Kernel Method: Data Analysis with Positive Definite Kernels

5. Theory on Positive Definite Kernel and Reproducing Kernel Hilbert Space

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Outline

Positive and negative definite kernels

- Review on positive definite kernels
- Negative definite kernel and its relation to positive definite kernel

Bochner's theorem

- Bochner's theorem
- Explicit form of some RKHS

Mercer's theorem

- Basic facts of Hilbert space
- Integral operator and Hilbert-Schmidt operator
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Restriction, Sum, and Product of RKHS

- Restriction, Sum, and Product of RKHS

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Review on Positive Definite Kernels I

Proposition 1

If $k_i : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ ($i = 1, 2, \ldots$) are positive definite kernels, then so are the following:

1. *(positive combination)* $ak_1 + bk_2 \qquad (a, b \geq 0)$.
2. *(product)* $k_1 k_2 \qquad (k_1(x, y)k_2(x, y))$.
3. *(limit)* $lim_{i\to\infty} k_i(x, y)$, *assuming the limit exists.*

Remark. Proposition 1 says that the set of all positive definite kernels is closed (w.r.t. pointwise convergence) convex cone stable under multiplication.

Example: If $k(x, y)$ is positive definite,

$$e^{k(x,y)} = 1 + k + \frac{1}{2}k^2 + \frac{1}{3!}k^3 + \cdots$$

is also positive definite.

Review on Positive Definite Kernels II

Proposition 2

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ be a positive definite kernel and $f : \mathcal{X} \to \mathbb{C}$ be an arbitrary function. Then,

$$\tilde{k}(x, y) = f(x)k(x, y)\overline{f(y)}$$

is positive definite. In particular,

$$f(x)\overline{f(y)}$$

is a positive definite kernel.

Example. Normalization:

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

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Negative Definite Kernel

Definition. A function $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is called a negative definite kernel if it is Hermitian i.e. $\psi(y, x) = \overline{\psi(x, y)}$, and

$$\sum_{i,j=1}^{n} c_i \overline{c_j} \psi(x_i, x_j) \leq 0$$

for any $x_1, \ldots, x_n$ ($n \geq 2$) in $\mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{C}$ with $\sum_{i=1}^{n} c_i = 0$.

Note: a negative definite kernel is not necessarily minus positive definite kernel, because we need the condition $\sum_{i=1}^{n} c_i = 0$.

Properties of negative definite kernels

Proposition 3

1. *If k is positive definite, $\psi = -k$ is negative definite.*
2. *Constant functions are negative definite.*

Proof. (2) $\sum_{i,j=1}^{n} c_i c_j = \sum_{i=1}^{n} c_i \sum_{j=1}^{n} c_j = 0$.

Proposition 4

If $\psi_i : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ ($i = 1, 2, \ldots$) are negative definite kernels, then so are the following:

1. *(positive combination)* $a\psi_1 + b\psi_2 \qquad (a, b \geq 0)$.
2. *(limit)* $lim_{i\to\infty} \psi_i(x, y)$, *assuming the limit exists.*

- The set of all negative definite kernels is a closed convex cone.
- Multiplication does not preserve negative definiteness.

Example of Negative Definite Kernel

Proposition 5

Let V be an inner product space, and $\phi : \mathcal{X} \to V$. Then,

$$\psi(x, y) = \|\phi(x) - \phi(y)\|^2$$

is a negative definite kernel on $\mathcal{X}$.

Proof. [Exercise]

Relation Between Positive and Negative Definite Kernels

Lemma 6

Let $\psi(x,y)$ be a hermitian kernel on $\mathcal{X}$. Fix $x_0 \in \mathcal{X}$ and define

$$\varphi(x,y) = -\psi(x,y) + \psi(x,x_0) + \psi(x_0,y) - \psi(x_0,x_0).$$

Then, ψ is negative definite if and only if φ is positive definite.

Proof. "If" part is easy (exercise). Suppose ψ is neg. def. Take any $x_i \in \mathcal{X}$ and $c_i \in \mathbb{C}$ $(1 = 1, \ldots, n)$. Define $c_0 = -\sum_{i=1}^n c_i$. Then,

$$\begin{aligned}
0 &\geq \textstyle\sum_{i,j=0}^n c_i \overline{c_j} \psi(x_i,x_j) \qquad\qquad \text{[for } x_0, x_1, \ldots, x_n\text{]} \\
&= \textstyle\sum_{i,j=1}^n c_i \overline{c_j} \psi(x_i,x_j) + \overline{c_0} \sum_{i=1}^n c_i \psi(x_i,x_0) + c_0 \sum_{j=1}^n c_i \psi(x_0,x_j) \\
&\qquad + |c_0|^2 \psi(x_0,x_0) \\
&= \textstyle\sum_{i,j=1}^n c_i \overline{c_j} \{\psi(x_i,x_j) - \psi(x_i,x_0) - \psi(x_0,x_j) + \psi(x_0,y_0)\} \\
&= -\textstyle\sum_{i,j=1}^n c_i \overline{c_j} \varphi(x_i,x_j).
\end{aligned}$$

Schoenberg's Theorem

Theorem 7 (Schoenberg's theorem)

Let $\mathcal{X}$ be a nonempty set, and $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ be a kernel. ψ is negative definite if and only if $\exp(-t\psi)$ is positive definite for all $t > 0$.

Proof.

If part:

$$\psi(x, y) = \lim_{t \downarrow 0} \frac{1 - \exp(-t\psi(x, y))}{t}.$$

Only if part: We can prove only for $t = 1$. Take $x_0 \in \mathcal{X}$ and define

$$\varphi(x, y) = -\psi(x, y) + \psi(x, x_0) + \psi(x_0, y) - \psi(x_0, x_0).$$

φ is positive definite (Lemma 6).

$$e^{-\psi(x,y)} = e^{\varphi(x,y)} e^{-\psi(x,x_0)} \overline{e^{-\psi(y,x_0)}} e^{\psi(x_0,x_0)}.$$

This is also positive definite. $\square$

Generating New Kernels I

Proposition 8

If $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ *is negative definite and* $\psi(x,x) \geq 0$*. Then, for any* $0 < p \leq 1$*,*

$$\psi(x,y)^p$$

is negative definite.

Proof. Use the formula

$$z^p = \frac{p}{\Gamma(1-p)} \int_0^\infty t^{-p-1}(1 - e^{-tz})dt \quad (z \in \mathbb{C}).$$

Then,

$$\psi(x,y)^p = \frac{p}{\Gamma(1-p)} \int_0^\infty t^{-p-1}(1 - e^{-t\psi(x,y)})dt$$

The integrand is negative definite for all $t > 0$. $\square$.

Generating New Kernels II

- For any $0 \le p \le 2$,

$$\|x - y\|^p$$

is negative definite on $\mathbb{R}^m$.

- For any $0 \le p \le 2$ and $\alpha > 0$,

$$\exp(-\alpha \|x - y\|^p)$$

is positive definite on $\mathbb{R}^n$.

  - $\alpha = 2 \Rightarrow$ Gaussian kernel.
  - $\alpha = 1 \Rightarrow$ Laplacian kernel.

Generating New Kernels III

Proposition 9

If $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is negative definite and $\mathrm{Re}\psi(x,y) \geq 0$. Then, for any $a > 0$,

$$\frac{1}{\psi(x,y) + a}$$

is positive definite.

Proof.

$$\frac{1}{\psi(x,y) + a} = \int_0^\infty e^{-t(\psi(x,y)+a)} dt.$$

The integrand is positive definite for all $t > 0$. $\square$.

For any $0 < p \leq 2$,

$$\frac{1}{1 + \|x - y\|^p}$$

is positive definite on $\mathbb{R}^m$. ($p = 2$: Cauchy kernel.)

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Positive definite functions

Definition. Let $\phi : \mathbb{R}^n \to \mathbb{C}$ be a function. ϕ is called a positive definite function (or function of positive type) if

$$k(x, y) = \phi(x - y)$$

is a positive definite kernel on $\mathbb{R}^n$, *i.e.*,

$$\sum_{i,j=1}^{n} c_i \overline{c_j} \phi(x_i - x_j) \geq 0$$

for any $x_1, \ldots, x_n \in \mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{C}$.

- A positive definite kernel of the form $\phi(x - y)$ is called shift invariant (or translation invariant).
- Examples: Gaussian and Laplacian kernels.

Bochner's theorem I

The Bochner's theorem characterizes *all* the continuous shift-invariant kernels on $\mathbb{R}^n$.

Theorem 10 (Bochner)

Let ϕ be a continuous function on $\mathbb{R}^n$. Then, ϕ is positive definite if and only if there is a finite non-negative Borel measure Λ on R^n such that

$$\phi(x) = \int e^{\sqrt{-1}\omega^T x} d\Lambda(\omega).$$

- ϕ is the inverse Fourier (or Fourier-Stieltjes) transform of Λ.
- Roughly speaking, the shift invariant functions are the class that have non-negative Fourier transform.

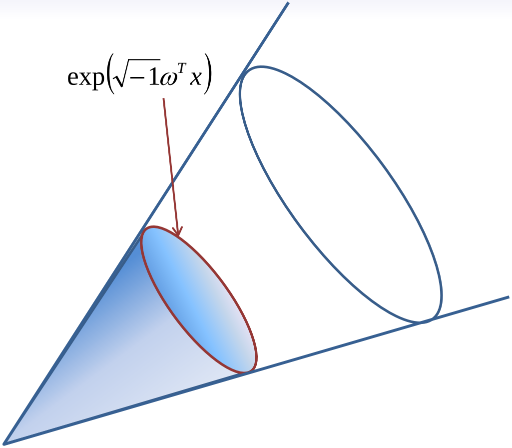
Bochner's Theorem II

- The Fourier kernel $e^{\sqrt{-1}x^T\omega}$ is a positive definite function for every $\omega \in \mathbb{R}^n$.

$$\exp(\sqrt{-1}(x-y)^T\omega) = \exp(\sqrt{-1}x^T\omega)\overline{\exp(\sqrt{-1}y^T\omega)}.$$

- The set of all positive definite functions is a convex cone, which is closed under the pointwise-convergence topology.

- The generator of the convex cone is the Fourier kernels $\{e^{\sqrt{-1}x^T\omega} \mid \omega \in \mathbb{R}^n\}$.



The closed cone of positive definite functions.

Bochner's theorem III

- Example on $\mathbb{R}$: (positive constants are neglected)

p.d. function	Fourier transform
$\exp(-\frac{1}{2\sigma^2}x^2)$	$\exp(-\frac{\sigma^2}{2}\|\omega\|^2)$
$\exp(-\alpha\|x\|)$	$\dfrac{1}{\omega^2+\alpha^2}$
$\dfrac{1}{x^2+\alpha^2}$	$\exp(-\alpha\|\omega\|)$

- Bochner's theorem can be extended to toplogical groups and semigroups [BCR84].

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Explicit Realization of RKHS by Bochner's Theorem I

Assume in the Bochner's theorem $d\Lambda = \rho(\omega)d\omega$, *i.e.*,

$$k(x, y) = \int e^{\sqrt{-1}\omega^T(x-y)}\rho(\omega)d\omega,$$

$\rho(\omega)$ is continuous for every ω, and $\int \rho(\omega)d\omega < \infty$.
(*e.g.* Gaussian, Laplacian, Cauchy.)

Then, the RKHS $\mathcal{H}_k$ is given by[1]

$$\mathcal{H}_k = \Big\{ f \in L^2(\mathbb{R}^m, dx) \;\Big|\; \int \frac{|\hat{f}(t)|^2}{\rho(t)} dt < \infty \Big\},$$

$$\langle f, g \rangle_{\mathcal{H}_k} = \int \frac{\hat{f}(t)\overline{\hat{g}(t)}}{\rho(t)} dt.$$

[1] $\hat{f}$ denotes the Fourier transform defined by $\hat{f} = \frac{1}{(2\pi)^m}\int e^{-\sqrt{1}\omega^T x} f(x)dx$.

Explicit Realization of RKHS by Bochner's Theorem II

- $\mathcal{H}_k$ is a Hilbert space consisting of functions on $\mathbb{R}^m$.
- $\langle \cdot, \cdot \rangle_{\mathcal{H}_k}$ defines an inner product on $\mathcal{H}_k$.
- $k(\cdot, x)$ is the reproducing kernel of $\mathcal{H}_k$:
  Proof. From
  $$k(x, y) = \int e^{\sqrt{-1}\omega^T(x-y)} \rho(\omega) d\omega = \int e^{\sqrt{-1}\omega^T x} e^{-\sqrt{-1}\omega^T y} \rho(\omega) d\omega,$$
  the Fourier transform of $k(\cdot, y)$ (y fixed) is given by
  $$\widehat{k(\cdot, y)}(\omega) = e^{-\sqrt{-1}\omega^T y} \rho(\omega).$$
  Thus,
  $$\langle f, k(\cdot, y) \rangle_{\mathcal{H}_k} = \int \frac{\hat{f}(\omega) e^{\sqrt{-1}\omega^T y} \rho(\omega)}{\rho(\omega)} d\omega$$
  $$= \int \hat{f}(\omega) e^{\sqrt{-1}\omega^T y} d\omega = f(y).$$

Examples

- Gaussian RBF kernel: $\rho(t) = \frac{1}{2\pi}\exp\{-\frac{\sigma^2}{2}\omega^2\}$,

$$\mathcal{H}_k = \Big\{ f \in L^2(\mathbb{R}, dx) \,\Big|\, \int |\hat{f}(\omega)|^2 \exp\big(\frac{\sigma^2}{2}\omega^2\big) d\omega < \infty \Big\},$$

$$\langle f, g \rangle_{\mathcal{H}_k} = \int \hat{f}(\omega)\overline{\hat{g}(\omega)} \exp\big(\frac{\sigma^2}{2}\omega^2\big) d\omega$$

- Laplacian kernel: $\rho(\omega) = \frac{1}{2\pi}\frac{1}{\omega^2+\beta^2}$,

$$\mathcal{H}_k = \Big\{ f \in L^2(\mathbb{R}, dx) \,\Big|\, \int |\hat{f}(\omega)|^2 (\omega^2 + \beta^2) dt < \infty \Big\},$$

$$\langle f, g \rangle = \int \hat{f}(\omega)\overline{\hat{g}(\omega)} (\omega^2 + \beta^2) d\omega.$$

- Cauchy kernel: $\rho(\omega) = \frac{1}{2\pi} e^{-\alpha|\omega|}$,

$$\mathcal{H}_k = \left\{ f \in L^2(\mathbb{R}, dx) \;\Big|\; \int |\hat{f}(\omega)|^2 e^{\alpha|\omega|} d\omega < \infty \right\},$$

$$\langle f, g \rangle_{\mathcal{H}_k} = \int \hat{f}(\omega) \overline{\hat{g}(\omega)} e^{\alpha|\omega|} d\omega.$$

- Note in the above three examples the RKHS's admits different decay rates of frequency.

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Complete Orthonormal System

- A subset $\{u_i\}_{i \in I}$ of $\mathcal{H}$ is called an orthonormal system (ONS) if $(u_i, u_j) = \delta_{ij}$ (δ_{ij} is Kronecker's delta).
- A subset $\{u_i\}_{i \in I}$ of $\mathcal{H}$ is called a complete orthonormal system (CONS) (orthonormal basis) if it is ONS and if $(x, u_i) = 0$ ($\forall i \in I$) implies $x = 0$.
- A Hilbert space is called separable if it has a countable CONS.

Fourier Expansion

Theorem 11 (Fourier series expansion)

Let $\{u_i\}_{i=1}^{\infty}$ *be a CONS of a separable Hilbert space. For each* $x \in \mathcal{H}$*,*

$$x = \sum_{i=1}^{\infty} (x, u_i) u_i, \qquad \textit{(Fourier expansion)}$$

$$\|x\|^2 = \sum_{i=1}^{\infty} |(x, u_i)|^2. \qquad \textit{(Parseval's equality)}$$

Proof omitted.

Example: CONS of $L^2([0\ 2\pi], dx)$

$$u_n(t) = \frac{1}{\sqrt{2\pi}} e^{\sqrt{-1}nt} \qquad (n = 0, 1, 2, \dots)$$

Then,

$$f(t) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} a_n e^{\sqrt{-1}nt}$$

is the (ordinary) Fourier expansion of a periodic function.

Bounded Operator I

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. A linear transform $T : \mathcal{H}_1 \to \mathcal{H}_2$ is often called operator.

Definition. A linear operator $\mathcal{H}_1$ and $\mathcal{H}_2$ is called bounded if

$$\sup_{\|x\|_{\mathcal{H}_1}=1} \|Tx\|_{\mathcal{H}_2} < \infty.$$

The operator norm of a bounded operator T is defined by

$$\|T\| = \sup_{\|x\|_{\mathcal{H}_1}=1} \|Tx\|_{\mathcal{H}_2} = \sup_{x \neq 0} \frac{\|Tx\|_{\mathcal{H}_2}}{\|x\|_{\mathcal{H}_1}}.$$

(Corresponds to the largest singular value of a matrix.)

Fact. If $T : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded,

$$\|Tx\|_{\mathcal{H}_2} \leq \|T\| \|x\|_{\mathcal{H}_1}.$$

Bounded Operator II

Proposition 12

A linear operator is bounded if and only if it is continuous.

Proof. Assume $T : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded. Then,

$$\|Tx - Tx_0\| = \|T(x - x_0)\| \leq \|T\|\|x - x_0\|$$

means continuity of T.

Assume T is continuous. For any $\varepsilon > 0$, there is $\delta > 0$ such that $\|Tx\| < \varepsilon$ for all $x \in \mathcal{H}_1$ with $\|x\| < 2\delta$.
Then,

$$\sup_{\|x\|=1} \|Tx\| = \sup_{\|x\|=\delta} \frac{1}{\delta}\|Tx\| \leq \frac{\varepsilon}{\delta}.$$

□

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Overview

Hermitian kernel:

$K \Longrightarrow T_K \Longrightarrow$ Eigendecomposition of T_K in L^2

self-adjoint operator

$\Downarrow$

Eigendecomposition of K in L^2

$$K(x,y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)}$$

Positive definite kernel on a compact set:

$K \Longrightarrow T_K \Longrightarrow$ Eigendecomposition of T_K in L^2

positive self-adjoint operator

$\Downarrow$

Eigendecomposition of K

$$K(x,y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)}$$

uniformly and absolutely

Hilbert-Schmidt Operator I

$\mathcal{H}$: separable Hilbert space.

Definition. An operator T on $\mathcal{H}$ is called Hilbert-Schmidt if for a CONS $\{\varphi_i\}_{i=1}^{\infty}$

$$\sum_{i=1}^{\infty} \|T\varphi_i\|^2 < \infty,$$

and its Hilbert-Schmidt norm $\|T\|_{HS}$ is defined by

$$\|T\|_{HS} = \left(\sum_{i=1}^{\infty} \|T\varphi_i\|^2\right)^{1/2}.$$

- $\|T\|_{HS}$ does not depend on the choice of a CONS.

  $\because$) From Parseval's equality, for a CONS $\{\psi_j\}_{j=1}^{\infty}$,

$$\begin{aligned}\|T\|_{HS}^2 = \sum_{i=1}^{\infty} \|T\varphi_i\|^2 &= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} |(\psi_j, T\varphi_i)|^2 \\ &= \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} |(T^*\psi_j, \varphi_i)|^2 = \sum_{j=1}^{\infty} \|T^*\psi_j\|^2.\end{aligned}$$

Hilbert-Schmidt Operator II

- Fact: $\|T\| \leq \|T\|_{HS}$.

  ($\because$) Let u_1 be the unit vector such that $\|Tu_1\| \geq \|T\| - \varepsilon$. Make CONS including u_1 and compute $\|T\|_{HS}^2$.)

- Hilbert-Schmidt norm is an extension of Frobenius norm of a matrix:

$$\|T\|_{HS}^2 = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} |(\psi_j, T\varphi_i)|^2.$$

  $(\psi_j, T\varphi_i)$ is the component of the matrix expression of T with the CONS's $\{\varphi_i\}$ and $\{\psi_j\}$.

Integral Kernel

$(\Omega, \mathcal{B}, \mu)$: measure space.

$K(x,y)$: measurable function on $\Omega \times \Omega$ such that

$$\int_\Omega \int_\Omega |K(x,y)|^2 d\mu(x) d\mu(y) < \infty. \qquad \text{(square integrability)}$$

Def. Operator $T_K : L^2(\Omega,\mu) \to L^2(\Omega,\mu)$ by

$$(T_K f)(x) = \int_\Omega K(x,y) f(y) d\mu(y) \qquad (f \in L^2(\Omega,\mu)).$$

T_K: integral operator with integral kernel K.

Fact: $T_K f \in L^2(\Omega,\mu)$.

$$\begin{aligned} \because) \quad \int |T_K f(x)|^2 dx &= \int \left| \int K(x,y) f(y) d\mu(y) \right|^2 d\mu(x) \\ &\leq \int \int |K(x,y)|^2 d\mu(y) \int |f(y)|^2 d\mu(y) d\mu(x) \\ &= \int \int |K(x,y)|^2 d\mu(x) d\mu(y) \|f\|_{L^2}^2. \end{aligned}$$

Hilbert-Schmidt Operator and Integral Kernel I

Theorem 13

Let $(\Omega, \mathcal{B}, \mu)$ be a measure space, and assume $L^2(\Omega, \mu)$ is separable. Then, T_K is a Hilbert-Schmidt operator, and

$$\|T_K\|_{HS}^2 = \int\int_{\Omega\times\Omega} |K(x,y)|^2 d\mu(x) d\mu(y).$$

Proof. Let $\{\varphi_i\}$ be a CONS. From Parseval's equality,

$$\int |K(x,y)|^2 dy = \sum_i \left|(K(x,\cdot), \varphi_i)_{L^2}\right|^2 = \sum_i \left|\int K(x,y)\overline{\varphi_i(y)} dy\right|^2 = \sum_i |T_K \overline{\varphi_i}(x)|^2.$$

Integrate w.r.t. x, ($\{\overline{\varphi_i}\}$ is also a CONS)

$$\int\int |K(x,y)|^2 dx dy = \sum_i \|T_K \overline{\varphi_i}\|^2 = \|T_K\|_{HS}^2.$$

$\square$

Hilbert-Schmidt Operator and Integral Kernel II

Converse is also true!

Theorem 14

Let $(\Omega, \mathcal{B}, \mu)$ *be a measure space, and assume* $L^2(\Omega, \mu)$ *is separable. For any Hilbert-Schmidt operator* T *on* $L^2(\Omega, \mu)$*, there is a square integrable kernel* $K(x, y)$ *such that*

$$T\varphi = \int K(x, y)\varphi(y)d\mu(y) \ \ \big(= T_K\varphi\big).$$

Proof omitted.

Hilbert-Schmidt Expansion I

- $(\Omega, \mathcal{B}, \mu)$: measure space.
- $K(x, y)$: Hermitian ($K(y, x) = \overline{K(x, y)}$) square integrable kernel.

- Fact: T_K is self-adjoint, *i.e.*,

$$(T_K f, g) = (f, T_K g) \qquad (\forall f, g \in L^2(\Omega, \mu)).$$

Proof.

$$\begin{aligned}(T_K f, g) &= \int\int K(x, y) f(y) \overline{g(x)} d\mu(x) d\mu(Y) \\ &= \int f(y) \overline{\int K(y, x) g(x) d\mu(x)} d\mu(y) = (f, T_K g).\end{aligned}$$

- For Hermite kernels, T_K admits eigendecompsition in an analogous way to Hermitian (or symmetric) matrices.

Hilbert-Schmidt Expansion II

A self-adjoint Hilbert-Schmidt operator admits Hilbert-Schmidt expansion:

- Every eigenvalue of T_K is a real value.
- The eigenspace of each eigenvalue is finite dimensional.
- Let

  $$|\lambda_1| \geq |\lambda_2| \geq \cdots > 0$$

  be the non-zero eigenvalues (counted as multiplicity).
- Let ϕ_i be the unit eigenvector w.r.t. λ_i.
- Hilbert-Schmidt expansion

$$T_K f = \sum_{i=1}^{\infty} \lambda_i (f, \phi_i) \phi_i.$$

Hilbert-Schmidt Expansion III

Theorem 15

Let K be a Hermitian square integrable kernel, and λ_i, ϕ_i as above.

$$K(x,y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)}$$

in $L^2(\Omega \times \Omega, \mu \times \mu)$.

(Proof omitted.) This is a generalization of eigendecomposition.

c.f. A: $m \times m$ Hermitian (or symmetric) matrix.
$\{\lambda_i\}_{i=1}^m$: the eigenvalues of A. u_i: unit eigenvector w.r.t. λ_i.
Then,

$$A = \sum_{i=1}^{m} \lambda_i u_i u_i^*,$$

$$Av = \sum_{i=1}^{m} \lambda_i (v, u_i) u_i.$$

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Integral Kernel and Positive Definiteness I

Consider positive definite $K(x, y)$.

Proposition 16 (Positive definiteness)

Let D be a compact subset of $\mathbb{R}^m$, and $K(x, y)$ be a continuous symmetric kernel on $\Omega \times \Omega$.
$K(x, y)$ is positive definite on Ω if and only if

$$\int\int_{D\times D} K(x, y) f(x) \overline{f(y)} dxdy \geq 0$$

for any $f \in L^2(D)$.

c.f. Definition of positive definiteness:

$$\sum_{i,j} K(x_i, x_j) c_i \overline{c_j} \geq 0.$$

Integral Kernel and Positive Definiteness II

Proof.

($\Rightarrow$). For a continuous function f, a Riemann sum satisfies

$$\sum_{i,j} K(x_i, x_j) f(x_i) \overline{f(x_j)} |E_i||E_j| \geq 0.$$

The integral is the limit of such sums, thus non-negative. For $f \in L^2(\Omega, \mu)$, approximate it by a continuous function.

($\Leftarrow$). Omitted. See [Fuk10, Sec. 6.3]

Integral Operator by Positive Definite Kernel

D: compact subset of $\mathbb{R}^m$.

$K(x, y)$: continuous positive definite kernel on D.

$$(T_K f)(x) = \int_D K(x, y) f(y) dy \qquad (f \in L^2(D))$$

Fact: Recall from Proposition 16

$$(T_K f, f)_{L^2(D)} \geq 0 \qquad (\forall f \in L^2(D)).$$

In particular, every eigenvalue of T_K is non-negative.

Mercer's Theorem

$\{\lambda_i\}_{i=1}^{\infty}$ $(\lambda_1 \geq \lambda_2 \geq \cdots > 0)$, $\{\phi_i\}_{i=1}^{\infty}$: the positive eigenvalues and unit eigenfunctions of T_K.

From Hilbert-Schmidt expansion,

$$K(x, y) = \textstyle\sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)},$$

in $L^2(D \times D)$.

Theorem 17 (Mercer)

Let K be a continuous positive definite kernel on a compact subset D in $\mathbb{R}^m$. Then,

$$K(x, y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)},$$

where the convergence is absolute and uniform over $D \times D$.

Proof is omitted. See [RSN65], Sec. 98, or [Ito78], Chap. 13.

Explicit Expression of RKHS

Let $K(x, y)$ be a continuous positive definite kernel on a compact subset D in $\mathbb{R}^m$.

$\{\lambda_i\}_{i=1}^{\infty}$ ($\lambda_1 \geq \lambda_2 \geq \cdots > 0$), $\{\phi_i\}_{i=1}^{\infty}$: the positive eigenvalues and unit eigenfunctions of T_K.

By adding the northonormal basis of $\mathcal{N}(T_K)$, we have a CONS $\{\phi_i\}$ of $\mathcal{H}_K$ consisting of eigenvectors of T_K.

Theorem 18

$$\mathcal{H}_k = \left\{ f \in L^2(D) \;\middle|\; f = \sum_{i=1}^{\infty} a_i \phi_i, \sum_{i=1}^{\infty} \frac{|a_i|^2}{\lambda_i} < \infty \right\},$$

and for $f = \sum_{i=1}^{\infty} a_i \phi_i$ *and* $g = \sum_{i=1}^{\infty} b_i \phi_i$*,*

$$\langle f, g \rangle_{\mathcal{H}_k} = \sum_{i=1}^{\infty} \frac{a_i \overline{b_i}}{\lambda_i},$$

where a_i *and* b_i *are set 0 if* $\lambda_i = 0$*.*

- It is not difficult to show $\mathcal{H}_k$ is a Hilbert space.
- Reproducing property:
  First note that by Mercer's theorem,

$$\textstyle\sum_{i=1}^{\infty} \lambda_i |\phi_i(x)|^2 < \infty,$$

  which means $K(\cdot, x) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\cdot) \overline{\phi_i(x)} \in \mathcal{H}_k$.
  For arbitrary $f = \sum_{i=1} a_i \phi_i \in \mathcal{H}_k$

$$\langle f, K(\cdot, x) \rangle = \sum_{i=1}^{\infty} \frac{a_i \lambda_i \phi_i(x)}{\lambda_i} = \sum_{i=1}^{\infty} a_i \phi_i(x) = f(x).$$

- *C.f.*, RKHS on a finite set.

Positive and negative definite kernels

- Review on positive definite kernels
- Negative definite kernel and its relation to positive definite kernel

Bochner's theorem

- Bochner's theorem
- Explicit form of some RKHS

Mercer's theorem

- Basic facts of Hilbert space
- Integral operator and Hilbert-Schmidt operator
- Mercer's theorem

Restriction, Sum, and Product of RKHS

- Restriction, Sum, and Product of RKHS

Restriction of RKHS

k: positive definite kernel on a set $\mathcal{X}$. $\mathcal{H}_k$: corresponding RKHS.
$\mathcal{Y}$: subset of $\mathcal{X}$.

$\tilde{k}$: restriction of k to $\mathcal{Y} \times \mathcal{Y}$ $\Rightarrow$ positive definite kernel on $\mathcal{Y}$.

Theorem 19

The RKHS corresponding to $\tilde{k}$ is $\{f|_{\mathcal{Y}} \mid f \in \mathcal{H}_k\}$.

Sum of RKHS

k_1, k_2: positive definite kernels on a set $\mathcal{X}$.
$\mathcal{H}_1, \mathcal{H}_2$: corresponding RKHS's.

$k_1 + k_2$: positive definite kernel on $\mathcal{X}$.

Theorem 20

The RKHS corresponding to $k_1 + k_2$ is given by

$$\mathcal{H} = \{f_1 + f_2 : \mathcal{X} \to \mathbb{R} \mid f_1 \in \mathcal{H}_1, f_2 \in \mathcal{H}_2\},$$

and its norm is given by

$$\|f\|_{\mathcal{H}}^2 = \min\{\|f_1\|_{\mathcal{H}_1}^2 + \|f_2\|_{\mathcal{H}_2}^2 \mid f = f_1 + f_2, f_1 \in \mathcal{H}_1, f_2 \in \mathcal{H}_2\}.$$

Product of RKSH

k_1, k_2: positive definite kernels on set $\mathcal{X}_1, \mathcal{X}_2$, resp.
$\mathcal{H}_1, \mathcal{H}_2$: corresponding RKHS's.

$k((x_1, x_2), (y_1, y_2)) := k_1(x_1, y_1)k_2(x_2, y_2)$: positive definite kernel on $\mathcal{X}_1 \times \mathcal{X}_2$.

Theorem 21

The RKHS corresponding to k is the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Corollary 22

If k_1 and k_2 are positive definite kernels on $\mathcal{X}$, the RKHS corresponding to $k(x, y) = k_1(x, y)k_2(x, y)$ is the restriction of $\mathcal{H}_1 \otimes \mathcal{H}_2$ to the diagonal set $\{(x, x) \in \mathcal{X} \times \mathcal{X} \mid x \in \mathcal{X}\}$.

Tensor Product

Define inner product space $\mathcal{H}_1 \tilde{\otimes} \mathcal{H}_2$ by

$$\mathcal{H}_1 \tilde{\otimes} \mathcal{H}_2 := \left\{ \sum_{i=1}^{n} f_i^{(1)} \otimes f_i^{(2)} \;\middle|\; f_i^{(1)} \in \mathcal{H}_1, f_i^{(2)} \in \mathcal{H}_2, i = 1, \ldots, n \right\}.$$

$$\left\langle \sum_{i=1}^{n} f_i^{(1)} \otimes f_i^{(2)}, \sum_{j=1}^{m} g_j^{(1)} \otimes g_j^{(2)} \right\rangle := \sum_{i=1}^{n} \sum_{j=1}^{m} \langle f_i^{(1)}, g_j^{(1)} \rangle_{\mathcal{H}_1} \langle f_i^{(2)}, g_j^{(2)} \rangle_{\mathcal{H}_2}.$$

The tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the completion of $\mathcal{H}_1 \tilde{\otimes} \mathcal{H}_2$.

Summary of Section 5

- Negative definite kernels and positive definite kernels are related by Schoenberg's theorem.
- Various examples of positive definite kernels can be derived by functional operations.
- Bochner's theorem: characterization of continuous shift-invariant kernels on $\mathbb{R}^m$ by Fourier transform.
- Based on Bochner's theorem, RKHS for shift-invariant kernels can be written explicitly by Fourier transform.
- Mercer's theorem: eigendecomposition of positive definite kernel.

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