Kernel Method: Data Analysis with Positive Definite Kernels

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

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Outline

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

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  Bochner’s theorem
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Restriction, Sum, and Product of RKHS
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) $ak_1 + bk_2$ ($a, b \geq 0$).
2. (product) $k_1 k_2$ ($k_1(x, y)k_2(x, y)$).
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.
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,

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

is positive definite. In particular,

$$f(x)f(y)$$

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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Restriction, Sum, and Product of RKHS
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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)* \[ a\psi_1 + b\psi_2 \quad (a, b \geq 0). \]
2. *(limit)* \[ \lim_{i \to \infty} \psi_i(x, y), \quad \text{assuming the limit exists.} \]

- The set of all negative definite kernels is a closed convex cone.
- Multiplication does not preserve negative definiteness.
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]
Lemma 6

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

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

Then, $\psi$ is negative definite if and only if $\varphi$ is positive definite.

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

$$0 \geq \sum_{i,j=0}^{n} c_i \overline{c_j} \psi(x_i, x_j) \quad [\text{for } x_0, x_1, \ldots, x_n]$$

$$= \sum_{i,j=1}^{n} c_i \overline{c_j} \psi(x_i, x_j) + \overline{c_0} \sum_{i=1}^{n} c_i \psi(x_i, x_0) + c_0 \sum_{j=1}^{n} c_i \psi(x_0, x_j)$$

$$+ |c_0|^2 \psi(x_0, x_0)$$

$$= \sum_{i,j=1}^{n} c_i \overline{c_j} \left\{ \psi(x_i, x_j) - \psi(x_i, x_0) - \psi(x_0, x_j) + \psi(x_0, y_0) \right\}$$

$$= -\sum_{i,j=1}^{n} c_i \overline{c_j} \varphi(x_i, x_j).$$
Theorem 7 (Schoenberg’s theorem)

Let $X$ be a nonempty set, and $\psi : X \times X \to \mathbb{C}$ be a kernel. \( \psi \) 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 $x_0 \in X$ and define

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

$\varphi$ is positive definite (Lemma 6).

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

This is also positive definite.
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 \( t > 0 \). \( \square \).
For any \( 0 \leq p \leq 2 \),
\[
\| x - y \|_p
\]
is negative definite on \( \mathbb{R}^m \).

For any \( 0 \leq p \leq 2 \) and \( \alpha > 0 \),
\[
exp(-\alpha \| x - y \|_p)
\]
is positive definite on \( \mathbb{R}^n \).
- \( \alpha = 2 \Rightarrow \text{Gaussian kernel} \).
- \( \alpha = 1 \Rightarrow \text{Laplacian kernel} \).
Proposition 9

If \( \psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C} \) is negative definite and \( \Re \psi(x, y) \geq 0 \). 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 $\phi : \mathbb{R}^n \rightarrow \mathbb{C}$ be a function. $\phi$ 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.
The Bochner’s theorem characterizes *all* the continuous shift-invariant kernels on $\mathbb{R}^n$.

**Theorem 10 (Bochner)**

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

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

- $\phi$ is the inverse Fourier (or Fourier-Stieltjes) transform of $\Lambda$.
- Roughly speaking, the shift invariant functions are the class that have non-negative Fourier transform.
The Fourier kernel $e^{\sqrt{-1}x^T\.\omega}$ is a positive definite function for every $\omega \in \mathbb{R}^n$.

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

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 $\{e^{\sqrt{-1}x^T\omega} \mid \omega \in \mathbb{R}^n\}$. 

Bochner’s Theorem II
The closed cone of positive definite functions.

\[ \exp(\sqrt{-1} \omega^T x) \]
Bochner’s theorem III

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

<table>
<thead>
<tr>
<th>p.d. function</th>
<th>Fourier transform</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\exp\left(-\frac{1}{2\sigma^2} x^2\right)$</td>
<td>$\exp\left(-\frac{\sigma^2}{2}</td>
</tr>
<tr>
<td>$\exp(-\alpha</td>
<td>x</td>
</tr>
<tr>
<td>$\frac{1}{x^2 + \alpha^2}$</td>
<td>$\exp(-\alpha</td>
</tr>
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- Bochner’s theorem can be extended to topological groups and semigroups [BCR84].
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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 \( \omega \), and \( \int \rho(\omega)d\omega < \infty \).
(e.g. Gaussian, Laplacian, Cauchy.)

Then, the RKHS \( \mathcal{H}_k \) is given by\(^1\)

\[
\mathcal{H}_k = \left\{ f \in L^2(\mathbb{R}^m, dx) \mid \int \frac{|\hat{f}(t)|^2}{\rho(t)}dt < \infty \right\},
\]

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

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

$$\hat{k}(\cdot, y)(\omega) = e^{-\sqrt{-1}\omega^Ty} \rho(\omega).$$

Thus,

$$\langle f, k(\cdot, y) \rangle_{\mathcal{H}_k} = \int \frac{\hat{f}(\omega) e^{\sqrt{-1}\omega^Ty} \rho(\omega)}{\rho(\omega)} d\omega$$

$$= \int \hat{f}(\omega) e^{\sqrt{-1}\omega^Ty} d\omega = f(y).$$
Examples

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

\[
\mathcal{H}_k = \left\{ f \in L^2(\mathbb{R}, dx) \mid \int |\hat{f}(\omega)|^2 \exp\left(\frac{\sigma^2}{2} \omega^2 \right) d\omega < \infty \right\},
\]

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

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

\[
\mathcal{H}_k = \left\{ f \in L^2(\mathbb{R}, dx) \mid \int |\hat{f}(\omega)|^2 (\omega^2 + \beta^2) dt < \infty \right\},
\]

\[
\langle f, g \rangle = \int \hat{f}(\omega)\overline{\hat{g}(\omega)} (\omega^2 + \beta^2) d\omega.
\]
• Cauchy kernel: $\rho(\omega) = \frac{1}{2\pi} e^{-\alpha|\omega|},$

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

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

• Note in the above three examples the RKHS’s admits different decay rates of frequency.
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• A subset \( \{ u_i \}_{i \in I} \) of \( \mathcal{H} \) is called an orthonormal system (ONS) if \( (u_i, u_j) = \delta_{ij} \) (\( \delta_{ij} \) 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 \( x \in \mathcal{H} \),

\[
x = \sum_{i=1}^{\infty} (x, u_i) u_i,
\]

(Fourier expansion)

\[
\|x\|^2 = \sum_{i=1}^{\infty} |(x, u_i)|^2.
\]

(Parseval’s equality)

Proof omitted.

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

\[
u_n(t) = \frac{1}{\sqrt{2\pi}} e^{\sqrt{-1}nt} \quad (n = 0, 1, 2, \ldots)
\]

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

\[
\|Tx\| < \varepsilon \text{ for all } x \in \mathcal{H}_1 \text{ with } \|x\| < 2\delta.
\]

Then,

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

\[
\text{\therefore From Parseval's equality, for a CONS } \{ \psi_j \}_{j=1}^{\infty},
\]

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

\[
= \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} |(T^* \psi_j, \varphi_i)|^2 = \sum_{j=1}^{\infty} \| T^* \psi_j \|^2.
\]
• Fact: $\|T\| \leq \|T\|_{HS}$.

(vature) 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

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

**Def.** Operator \(T_K : L^2(\Omega, \mu) \rightarrow L^2(\Omega, \mu)\) by

\[
(T_K f)(x) = \int_{\Omega} K(x, y) f(y) d\mu(y) \quad (f \in L^2(\Omega, \mu)).
\]

\(T_K\): integral operator with integral kernel \(K\).

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

\[
\therefore \int |T_K f(x)|^2 dx = \int \left| \int K(x, y) f(y) d\mu(y) \right|^2 d\mu(x)
\leq \int \int |K(x, y)|^2 d\mu(y) \int |f(y)|^2 d\mu(y) d\mu(x)
= \int \int |K(x, y)|^2 d\mu(x) d\mu(y) \|f\|_{L^2}^2.
\]
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

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

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

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

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

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

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

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.,

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

**Proof.**

$$
(T_K f, g) = \int \int K(x, y) f(y) \overline{g(x)} d\mu(x) d\mu(y) \\
= \int f(y) \int K(y, x) \overline{g(x)} d\mu(x) d\mu(y) = (f, T_K g).
$$

- For Hermite kernels, $T_K$ admits eigendecomposition 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 $\phi_i$ be the unit eigenvector w.r.t. $\lambda_i$.
- Hilbert-Schmidt expansion

$$T_K f = \sum_{i=1}^{\infty} \lambda_i (f, \phi_i) \phi_i.$$
Theorem 15

Let $K$ be a Hermitian square integrable kernel, and $\lambda_i, \phi_i$ as above.

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

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. $\lambda_i$.

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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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 $\Omega$ if and only if

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

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

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

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

**Fact:** Recall from Proposition 16

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

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,

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

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

**Theorem 18**

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

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

\[
\langle f, g \rangle_{\mathcal{H}_k} = \sum_{i=1}^{\infty} \frac{a_i \bar{b}_i}{\lambda_i},
\]

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,
  \[
  \sum_{i=1}^{\infty} \lambda_i |\phi_i(x)|^2 < \infty, 
  \]
  which means $K(\cdot, x) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\cdot) \overline{\phi_i(x)} \in \mathcal{H}_k$.
  For arbitrary $f = \sum_{i=1}^{\infty} a_i \phi_i \in \mathcal{H}_k$

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

• 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 \( \{ f\mid_{\mathcal{Y}} \mid f \in \mathcal{H}_k \} \).*
$k_1, k_2$: 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

$$\|f\|_{\mathcal{H}}^2 = \min\{\|f_1\|_{\mathcal{H}_1}^2 + \|f_2\|_{\mathcal{H}_2}^2 \mid f = f_1 + f_2, f_1 \in \mathcal{H}_1, f_2 \in \mathcal{H}_2\}.$$
$k_1, k_2$: 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 $\{(x, x) \in \mathcal{X} \times \mathcal{X} \mid x \in \mathcal{X}\}$.***
Define inner product space $\mathcal{H}_1 \tilde{\otimes} \mathcal{H}_2$ by

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

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

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.
References


*Harmonic Analysis on Semigroups.*


*Introduction to Kernel Method (in Japanese).*
Asakura Shoten, 2010.

[Ito78] Seizo Ito.

*Kansu-Kaiseki III (Iwanami kouza Kiso-suugaku).*

[RSN65] Frigyes Riesz and Béla Sz.-Nagy.

*Functional Analysis (2nd ed.).*