On the Relation Between Universality, Characteristic Kernels and RKHS Embedding of Measures

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Outline

- RKHS embedding of probability measures
- *Characteristic kernels*
- *Universal kernels*
  - *Various notions* of universality
  - *Novel characterization of universality*
  - Relation to RKHS embedding of *signed measures*

RKHS Embedding of Probability Measures

- *Input space* : X
- *Feature space* : $\mathcal{H}$ (with reproducing kernel, k)
- *Feature map* : Φ

$$\Phi : X \to \mathcal{H} \qquad\qquad x \mapsto \Phi(x) := k(\cdot, x)$$

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$$\mathbb{P} \mapsto \Phi(\mathbb{P}) := \underbrace{\int_X k(\cdot, x)\, d\mathbb{P}(x)}_{E_{Y\sim\mathbb{P}}[\Phi(Y)]=E_{Y\sim\mathbb{P}}[k(\cdot,Y)]}$$

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$$\mathbb{P} \mapsto \Phi(\mathbb{P}) := \int_X k(\cdot, x)\, d\mathbb{P}(x)$$

Advantage: $\Phi(\mathbb{P})$ can distinguish $\mathbb{P}$ by *high-order moments.*

$$\begin{aligned} k(y, x) &= c_0 + c_1(xy) + c_2(xy)^2 + \cdots \quad (c_i \neq 0) \qquad \text{e.g. } k(y, x) = e^{xy} \\ \Phi(\mathbb{P})(y) &= c_0 + c_1 \left(\int_X x \, d\mathbb{P}(x) \right) y + c_2 \left(\int_X x^2 \, d\mathbb{P}(x) \right) y^2 + \cdots \end{aligned}$$

Applications

Two-sample problem:

- Given random samples $\{X_1, \ldots, X_m\}$ and $\{Y_1, \ldots, Y_n\}$ drawn i.i.d. from $\mathbb{P}$ and $\mathbb{Q}$, respectively.
- *Determine:* are $\mathbb{P}$ and $\mathbb{Q}$ different?

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- *Determine:* are $\mathbb{P}$ and $\mathbb{Q}$ different?
- $\gamma(\mathbb{P}, \mathbb{Q}) = \|\Phi(\mathbb{P}) - \Phi(\mathbb{Q})\|_{\mathcal{H}}$: distance metric between $\mathbb{P}$ and $\mathbb{Q}$.

$$\begin{matrix} H_0 : \mathbb{P} = \mathbb{Q} \\ \\ H_1 : \mathbb{P} \neq \mathbb{Q} \end{matrix} \quad \equiv \quad \begin{matrix} H_0 : \gamma(\mathbb{P}, \mathbb{Q}) = 0 \\ \\ H_1 : \gamma(\mathbb{P}, \mathbb{Q}) > 0 \end{matrix}$$

- *Test:* Say H_0 if $\widehat{\gamma}(\mathbb{P}, \mathbb{Q}) < \varepsilon$. Otherwise say H_1.

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Other applications:

- *Hypothesis testing* : Independence test, Goodness of fit test, etc.
- Feature selection, message passing, density estimation, etc.

Characteristic Kernels

Define: k is *characteristic* if

$$\mathbb{P} \mapsto \int_X k(\cdot, x)\, d\mathbb{P}(x) \ \textit{ is injective.}$$

In other words,

$$\int_X k(\cdot, x)\, d\mathbb{P}(x) = \int_X k(\cdot, x)\, d\mathbb{Q}(x) \Leftrightarrow \mathbb{P} = \mathbb{Q}.$$

- When $k(\cdot, x) = e^{\sqrt{-1}\langle \cdot, x \rangle}$, $\Phi(\mathbb{P})$ is the characteristic function of $\mathbb{P}$.

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- When $k(\cdot, x) = e^{\sqrt{-1}\langle \cdot, x\rangle}$, $\Phi(\mathbb{P})$ is the characteristic function of $\mathbb{P}$.
- Not all kernels are characteristic, e.g., $k(x, y) = x^T y$.

$$\mu_{\mathbb{P}} = \mu_{\mathbb{Q}} \not\Rightarrow \mathbb{P} = \mathbb{Q}$$

- *When is k characteristic?* [Gretton et al., 2007, Sriperumbudur et al., 2008, Fukumizu et al., 2008, Fukumizu et al., 2009, Sriperumbudur et al., 2009].

Universal Kernels

- *Regularization approach to supervised learning*

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \lambda \Omega[f], \qquad (1)$$

where $\lambda > 0$ and $\{(x_i, y_i)\}_{i=1}^{n}$ is the training data.

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- *Representer theorem :* The solution to (1) is of the form

$$f = \sum_{i=1}^{n} c_i k(\cdot, x_i),$$

  where $\{c_i\}_{i=1}^n \subset \mathbb{R}$ are the parameters typically obtained from the training data.

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- We need *$\mathcal{H}$ to be "dense" in the space of target functions — k is universal.*

Various Notions of Universality

- *Prior work*
  - *c-universality* [Steinwart, 2001]
  - *cc-universality* [Micchelli et al., 2006]
- Proposed notion: c_0*-universality*
- *Characterization of c-, cc- and* c_0*-universality* : Relation to RKHS embedding of measures
  - Translation invariant kernels on $\mathbb{R}^d$
  - Radial kernels on $\mathbb{R}^d$

c-universality [Steinwart, 2001]

- X : compact metric space
- k : continuous on $X \times X$
- *Target function space* : $C(X)$, continuous functions on X

Define k to be *c-universal* if $\mathcal{H}$ is dense in $C(X)$ w.r.t. the uniform norm ($\|f\|_u := \sup_{x \in X} |f(x)|$).

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- *Sufficient conditions* are obtained based on the Stone-Weierstraß theorem. *Not easy to check!*
- *Examples:* Gaussian and Laplacian kernels on any compact subset of $\mathbb{R}^d$.

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Issue: X is compact which excludes many interesting spaces, such as $\mathbb{R}^d$.

cc-universality [Micchelli et al., 2006]

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Define k to be *cc-universal* if $\mathcal{H}$ is dense in $C(X)$ endowed with the *topology of compact convergence.*

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In other words, for any compact set $Z \subset X$, $\mathcal{H}_{|Z} := \{f_{|Z} : f \in \mathcal{H}\}$ is dense in $C(Z)$ w.r.t. $\|\cdot\|_u$.

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Define k to be *cc-universal* if $\mathcal{H}$ is dense in $C(X)$ endowed with the *topology of compact convergence.*

- *Necessary and sufficient conditions* are obtained, which are related to the injectivity of RKHS embedding of measures.
- *Examples:* Gaussian, Laplacian and Sinc kernels on $\mathbb{R}^d$.

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Issue: Topology of compact convergence is *weaker* than the topology of uniform convergence.

Proposed Notion: c_0-universality

- X : locally compact Hausdorff (LCH) space
- *Target function space* : $C_0(X)$, the space of bounded continuous functions that "vanish at infinity" (for every $\epsilon > 0$, $\{x \in X : |f(x)| \geq \epsilon\}$ is compact).
- k is bounded and $k(\cdot, x) \in C_0(X)$ for all $x \in X$.

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Define k to be *c_0-universal* if $\mathcal{H}$ is dense in $C_0(X)$ w.r.t. $\|\cdot\|_u$.

- Handles non-compact X and ensures uniform convergence over entire X.

Embedding Characterization of Universality

Theorem

- *k is c_0-universal if and only if*

$$\mu \mapsto \int_X k(\cdot, x)\, d\mu(x),\ \mu \in M_b(X),$$

is injective. $M_b(X)$ is the space of finite signed Radon measures on X.

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Postive Definite Characterization of Universality

Theorem

- *k is c_0-universal (resp. c-universal) if and only if*

$$\int_X \int_X k(x,y)\, d\mu(x)\, d\mu(y) > 0, \forall\, \mu \in M_b(X)\backslash\{0\}.$$

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- *If k is c-, cc- or c_0-universal, then it is strictly positive definite.*

X is an LCH space: Summary

$$\begin{array}{ccc}
\clubsuit \text{ holds} & \begin{array}{c}\Longrightarrow\\ \not\Longleftarrow\end{array} & \clubsuit \text{ holds}\\
\forall\, \mu \in M_b(X) & & \forall\, \mu \in M_{bc}(X)\\
\Updownarrow & & \Updownarrow\\
c_0\text{-}\mathit{universal} & \begin{array}{c}\Longrightarrow\\ \not\Longleftarrow\end{array} & cc\text{-}\mathit{universal}\\
\Downarrow \quad \not\Uparrow & & \Downarrow \quad \not\Uparrow\\
\mathit{characteristic} & \begin{array}{c}\overset{?}{\Longrightarrow}\\ \not\Longleftarrow\end{array} & \mathit{strictly\ pd}
\end{array}$$

$$\clubsuit \;:\; \iint_X k(x,y)\, d\mu(x)\, d\mu(y) > 0$$

Translation Invariant Kernels on $\mathbb{R}^d$

$X = \mathbb{R}^d$ and $k(x, y) = \psi(x - y)$, where

$$\psi(x) = \int_{\mathbb{R}^d} e^{\sqrt{-1}x^T\omega}\, d\Lambda(\omega),\ x \in \mathbb{R}^d,$$

and Λ is a non-negative finite Borel measure.

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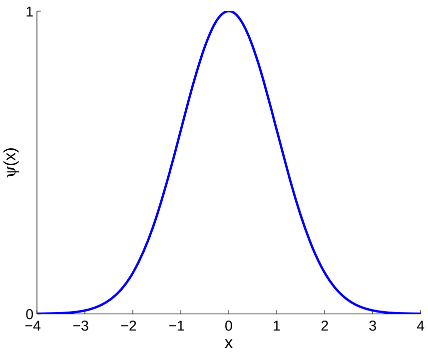
and Λ is a non-negative finite Borel measure.

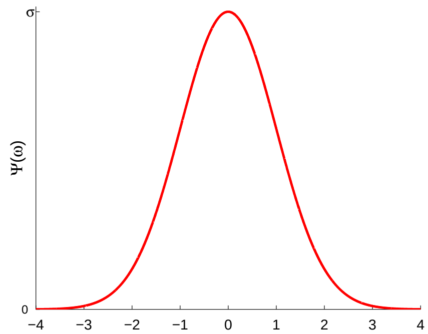
Theorem

- *k is c_0-universal if and only if $supp(\Lambda) = \mathbb{R}^d$.*
- *k is c_0-universal if and only if it is characteristic.*
- *If $supp(\Lambda)$ has a non-empty interior, then k is cc-universal. [Micchelli et al., 2006]*

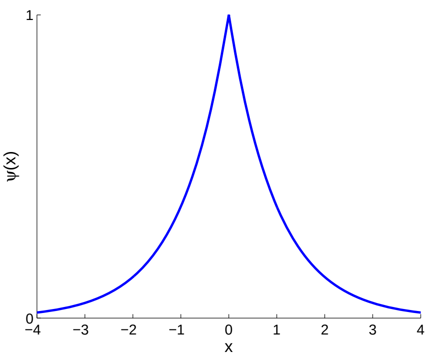
Examples

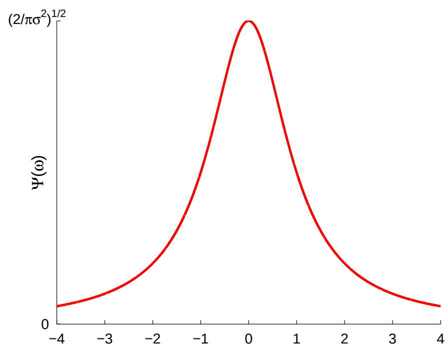
- Gaussian kernel: $\psi(x) = e^{-x^2/2\sigma^2}$; $\Psi(\omega) = \sigma e^{-\sigma^2\omega^2/2}$; $d\Lambda(\omega) = \Psi(\omega)\, d\omega$.



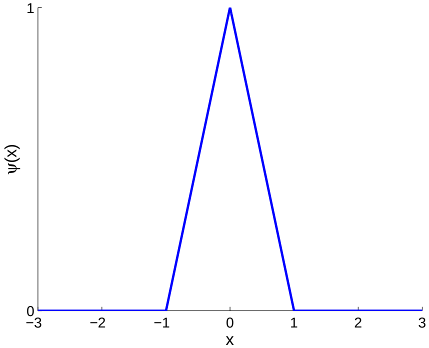


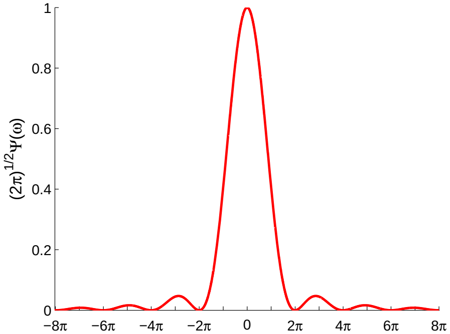
- Laplacian kernel: $\psi(x) = e^{-\sigma|x|}$; $\Psi(\omega) = \sqrt{\frac{2}{\pi}} \frac{\sigma}{\sigma^2+\omega^2}$.



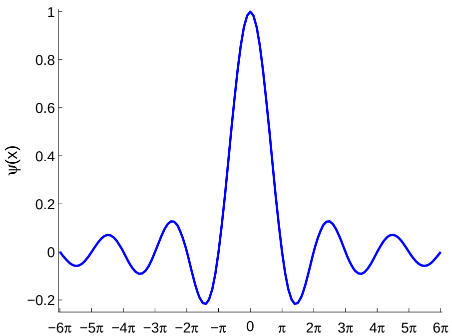


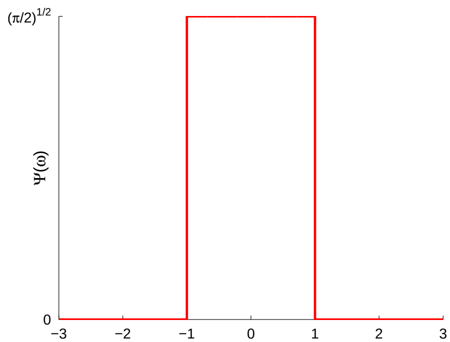
- B_1-spline kernel: $\psi(x) = (1 - |x|)\mathbb{1}_{[-1,1]}(x)$; $\Psi(\omega) = \frac{2\sqrt{2}}{\sqrt{\pi}} \frac{\sin^2(\frac{\omega}{2})}{\omega^2}$.





- Sinc kernel: $\psi(x) = \frac{\sin(\sigma x)}{x}$; $\Psi(\omega) = \sqrt{\frac{\pi}{2}}\mathbb{1}_{[-\sigma,\sigma]}(\omega)$.





Translation Invariant Kernels on $\mathbb{R}^d$: Summary

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\operatorname{supp}(\Lambda) = \mathbb{R}^d \arrow[r, Rightarrow, shift left] \arrow[d, Leftrightarrow] & (\operatorname{supp}(\Lambda))^\circ \neq \emptyset \arrow[l, Rightarrow, shift left, "/" marking] \arrow[d, Rightarrow, shift right] \\
c_0\text{-}universal \arrow[r, Rightarrow, shift left] \arrow[d, Leftrightarrow] & cc\text{-}universal \arrow[l, Rightarrow, shift left, "/" marking] \arrow[u, Rightarrow, shift right, "?"'] \arrow[d, Rightarrow, shift right] \\
characteristic \arrow[r, Rightarrow, shift left] & strictly\ pd \arrow[l, Rightarrow, shift left, "/" marking] \arrow[u, Rightarrow, shift right, "?\ (\spadesuit)"']
\end{tikzcd}
$$

$$\spadesuit \; : \; \psi \in C_b(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$$

Radial Kernels on $\mathbb{R}^d$

Let

$$k(x,y) = \int_{[0,\infty)} e^{-t\|x-y\|_2^2}\, d\nu(t),$$

where ν is a finite non-negative Borel measure on $[0,\infty)$.

- *Examples:* Gaussian kernel, Inverse multi-quadratic kernel, $k(x,y) = (c^2 + \|x-y\|_2^2)^{-\beta}$, $\beta > \frac{d}{2}$, $c > 0$, etc.

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Theorem

The following conditions are equivalent.

- *supp*$(\nu) \neq \{0\}$.
- k *is* c_0*-universal.*
- k *is cc-universal.*
- k *is characteristic.*
- k *is strictly pd.*

Radial Kernels on $\mathbb{R}^d$: Summary

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\begin{tikzcd}
\operatorname{supp}(\nu) \neq \{0\} \arrow[d, Leftrightarrow] & \\
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Summary

- *Characteristic kernel*
  - Injective RKHS embedding of probability measures.
  - *Applications:* Hypothesis testing, feature selection, etc.
- *Universal kernel*
  - Consistency of learning algorithms.
  - Injective RKHS embedding of finite signed Radon measures.
- *Clarified the relation* between various notions of universality and characteristic kernels.

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