ &\stackrel{(d)}{=} \int_{\mathcal{X}} \int_{\mathcal{X}} \langle k(\cdot, x) k(\cdot, y) \rangle_{\mathcal{H}_k} d\gamma(x) d\eta(y)\end{aligned}$$

(a): μ_k definition, (b): $S(\int_{\mathcal{X}} f d\mu) = \int_{\mathcal{X}} S f d\mu$, $S(z) = \langle \mu_k(\gamma), z \rangle_{\mathcal{H}_k}$ [\Leftarrow Hille's theorem], (c): μ_k definition, (d): (b) with $S_y(z) = \langle z, k(\cdot, y) \rangle_{\mathcal{H}_k}$

Mean embedding: expected kernel trick

$$\begin{aligned}\langle \mu_k(\gamma), \mu_k(\eta) \rangle_{\mathcal{H}_k} &\stackrel{(a)}{=} \langle \mu_k(\gamma), \int_{\mathcal{X}} k(\cdot, y) d\eta(y) \rangle_{\mathcal{H}_k} \\ &\stackrel{(b)}{=} \int_{\mathcal{X}} \langle \mu_k(\gamma), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y) \\ &\stackrel{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) d\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} d\eta(y) \\ &\stackrel{(d)}{=} \int_{\mathcal{X}} \int_{\mathcal{X}} \langle k(\cdot, x) k(\cdot, y) \rangle_{\mathcal{H}_k} d\gamma(x) d\eta(y) \\ &\stackrel{(e)}{=} \int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) d\gamma(x) d\eta(y),\end{aligned}$$

(a): μ_k definition, (b): $S(\int_{\mathcal{X}} f d\mu) = \int_{\mathcal{X}} S f d\mu$, $S(z) = \langle \mu_k(\gamma), z \rangle_{\mathcal{H}_k}$ [\Leftarrow Hille's theorem], (c): μ_k definition, (d): (b) with $S_y(z) = \langle z, k(\cdot, y) \rangle_{\mathcal{H}_k}$, (e): reproducing property.

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