# The Power of Cumulants in Reproducing Kernel Hilbert Spaces

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

$$\mu^{(i)}(\gamma) := \mathbb{E}\left( X^i \right) \in \mathbb{R}, \qquad \mu^{(0)}(\gamma) := 1.$$

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

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- Cumulants $\kappa(\gamma) = \left( \kappa^{(i)}(\gamma) \right)_{i \in \mathbb{N}}$: 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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$$\kappa^{(1)}(\gamma) = \mathbb{E}(X) \qquad\qquad \text{mean}$$
$$\kappa^{(2)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^2 \qquad\qquad \text{variance}$$
$$\kappa^{(3)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^3 \qquad\qquad \text{3rd central moment}$$
$$\kappa^{(4)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^4 - 3 \left[ \mathbb{E}(X - \mathbb{E}X)^2 \right]^2$$
$$\kappa^{(5)}(\gamma) = \mathbb{E}(X - \mathbb{E}X)^5 - 10\mathbb{E}(X - \mathbb{E}X)^3 \mathbb{E}(X - \mathbb{E}X)^2$$

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

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

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

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

<span style="color:red">{{1}}</span>

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$\dots$

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

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

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

## Moment and cumulants on $\mathbb{R}^d$

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

## Known theorem [Billingsley, 2012]

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

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

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

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## Motivation

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

# Idea

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

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Ingredients:

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

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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:
   - log on tensor algebras, or
   - 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):

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

- 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

- $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k = \overline{\mathsf{Span}}(k(\cdot, x) : x \in \mathcal{X})$: Fourier analysis, approximation with polynomials, splines, …
- Examples ($c \geq 0$, $p \in \mathbb{N}$): $k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^p$, $k_G(\mathbf{x}, \mathbf{y}) = e^{-c\|\mathbf{x}-\mathbf{y}\|_2^2}$.
- 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, Schulz et al., 2022, Nikolentzos and Vazirgiannis, 2023].

# Mean embedding

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

$$\mu_k(\gamma) := \int_{\mathcal{X}} \underbrace{k(\cdot, x)}_{\Phi(x) \in \mathcal{H}_k,\ \text{a la }\ \Phi(x) = e^{i\langle \cdot, x \rangle}} \mathrm{d}\gamma(x) \in \mathcal{H}_k.$$

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

$$\mathrm{HSIC}_k(\gamma) := \mathrm{MMD}_k\left(\gamma, \otimes_{j=1}^{d} \gamma|_{\mathcal{X}_j}\right)$$

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

# MMD, HSIC: information theoretical & statistical relations

- **M** MD :

$$\text{MMD}_k(\gamma, \eta) = \|\mu_k(\gamma) - \mu_k(\eta)\|_{\mathcal{H}_k} = \sup_{f \in B_k} \underbrace{\langle f, \mu_k(\gamma) - \mu_k(\eta) \rangle_{\mathcal{H}_k}}_{\mathbb{E}_{x \sim \gamma} f(x) - \mathbb{E}_{x \sim \eta} f(x)}$$

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- HSIC ($d = 2$) $\overset{\dagger}{\Leftrightarrow}$ distance covariance
  [Székely et al., 2007, Székely and Rizzo, 2009, Lyons, 2013].
- † [Sejdinovic et al., 2013b].

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

$$L(\gamma) := \gamma - \gamma|_{\mathcal{X}_1 \mathcal{X}_2} \otimes \gamma|_{\mathcal{X}_3} - \gamma|_{\mathcal{X}_2 \mathcal{X}_3} \otimes \gamma|_{\mathcal{X}_1} - \gamma|_{\mathcal{X}_1 \mathcal{X}_3} \otimes \gamma|_{\mathcal{X}_2}$$
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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** [Sejdinovic et al., 2013a]

$$\left\| \mu_{k_{\mathcal{X}_1} \otimes k_{\mathcal{X}_2} \otimes k_{\mathcal{X}_3}}(L(\gamma)) \right\|^2_{\mathcal{H}_{k_{\mathcal{X}_1}} \otimes \mathcal{H}_{k_{\mathcal{X}_2}} \otimes \mathcal{H}_{k_{\mathcal{X}_3}}} \overset{?}{>} 0 \Rightarrow \text{no factorization.}$$

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

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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

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

# Tensor product: $\bigotimes_{j=1}^{d} a_j$

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

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

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

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

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

  $\mathbf{a} \otimes \mathbf{b} := \mathbf{ab}^{\top}$ is an $\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R}$ bilinear form.
- For $a \in \mathcal{H}_1$, $b \in \mathcal{H}_2$ Hilbert spaces, i.e. for $d = 2$:

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

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

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

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

$$\left( \otimes_{j=1}^{d} a_j \right) (b_1, \ldots, b_d) := \prod_{j=1}^{d} \langle a_j, b_j \rangle_{\mathcal{H}_j}.$$

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

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

[Berlinet and Thomas-Agnan, 2004]

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

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

Validness:

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

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Properties:

① Injectivity of $\mu_k$ on probability / finite signed measures, so

$$\text{universal} \Rightarrow \text{characteristic}.$$

# Validness of MMD & HSIC, their estimation

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  $k_j$-s are universal [Steinwart, 2001, Micchelli et al., 2006].

Properties:

1. Injectivity of $\mu_k$ on probability / finite signed measures, so
   universal $\Rightarrow$ characteristic.

2. Easy-to-estimate: expected kernel trick

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

# 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], . . .

# Kernelized moments – towards kernelized cumulants

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

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

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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:

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

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  $$\kappa_k^{(1)}(\gamma) = \mathbb{E}[\Phi(X)]$$

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

$$\kappa_k^{(1)}(\gamma) = \mathbb{E}[\Phi(X)],$$

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$$\kappa_k^{(3)}(\gamma) = \mathbb{E}\big[\Phi^{\otimes 3}(X)\big] - \mathbb{E}\big[\Phi(X) \otimes \Phi(X) \otimes \Phi(X')\big]$$
$$- \mathbb{E}\big[\Phi(X) \otimes \Phi(X') \otimes \Phi(X)\big] - \mathbb{E}\big[\Phi(X') \otimes \Phi(X) \otimes \Phi(X)\big]$$
$$+ 2\mathbb{E}^{\otimes 3}\big[\Phi(X)\big].$$

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$$+ 2\mathbb{E}^{\otimes 3}\big[\Phi(X)\big].$$

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

$$\kappa_{k_1,k_2}^{(2,0)}(\gamma) = \mathbb{E}\Big[\Phi_1^{\otimes 2}(X_1)\Big] - \mathbb{E}^{\otimes 2}\big[\Phi_1(X_1)\big],$$

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

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

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

Wanted: repetition and partitioning. Weights: as before ($c_\pi$).

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

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

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$$\kappa_{k_1, \ldots, k_d}(\gamma) := \left(\kappa_{k_1, \ldots, k_d}^{\mathbf{i}}(\gamma)\right)_{\mathbf{i} \in \mathbb{N}^d},$$

$$\kappa_{k_1, \ldots, k_d}^{\mathbf{i}}(\gamma) := \sum_{\pi \in P(m)} c_\pi \mathbb{E}_{\gamma_\pi^{\mathbf{i}}} k^{\otimes \mathbf{i}}(\cdot, (X_1, \ldots, X_m)).$$

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

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$\Rightarrow$ expected kernel trick is applicable

# Cumulants characterize distributions

Point-separating $k$ := injectivity of $\Phi \Leftarrow$ characteristic $k \Leftarrow$ universal $k$.

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### Theorem

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

$$
\begin{aligned}
d^{\mathbf{i}}(\gamma, \eta) &:= \|\kappa_{k_1,\ldots,k_d}^{\mathbf{i}}(\gamma) - \kappa_{k_1,\ldots,k_d}^{\mathbf{i}}(\eta)\|_{\mathcal{H}^{\otimes \mathbf{i}}}^2 \\
&= \sum_{\pi,\tau \in P(m)} c_\pi c_\tau \Big[ \mathbb{E}_{\gamma_\pi^{\mathbf{i}} \otimes \gamma_\tau^{\mathbf{i}}} k^{\otimes \mathbf{i}}((X_1,\ldots,X_m),(Y_1,\ldots,Y_m)) \\
&\qquad + \mathbb{E}_{\eta_\pi^{\mathbf{i}} \otimes \eta_\tau^{\mathbf{i}}} k^{\otimes \mathbf{i}}((X_1,\ldots,X_m),(Y_1,\ldots,Y_m)) \\
&\qquad - 2\mathbb{E}_{\gamma_\pi^{\mathbf{i}} \otimes \eta_\tau^{\mathbf{i}}} k^{\otimes \mathbf{i}}((X_1,\ldots,X_m),(Y_1,\ldots,Y_m)) \Big].
\end{aligned}
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- Then, $\gamma = \gamma|_{\mathcal{X}_1} \otimes \cdots \otimes \gamma|_{\mathcal{X}_d} \Leftrightarrow \kappa_{k_1,\ldots,k_d}^{\mathbf{i}}(\gamma) = 0$ for every $\mathbf{i} \in \mathbb{N}_+^d$

# Cumulants characterize independence

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

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

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## Theorem

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

## Estimation in both cases

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

# Distance between kernel variance embeddings

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

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

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

# Distance between kernel variance/skewness embeddings

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

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

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

### 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 $\|\kappa_{k,\ell}^{(1,2)}(\gamma)\|_{\mathcal{H}_k^{\otimes 1} \otimes \mathcal{H}_\ell^{\otimes 2}}^2$:

$$\frac{1}{N^2}\bigg\langle \mathbf{K} \circ \mathbf{K} \circ \mathbf{L} - 4\mathbf{K} \circ \mathbf{KH} \circ \mathbf{L} - 2\mathbf{K} \circ \mathbf{K} \circ \mathbf{LH} + 4\mathbf{KH} \circ \mathbf{K} \circ \mathbf{LH}$$

$$+2\mathbf{K} \circ \mathbf{L} \left\langle \frac{\mathbf{K}}{N^2} \right\rangle + 2\mathbf{KH} \circ \mathbf{HK} \circ \mathbf{L} + 4\mathbf{K} \circ \mathbf{HK} \circ \mathbf{LH} + \mathbf{K} \circ \mathbf{K} \left\langle \frac{\mathbf{L}}{N^2} \right\rangle$$

$$-8\mathbf{K} \circ \mathbf{LH} \left\langle \frac{\mathbf{K}}{N^2} \right\rangle - 4\mathbf{K} \circ \mathbf{HK} \left\langle \frac{\mathbf{L}}{N^2} \right\rangle + 4 \left\langle \frac{\mathbf{K}}{N^2} \right\rangle^2 \mathbf{L} \bigg\rangle,$$

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

1. Seoul bicycle rental data [E et al., 2020]:
   - features: temperature, humidity, wind speed, visibility, rainfall, snowfall, . . .

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

1. Seoul bicycle rental data [E et al., 2020]:
   - features: temperature, humidity, wind speed, visibility, rainfall, snowfall, ...

   - two-sample test (MMD, $d^{(2)}$): winter vs fall, $d = 11$,

2. Brazilian traffic data [Ferreira, 2016]:
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② Brazilian traffic data [Ferreira, 2016]:
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  - two-sample test (MMD, $d^{(3)}$): slow vs fast moving traffic, $d = 16$; r.h.s.
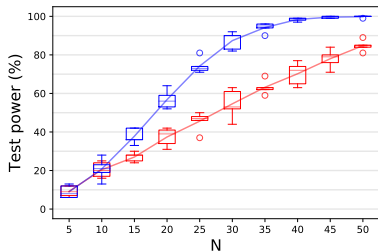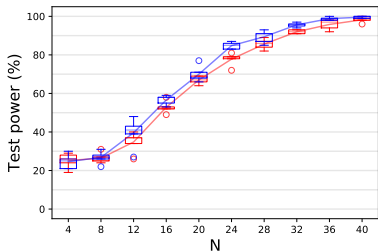
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# Appendix

- 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.

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

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- Recursion:

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

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

$$
\begin{array}{ccccc}
1 \\
1 & 2 \\
2 & 3 & 5 \\
5 & 7 & 10 & 15 \\
15 & 20 & 27 & 37 & 52 \\
52 & \ldots
\end{array}
$$

## Bell numbers – continued

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

$$
\begin{array}{cccccc}
1 & & & & & \\
1 & 2 & & & & \\
2 & 3 & 5 & & & \\
5 & 7 & 10 & 15 & & \\
15 & 20 & 27 & 37 & 52 & \\
52 & \cdots & & & &
\end{array}
$$

- 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 $m \to \infty$.

Contents

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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**Theorem ([Sriperumbudur et al., 2010])**

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

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

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

# Examples on $\mathbb{R}$; similarly $\mathbb{R}^d$ [Sriperumbudur et al., 2010]

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| kernel name | $k_0$ | $\widehat{k_0}(\omega)$ | $supp(\widehat{k_0})$ |
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| Cosine | $\cos(\sigma x)$ | $\sqrt{\frac{\pi}{2}} [\delta(\omega - \sigma) + \delta(\omega + \sigma)]$ | $\{-\sigma, \sigma\}$ |

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

Contents

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

**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 $(C(\mathcal{X}), \|\cdot\|_\infty)$.

# Universal kernel

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$\mathcal{X}$ assumption $\Rightarrow$

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

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$$\{0\} = \mathcal{H}_k^\perp = \Big\{ \mathbb{F} \in \underbrace{C(\mathcal{X})'}_{=\mathcal{M}_b(\mathcal{X})} : \forall f \in \mathcal{H}_k, 0 = T_{\mathbb{F}}(f) = \underbrace{\int_\mathcal{X} f \, d\mathbb{F}}_{\langle f, \mu_k(\mathbb{F})\rangle_{\mathcal{H}_k}} \Big\}$$

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

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$$= \{\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) : \mu_k(\mathbb{F}) = 0\}.$$

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- $k(x, x) > 0$ for all $x \in \mathcal{X}$.

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  is a metric.

- The normalized kernel (like $\mathrm{corr}$)

$$\tilde{k}(x, y) := \frac{k(x, y)}{\sqrt{k(x, x)k(y, y)}}$$

  is universal.

- For an $C^\infty \ni f : (-r, r) \to \mathbb{R}$

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

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

- $k(\mathbf{x}, \mathbf{y}) = e^{\alpha \langle \mathbf{x}, \mathbf{y} \rangle}$: 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.

- $k(\mathbf{x}, \mathbf{y}) = (1 - \langle \mathbf{x}, \mathbf{y} \rangle)^{-\alpha}$ 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 $\binom{b}{n} = \sum_{i=1}^{n} \frac{b-i+1}{i}$.

Contents

# 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 | $\mu^{(i)}(\gamma) := \mathbb{E}\left( X^i \right) \in \mathbb{R}$ | $\mu^{\mathbf{i}}(\gamma) := \mathbb{E}\left[ X_1^{i_1} \cdots X_d^{i_d} \right] \in \mathbb{R}$ |

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

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

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

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

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

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

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

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$$\langle \kappa_k^{(3)}(\gamma), \kappa_k^{(3)}(\eta) \rangle_{\mathcal{H}_k^{\otimes 3}} \approx \frac{1}{N^2} \bigg\langle \mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{K}_{xy} - 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy}$$

$$- 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} + 6\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \circ \mathbf{H}\mathbf{K}_{xy}$$

$$+ 3\mathbf{K}_{xy} \circ \mathbf{K}_{xy} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle + 2\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy}$$

$$+ 2\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \circ \mathbf{K}_{xy}\mathbf{H} - 6\mathbf{K}_{xy} \circ \mathbf{K}_{xy}\mathbf{H} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle$$

$$- 6\mathbf{K}_{xy} \circ \mathbf{H}\mathbf{K}_{xy} \left\langle \frac{\mathbf{K}_{xy}}{N^2} \right\rangle + 4 \left\langle \frac{\mathbf{K}}{N^2} \right\rangle^2 \mathbf{K}_{xy} \bigg\rangle.$$

Note: Matrix multiplication takes precedence over the Hadamard one.

$$\|\kappa_k^{(3)}(\gamma)\|_{\mathcal{H}_k^{\otimes 3}}^2 \approx \frac{1}{N^2}\Big\langle \mathbf{K}_x \circ \mathbf{K}_x \circ \mathbf{K}_x - 6\mathbf{K}_x \circ \mathbf{K}_x \mathbf{H} \circ \mathbf{K}_x$$

$$+ 4\mathbf{K}_x \mathbf{H} \circ \mathbf{K}_x \circ \mathbf{K}_x \mathbf{H} + 3\mathbf{K}_x \circ \mathbf{K}_x \Big\langle \frac{\mathbf{K}_x}{N^2} \Big\rangle$$

$$+ 6\mathbf{K}_x \mathbf{H} \circ \mathbf{H}\mathbf{K}_x \circ \mathbf{K}_x - 12\mathbf{K}_x \circ \mathbf{H}\mathbf{K}_x \Big\langle \frac{\mathbf{K}_x}{N^2} \Big\rangle$$

$$+ 4 \Big\langle \frac{\mathbf{K}_x}{N^2} \Big\rangle^2 \mathbf{K}_x \Big\rangle.$$

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

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

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

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- For $f = \sum_{i=1}^{n} c_i \chi_{A_i}$ ($A_i \in \mathcal{A}$, $c_i \in \mathcal{H}$) step functions

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

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

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

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

- $f : \mathcal{X} \to \mathcal{H}$ is Bochner integrable $\Leftrightarrow \int_{\mathcal{X}} \|f\|_{\mathcal{H}} \, d\gamma < \infty$.
- In this case $\left\| \int_{\mathcal{X}} f \, d\gamma \right\|_{\mathcal{H}} \leq \int_{\mathcal{X}} \|f\|_{\mathcal{H}} \, d\gamma$. ('Jensen inequality')

- $f : \mathcal{X} \to \mathcal{H}$ is Bochner integrable $\Leftrightarrow \int_{\mathcal{X}} \|f\|_{\mathcal{H}} \, \mathrm{d}\gamma < \infty$.
- In this case $\|\int_{\mathcal{X}} f \mathrm{d}\gamma\|_{\mathcal{H}} \le \int_{\mathcal{X}} \|f\|_{\mathcal{H}} \, \mathrm{d}\gamma$. ('Jensen inequality')
- In our context: $\mathcal{H} = \mathcal{H}_k$,

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

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

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

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

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**In short**

$|\int f \mathrm{d}\gamma| \leq \int |f| \mathrm{d}\gamma$ and $c \int f \mathrm{d}\gamma = \int c f \mathrm{d}\gamma$ generalize nicely.

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

(a): $\mu_k$ definition

# Mean embedding: expected kernel trick

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

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

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

# Mean embedding: expected kernel trick

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

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

$$\overset{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) \mathrm{d}\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} \mathrm{d}\eta(y)$$

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

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

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

$$\overset{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) \mathrm{d}\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} \mathrm{d}\eta(y)$$

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

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

# Mean embedding: expected kernel trick

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

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

$$\overset{(c)}{=} \int_{\mathcal{X}} \langle \int_{\mathcal{X}} k(\cdot, x) \mathrm{d}\gamma(x), k(\cdot, y) \rangle_{\mathcal{H}_k} \mathrm{d}\eta(y)$$

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

$$\overset{(e)}{=} \int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) \mathrm{d}\gamma(x) \mathrm{d}\eta(y),$$

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

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