Theory of Positive Definite Kernel and Reproducing Kernel Hilbert Space
Statistical Inference with Reproducing Kernel Hilbert Space

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Outline

1 Positive and negative definite kernels
   - Review on positive definite kernels
   - Negative definite kernel
   - Operations that generate new kernels

2 Bochner’s theorem
   - Bochner’s theorem

3 Mercer’s theorem
   - Mercer’s theorem
1. Positive and negative definite kernels
   - Review on positive definite kernels
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2. Bochner’s theorem
   - Bochner’s theorem

3. Mercer’s theorem
   - Mercer’s theorem
Review: operations that preserve positive definiteness

Proposition 1

If \( k_i : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C} \) (\( i = 1, 2, \ldots \)) 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)** \( \lim_{i \rightarrow \infty} k_i(x, y) \), 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.
Corollary 3 (Normalization)

Let $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C}$ be a positive definite kernel. If $k(x, x) > 0$ for any $x \in \mathcal{X}$, then

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

is positive definite. This is called normalization of $k$.

Note that

$$|\tilde{k}(x, y)| \leq 1$$

for any $x, y \in \mathcal{X}$.

Example: Polynomial kernel $k(x, y) = (x^Ty + c)^d$ ($c > 0$).

$$\tilde{k}(x, y) = \frac{(x^Ty + c)^d}{(x^Tx + c)^{d/2}(y^Ty + c)^{d/2}}.$$
1. Positive and negative definite kernels
   - Review on positive definite kernels
   - **Negative definite kernel**
   - Operations that generate new kernels

2. Bochner’s theorem
   - Bochner’s theorem

3. Mercer’s theorem
   - Mercer’s theorem
Definition. A function $\psi : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{C}$ 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 pos. def. kernel because of the condition $\sum_{i=1}^{n} c_i = 0$. 
Properties of negative definite kernels

**Proposition 4**

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

\[(2) \quad \sum_{i,j=1}^{n} c_i c_j = \sum_{i=1}^{n} c_i \sum_{j=1}^{n} c_j = 0.\]

**Proposition 5**

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

- The set of all negative definite kernels is closed (w.r.t. pointwise convergence) convex cone.
- Multiplication does not preserve negative definiteness.
Example of negative definite kernel

Proposition 6

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. Suppose \( \sum_{i=1}^{n} c_i = 0 \).

\[
\sum_{i,j=1}^{n} c_i c_j \|\phi(x_i) - \phi(x_j)\|^2 = \sum_{i,j=1}^{n} c_i c_j \left\{ \|\phi(x_i)\|^2 + \|\phi(x_j)\|^2 - (\phi(x_i), \phi(x_j)) - (\phi(x_j), \phi(x_i)) \right\}
\]

\[
= \sum_{i=1}^{n} c_i \|\phi(x_i)\|^2 \sum_{j=1}^{n} c_j + \sum_{j=1}^{n} c_j \|\phi(x_j)\|^2 \sum_{i=1}^{n} c_i
\]

\[
- (\sum_{i=1}^{n} c_i \phi(x_i), \sum_{j=1}^{n} c_j \phi(x_j)) - (\sum_{j=1}^{n} c_j \phi(x_j), \sum_{i=1}^{n} c_i \phi(x_i))
\]

\[
= -\|\sum_{i=1}^{n} c_i \phi(x_i)\|^2 - \|\sum_{i=1}^{n} c_i \phi(x_i)\|^2 \leq 0
\]
Relation between positive and negative definite kernels

Lemma 7

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

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

$$
0 \geq \sum_{i,j=0}^{n} c_i \overline{c_j} \psi(x_i, x_j) \quad \text{[for} \quad x_0, x_1, \ldots, x_n \text{]} \\
= \sum_{i,j=1}^{n} c_i \overline{c_j} \psi(x_i, x_j) + \overline{c_0} \sum_{i=1}^{n} c_i \psi(x_i, x_0) + c_0 \sum_{j=1}^{n} c_i \psi(x_0, x_j) \\
+ |c_0|^2 \psi(x_0, x_0) \\
= \sum_{i,j=1}^{n} c_i \overline{c_j} \left\{ \psi(x_i, x_j) - \psi(x_i, x_0) - \psi(x_0, x_j) + \psi(x_0, y_0) \right\} \\
= -\sum_{i,j=1}^{n} c_i \overline{c_j} \varphi(x_i, x_j).
$$
Schoenberg’s theorem

Theorem 8 (Schoenberg’s theorem)

Let $\mathcal{X}$ be a nonempty set, and $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ 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 $x_0 \in \mathcal{X}$ 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 7).

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

This is also positive definite.
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Proposition 9

If $\psi : X \times X \to \mathbb{C}$ 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 following formula.

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

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

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

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

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

- $\alpha = 2 \Rightarrow$ Gaussian kernel. $\alpha = 1 \Rightarrow$ Laplacian kernels.
Proposition 10

If $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C}$ is negative definite and $\psi(x, x) \geq 0$. Then,

$$\log(1 + \psi(x, y))$$

is negative definite.

Proof.

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

□.
Corollary 11

If \( \psi : \mathcal{X} \times \mathcal{X} \rightarrow (0, \infty) \) is negative definite. Then,

\[
\log \psi(x, y)
\]

is negative definite.

Proof. For any \( c > 0 \),

\[
\log(\psi + 1/c) = \log(1 + c\psi) - \log c
\]

is negative definite. Take the limit of \( c \rightarrow \infty \).

- \( \psi(x, y) = x + y \) is negative definite on \( \mathbb{R} \).
- \( \psi(x, y) = \log(x + y) \) is negative definite on \( (0, \infty) \).
More examples IV

**Proposition 12**

If \( \psi : \mathcal{X} \times \mathcal{X} \to \mathbb{C} \) is negative definite and \( \text{Re} \psi(x, y) \geq 0 \). 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 \( t > 0 \).

For any \( 0 < p \leq 2 \),

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

is positive definite on \( \mathbb{R} \).
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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).
- Gaussian and Laplacian kernels are examples of shift-invariant positive definite kernels.
The Bochner’s theorem characterizes all the continuous shift-invariant kernels on $\mathbb{R}^n$.

**Theorem 13 (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.
Bochner’s theorem II

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

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

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

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

\[
\exp\left(-\frac{1}{2\sigma^2}x^2\right) \quad \exp\left(-\frac{\sigma^2}{2} |\omega|^2\right) \\
\exp(-\alpha|x|) \quad \frac{1}{\omega^2 + \alpha^2}
\]

- Bochner’s theorem is extended to topological groups and semigroups [BCR84].
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Integral characterization of positive definite kernels I

Ω: compact Hausdorff space.
μ: finite Borel measure on Ω.

Proposition 14

Let \( K(x, y) \) be a continuous function on \( \Omega \times \Omega \).
\( K(x, y) \) is a positive definite kernel on \( \Omega \) if and only if

\[
\int_{\Omega} \int_{\Omega} K(x, y) f(x) \overline{f(y)} \, dx \, dy \geq 0
\]

for each function \( f \in L^2(\Omega, \mu) \).

c.f. Definition of positive definiteness:

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

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

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

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

($\Leftarrow$). Suppose

$$\sum_{i,j=1}^{n} c_i \overline{c_j} K(x_i, x_j) = -\delta < 0.$$ 

By continuity of $K$, there is an open neighborhood $U_i$ of $x_i$ such that

$$\sum_{i,j=1}^{n} c_i \overline{c_j} K(z_i, z_j) \leq -\delta/2.$$ 

for all $z_i \in U_i$.

We can approximate $\sum_i \frac{c_i}{\mu(U_i)} I_{U_i}$ by a continuous function $f$ with arbitrary accuracy.
Integral Kernel

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

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

$$\int_{\Omega} \int_{\Omega} |K(x,y)|^2 \, dx \, dy < \infty. \quad \text{(square integrability)}$$

Define an operator $T_K$ on $L^2(\Omega, \mu)$ by

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

$T_K$: integral operator with integral kernel $K$.

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

$$\therefore \quad \int |T_K f(x)|^2 \, dx = \int \left\{ \int K(x,y) f(y) \, dy \right\}^2 \, dx \leq \int \int |K(x,y)|^2 \, dy \int |f(y)|^2 \, dy \, dx = \int \int |K(x,y)|^2 \, dx \, dy \| f \|^2_{L^2}.$$
Hilbert-Schmidt operator I

\( \mathcal{H} \): separable Hilbert space.

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

\[
\sum_{i=1}^{\infty} \| T \varphi_i \|^2 < \infty.
\]

For a Hilbert-Schmidt operator \( T \), the 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.

\( \therefore \) 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: $\|T\| \leq \|T\|_{HS}$.

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 $\{\psi_j\}$. 
Recall

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

with square integrable kernel \(K\).

**Theorem 15**

Assume \(L^2(\Omega, \mu)\) is separable. Then, \(T_K\) is a Hilbert-Schmidt operator, and

\[\|T_K\|_{HS}^2 = \int \int |K(x, y)|^2 \, dx \, dy.\]

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

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

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

\[\int \int |K(x, y)|^2 \, dx \, dy = \sum_i \|T_K \overline{\varphi_i}\|^2 = \|T_K\|_{HS}^2.\]
Converse is true!

**Theorem 16**

*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*

$$T\varphi = \int K(x, y)\varphi(y)dy.$$  

**Outline of the proof.**

Fix a CONS $\{\varphi_i\}$. Define

$$K_n(x, y) = \sum_{i=1}^{n} (T\varphi_i)(x)\overline{\varphi_i(y)} \quad (n = 1, 2, 3, \ldots).$$

We can show $\{K_n(x, y)\}$ is a Cauchy sequence in $L^2(\Omega \times \Omega, \mu \times \mu)$, and the limit works as $K$ in the statement.
Integral operator by positive definite kernel

\( \Omega \): compact Hausdorff space.
\( \mu \): finite Borel measure on \( \Omega \).

\( K(x, y) \): continuous positive definite kernel on \( \Omega \).

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

**Fact:** From Proposition 14

\[(T_K f, f)_{L^2(\Omega, \mu)} \geq 0 \quad (\forall f \in L^2(\Omega, \mu)).\]

In particular, any eigenvalue of \( T_K \) is non-negative.
Mercer’s theorem

\( K(x, y) \): continuous positive definite kernel on \( \Omega \).

\( \{\lambda_i\}_{i=1}^{\infty}, \{\varphi_i\}_{i=1}^{\infty} \): the positive eigenvalues and eigenfunctions of \( T_K \).

\[ \lambda_1 \geq \lambda_2 \geq \cdots > 0, \quad \lim_{i \to \infty} \lambda_i = 0. \]

\[ T_K \varphi_i = \lambda_i \varphi_i, \quad \int K(x, y) \varphi_i(y) dy = \lambda_i \varphi_i(x). \]

**Theorem 17 (Mercer)**

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

where the convergence is absolute and uniform over \( \Omega \times \Omega \).

Proof is omitted. See [RSN65], Section 98, or [Ito78], Chapter 13.
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