Other Topics in Kernel Method

Statistical Inference with Reproducing Kernel Hilbert Space

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Outline

1. Relation to functional data analysis
2. Spline smoothing
3. Relation to random process

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3. Relation to random process

Functional data analysis

For functional data analysis, see Ramsay & Silverman (2005)

- What are functional data?

Data: $f_1(t),\ f_2(t),\ \ldots,\ f_N(t)$ -- functions on an interval $[a, b]$

Example: Berkeley Growth Study

See http://www.psych.mcgill.ca/misc/fda/index.html

Converting raw data into functional form

- Data are often given by a set of $\{(t_j,\ y_i(t_j)) \mid i = 1, \ldots, N,\ j = 1,\ldots, m_i\}$.
- Converting data by smoothing

  For each i, fit a curve $\phi_i(t)$ to individual data $\{(t_j,\ y_i(t_j)) \mid j = 1,\ldots, m_i\}$ by smoothing (e.g. B-spline)
- The converted data are of the form

$$\phi(t) = c_1\theta_1(t) + \cdots + c_\ell\theta_\ell(t), \qquad \theta_1(t),\ldots,\theta_\ell(t): \text{basis functions}$$

Analysis on functional data

- Apply linear methods to the “converted data” in a function space (typically L^2).
- Examples:
  - Functional PCA
  - Functional CCA
  - Functional linear modeling, etc.

Functional PCA

Functional data: $\phi_1(t), \ldots, \phi_N(t)$ (already converted)

Find a function to maximize

$$\mathrm{Var}_{emp}\left[\int \phi_i(t) f(t) dt\right] \qquad \text{subj.to} \quad \int f(t)^2 dt = 1.$$

Variance of the projections
on the direction of *f*

If basis functions $\theta_1(t), \ldots, \theta_\ell(t)$ are used,

$$\phi_i(t) = \sum_{j=1}^{\ell} c_{ij}\theta_j(t), \qquad f(t) = \sum_{j=1}^{\ell} \beta_j \theta_j(t)$$

Solve: $\max_\beta \beta^T V \beta \qquad \text{subj.to} \quad \beta^T R \beta = 1.$

where $V_{jk} = \frac{1}{N}\sum_{i=1}^{N}\sum_{s,t=1}^{\ell} c_{is}c_{it}R_{js}R_{kt}, \quad R_{jk} = \int \theta_j(t)\theta_k(t)dt.$

The integral in R is computed numerically, or by the property of the basis

Kernel method v.s. functional data analysis

- Similarity
  - Both the methods extends linear methods to “functional data”.

- Difference
  - In kernel methods, the data conversion is given by a positive definite kernel, while in FDA the data are assumed to be functional.
  - Kernel methods use RKHS as a function space, while the FDA uses L2 space in principle.

- Roughness penalty in FDA
  - In FDA, smoothness is sometimes imposed on the solution.

$$\int f(t)^2 = 1 \quad \Longrightarrow \int f(t)^2 + \lambda \int |Df(t)|^2 dt = 1$$

This is essentially the Sobolev norm (RKHS).

With roughness penalty, FDA is more similar to kernel methods.

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1. Relation to functional data analysis

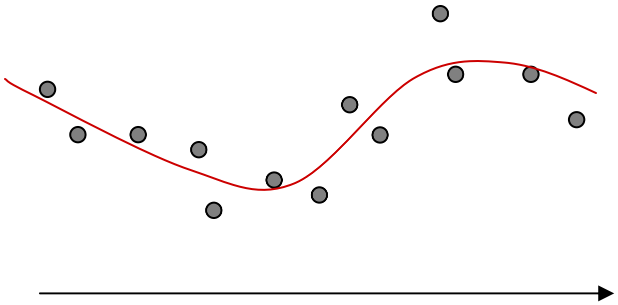
2. Spline smoothing

3. Relation to random process

Spline smoothing

$(X_1, Y_1), \ldots, (X_N, Y_N) \ : \ X_i \in \mathbf{R}^n, \ Y_i \in \mathbf{R}$

P: differential operator on $\mathbf{R}^n$



Spline smoothing:

$$\min_f \sum_{i=1}^{N} \left(Y^i - f(X^i) \right)^2 + \lambda \int | Pf(x) |^2 \, dx$$

Roughness penalty

Laplacian and Green function

- **Laplacian** $$\Delta f = \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \cdots + \frac{\partial^2 f}{\partial x_n^2}$$

Self-adjoint: if $|f(x)|, |g(x)| \rightarrow 0 \ (x \to \infty)$

$$\int \Delta f(x) g(x) dx = \int f(x) \Delta g(x) dx$$

- **Green function for Laplacian**

$$\Delta G(x,\xi) = \delta(x-\xi)$$

i.e. $$\int \Delta G(x,\xi) f(x) d\xi = f(\xi)$$

– Green function solves a differential equation: $\Delta f = \varphi$ given φ.

$\Longrightarrow$ $$f(x) = \int G(x,y)\varphi(y) dy$$

$\because$) $f(\xi) = \int f(x)\Delta G(x,\xi)dx = \int \Delta f(x) G(x,\xi)dx = \int \varphi(x) G(x,\xi) dx$

Smoothing penalty

- Regularization term

Consider functions on $\mathbf{R}^n$ for simplicity (no boundary)

$$J_m^n(f) = \sum_{\alpha_1+\cdots+\alpha_n=m} \frac{m!}{\alpha_1!\alpha_2!\cdots\alpha_n!} \left\| D^\alpha f \right\|_{L^2}^2$$

L^2 norm of m-th derivative

$$= \sum_{\alpha_1+\cdots+\alpha_n=m} \frac{m!}{\alpha_1!\alpha_2!\cdots\alpha_n!} \int \left| \frac{\partial^m f}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \cdots \partial x_n^{\alpha_n}} \right|^2 dx$$

– example (n = m = 2)

$$J_2^2(f) = \int \left\{ \left| \frac{\partial^2 f}{\partial x_1^2} \right|^2 + 2 \left| \frac{\partial^2 f}{\partial x_1 \partial x_2} \right|^2 + \left| \frac{\partial^2 f}{\partial x_2^2} \right|^2 \right\} dx$$

Smoothing

$$\min_f \sum_{i=1}^{N} \left(Y^i - f(X^i) \right)^2 + \lambda \sum_{m=0}^{\infty} a_m J_m^n(f) \qquad (a_m \geq 0)$$

Expression by Laplacian

Partial integral shows

$$J_m^n(f) = (-1)^m \left(f, \Delta^m f \right)_{L^2}$$

The smoothing problem is expressed by

$$\min_f \sum_{i=1}^{N} \left(Y^i - f(X^i) \right)^2 + \lambda \left(f, Af \right)_{L^2}$$

where $A = \sum_{m=0}^{\infty} (-1)^m a_m \Delta^m$

Two cases

- Case $a_0 \neq 0$
  - The Green function is a positive definite kernel.
  - The penalty term is equal to the squared RKHS norm.

- Case $a_0 = 0$
  - Spline smoothing
  - The Green functions is conditionally positive definite.
  - The functional space is RKHS + polynomial of some order
  - The penalty term is equal to the squared RKHS norm of the projection of f onto the RKHS.

$a_0 \neq 0$: RKHS regularization

- Solution

$$\min_f \sum_{i=1}^{N}\left(Y^i - f(X^i)\right)^2 + \lambda(f, Af)_{L^2}$$

Variational calculus

$$\sum_{i=1}^{N}\left(Y^i - f(x)\right)\delta(x - X^i) + \lambda Af = 0$$

$$Af = -\frac{1}{\lambda}\sum_{i=1}^{N}\left(Y^i - f(x)\right)\delta(x - X^i)$$

If we have the Green function G for A $\;i.e.\; AG = \delta$

$$f(\xi) = -\frac{1}{\lambda}\sum_{i=1}^{N}\int (Y^i - f(x))\delta(x - X^i)G(x,\xi)dx$$

$$= -\frac{1}{\lambda}\sum_{i=1}^{N}(Y^i - f(X^i))G(\xi, X^i)$$

Note: $f(X_i)$ unknown

The solution is to have the form:

$$f = \sum_{i=1}^{N} c_i G(\cdot, X^i)$$

Plug it into the original problem:

$$\min_{c \in \mathbf{R}^N} \quad \sum_{i=1}^{N} \left(Y^i - \sum_{j=1}^{N} c_j G(X^i, X^j) \right)^2 + \lambda \sum_{i,j=1}^{N} c_i c_j G(X^i, X^j)$$

$$\because) \quad (Af, f)_{L^2} = \sum_{i.j} c_i c_j (AG(\cdot, X_i), G(\cdot, X_j))_{L^2} = \sum_{i.j} c_i c_j G(X_i, X_j)$$

By differentiation,

$$c = (G + \lambda I)^{-1} \mathbf{Y}$$

where $\quad G_{ij} = G(X^i, X^j) \quad \mathbf{Y} = (Y^1, \ldots, Y^N)^T$

The solution:

$$f(x) = \mathbf{Y}^T (G + \lambda I)^{-1} g(x)$$ where $g_i(x) = G(x, X^i)$

Green function

Theorem

If $a_0 \neq 0, a_j \neq 0 (\exists j \geq 1)$, the Green function of A is a positive definite kernel.

Proof.

Since A is shift invariant, so is G. Thus,

$$\sum_{m=0}^{\infty} (-1)^m a_m \Delta^m G(z) = \delta(z)$$

By Fourier transform

$$\sum_{m=0}^{\infty} a_m \|u\|^{2m} \widehat{G}(u) = \frac{1}{(2\pi)^{n/2}}$$

$$\widehat{G}(u) = \frac{1}{(2\pi)^{n/2}(a_0 + \sum_{m=1}^{\infty} a_m \|u\|^{2m})}$$

If $a_0 \neq 0, a_j \neq 0 (\exists j \geq 1)$, the Fourier inversion is possible.
Use Bochner's theorem.

Regularization by RKHS norm

Assume $a_0 \neq 0, a_1 \neq 0$

G: Green function of A.

H_G: RKHS w.r.t. G.

$$\min_f \quad \sum_{i=1}^{N} \left(Y^i - f(X^i) \right)^2 + \lambda \sum_{m=0}^{\infty} a_m J_m^n(f)$$

The solution is given by $f = \sum_{i=1}^{N} c_i G(\cdot, X^i)$

The penalty term is, then,

$$\sum_{m=0}^{\infty} a_m J_m^n(f) = \sum_{i,j} c_i c_j G(X_i, X_j) = \|f\|_{H_G}^2.$$

The above regularization is equivalent to the kernel ridge regression

$$\min_f \quad \sum_{i=1}^{N} \left(Y^i - f(X^i) \right)^2 + \lambda \| f \|_{H_G}^2$$

$a_0 = 0$: Spline smoothing

- Thin-plate spline

$$\min_f \sum_{i=1}^{N} \left(Y^i - f(X^i)\right)^2 + \lambda J_m^n(f)$$

$$J_m^n(f) = \sum_{\alpha_1+\cdots+\alpha_n=m} \frac{m!}{\alpha_1!\alpha_2!\cdots\alpha_n!} \left\| D^\alpha f \right\|_{L^2}^2$$

  – The Green function of J_m^n is not necessarily positive definite, but conditionally positive definite

  – The function space for f is

$$B_m^n: \quad D^\alpha f \in L^2(\mathbf{R}^n) \quad (|\alpha| = m)$$

and

$$J_m^n(f) = 0 \quad \Leftrightarrow \quad f \in \mathcal{P}_{m-1}$$

$\mathcal{P}_{m\text{-}1}$: Polynomials of degree at most m - 1

Let $B_m^n = \mathcal{P}_{m-1} \oplus H_*$ be decomposition by direct sum.

<u>Theorem</u> (Meinguet 1979)

If $m > n/2$, the subspace H_* is a RKHS with inner product

$$\langle f, g \rangle_{H_*} = \sum_{|\alpha|=m} \frac{m!}{\alpha_1! \cdots \alpha_n!} \left(D^\alpha f, D^\alpha g \right)_{L^2} = \left((-1)^m \Delta^m f, g \right)_{L^2}$$

In particular, the norm is given by

$$\| f \|_{H_*}^2 = J_m^n(f)$$

$$\min_f \quad \sum_{i=1}^N \left(Y^i - f(X^i) \right)^2 + \lambda J_m^n(f)$$

$\Longleftrightarrow$

$$\min_{g \in H_*, p \in \mathcal{P}_{m-1}} \quad \sum_{i=1}^N \left(Y^i - (g(X^i) + p(X^i)) \right)^2 + \lambda \| g \|_{H_*}^2$$

Solution of spline smoothing

By the representer theorem, the solution is to be of the form:

$$f(x) = \sum_{i=1}^{N} c_i K(x - X_i) + \sum_{\ell=1}^{M} b_\ell \phi_\ell (x)$$

By plugging it,

$$\min_{c,b} \quad (Y - Kc - Hb)^T (Y - Kc - Hb) + \lambda c^T K c$$

The solution:

$$(K + \lambda I)c + Hb = Y, \qquad H^T c = 0.$$

⇨

$$\begin{cases} c = (I_N - H(H^T H)^{-1} H^T)(K + \lambda I)^{-1} Y \\ b = (H^T H)^{-1} H^T (K + \lambda I)^{-1} Y \end{cases}$$

Conditionally positive definite

Definition. $K(x,y) : \Omega \times \Omega \rightarrow \mathbf{R}$ is said to be conditionally positive definite of order m if

1. $K(x,y) = K(y,x)$
2. If points $x_1, \ldots, x_n$ in Ω and real numbers $c_1,\ldots, c_n$ satisfy

$$\sum_{i=1}^{n} c_i p(x_i) = 0$$

for any polynomial $p(x) \in \mathcal{P}_{m-1}$ (generalized increment of order m), then

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

– A positive definite kernel is conditionally positive definite of order 0.
– A negative definite kernel is negation of a conditionally positive definite kernel of order 1.
– Intuition: the above $c_1,\ldots, c_n$ is a generalization of the m-th order difference. Thus, the definition intuitively says that the m-th derivative of K is positive definite.

1st order diff.: $\dfrac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i}$

Coeff. of $f(t_i)$

c_1	c_2	c_3	
$\frac{-1}{t_2 - t_1}$	$\frac{1}{t_2 - t_1}$	0	...
0	$\frac{-1}{t_3 - t_2}$	$\frac{1}{t_3 - t_2}$	

$c_1 + c_2 + \cdots + c_n = 0$ → coefficients of 1st order difference

2nd order diff.: $\left\{ \dfrac{f(t_{i+2}) - f(t_{i+1})}{t_{i+2} - t_{i+1}} - \dfrac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i} \right\} \Big/ t_{i+2} - t_{i+1}$

Coeff. of $f(t_i)$

c_1	c_2	c_3	c_4	
$\frac{1}{t_2 - t_1} \Big/ t_3 - t_2$	$\frac{-1}{t_2 - t_1} + \frac{-1}{t_3 - t_2} \Big/ t_3 - t_2$	$\frac{1}{t_3 - t_2} \Big/ t_3 - t_2$	0	...
0	$\frac{1}{t_3 - t_2} \Big/ t_4 - t_3$	$\frac{-1}{t_3 - t_2} + \frac{-1}{t_4 - t_3} \Big/ t_4 - t_3$	$\frac{1}{t_4 - t_3} \Big/ t_4 - t_3$	

$$\begin{cases} c_1 + c_2 + \cdots + c_n = 0 \\ c_1 \times t_1 + c_2 \times t_2 + \cdots + c_n \times t_n = 0 \end{cases}$$

→ coefficients of 2nd order difference

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Gaussian process

– A Gaussian process is a random process $\{X_t\}_{t\in\Omega}$ (random variables with index Ω) such that for any finite subset $\{t_1, ..., t_n\}$ of Ω, the random vector $(X_{t_1},\ldots,X_{t_n})$ is a Gaussian random vector.

– Mean function $\mu(t) = E[X_t]$

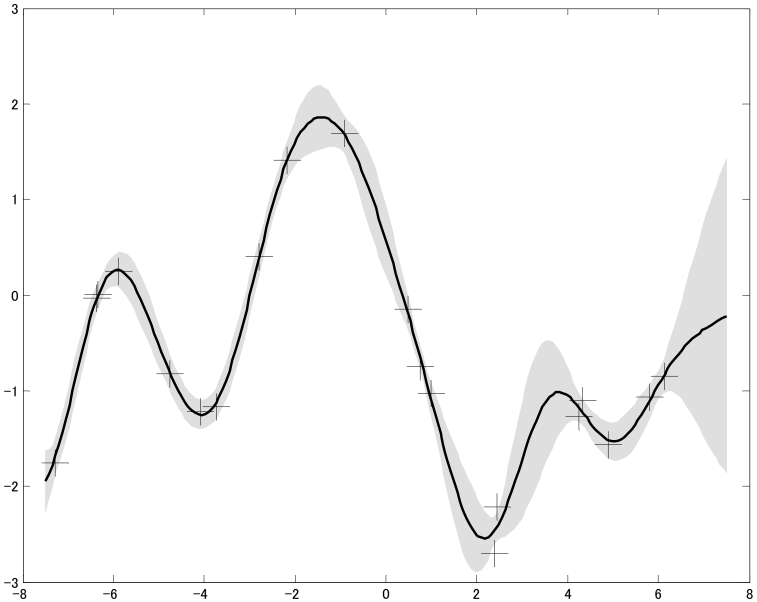
– Covariance function $R(t,s) = \mathrm{Cov}[X_t, X_s]$

– A Gaussian process is uniquely determined by the mean and covariance function.

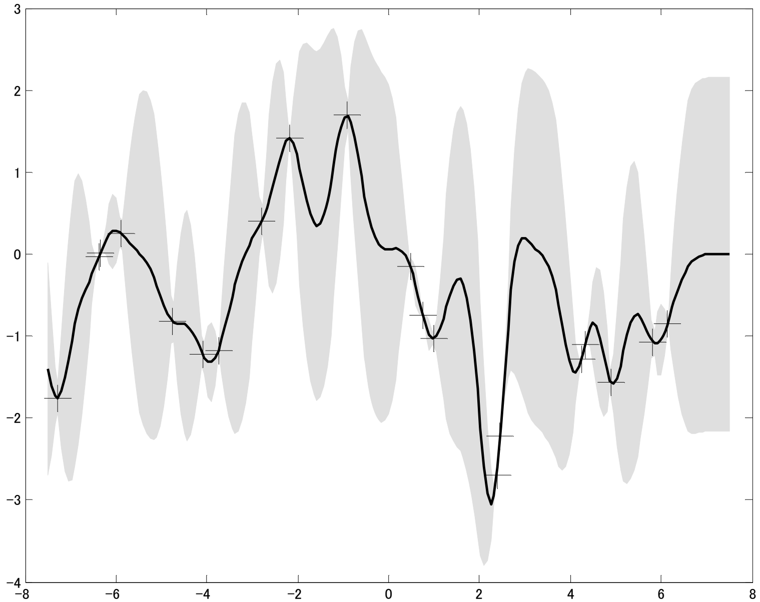
$$\mathbf{X} = (X_{t_1},\ldots,X_{t_n}) \sim N(\mu_{\mathrm{X}}, \Sigma_{\mathrm{X}})$$

$$\mu_{\mathbf{X}} = (\mu(t_1),\ldots,\mu(t_n)), \qquad \Sigma_{\mathbf{X}} = \begin{pmatrix} R(t_1,t_1) & R(t_1,t_2) & \cdots & R(t_1,t_n) \\ R(t_2,t_1) & R(t_2,t_2) & \cdots & R(t_2,t_n) \\ \vdots & \vdots & \ddots & \vdots \\ R(t_n,t_1) & R(t_n,t_2) & \cdots & R(t_n,t_n) \end{pmatrix}$$

– Examples



$\sigma = 1$



$\sigma = 0.3$

mean zero

covariance function $R(s,t) = \exp\left(-\frac{1}{2\sigma^2}(s-t)^2\right)$

Generated by Matlab gpml toolbox (Rasmussen and Williams)

Random process and positive definite kernel

- Covariance function is a positive definite kernel

<u>Theorem</u>

The covariance function $R(s,t)$ of a random process $\{X_t\}_{t\in\Omega}$ is a positive definite kernel.

$\because$) For simplicity, mean = 0.

$$\sum_{i,j=1}^n c_i c_j R(t_i,t_j) = \sum_{i,j=1}^n c_i c_j E[X_{t_i}, X_{t_j}]$$
$$= E\left[\sum_{i=1}^n c_i X_{t_i}, \sum_{j=1}^n c_j X_{t_j}\right] = E\left[\left(\sum_{i=1}^n c_i X_{t_i}\right)^2\right] \geq 0$$

– A random process on Ω determines a RKHS on Ω.

Positive definite kernel defines Gaussian process

$k(s,t)$: positive definite kernel on Ω.

For any finite subset $\mathbf{t} = (t_1, \ldots, t_n)$ of Ω, the Gram matrix $\Sigma_{\mathbf{t}} = (k(t_i, t_j))$ is always positive semidefinite.

By Kolmogorov extension theorem, there is a Gaussian process with index set Ω such that

$$\mathbf{X} = (X_{t_1}, \ldots, X_{t_n}) \quad \sim N(0, \Sigma_t)$$

The covariance function = $k(s,t)$.

RKHS by random process

$\{X_t\}_{t\in\Omega}$: random process on Ω with mean zero and finite 2nd moments.

$X_t : \Xi \to \mathbf{R}$ random variable defined by a probability space.

$\Rightarrow$

$$X_t \in L^2(\Xi, \mathcal{B}, P)$$

$$\overline{\mathcal{L}}(X) \equiv \overline{LH\{X_t \in L^2(\Xi) \mid t \in \Omega\}}$$ closed subspace of $L^2(\Xi)$

Hilbert space generated by $\{X_t\}_{t\in\Omega}$

Inner product

$$(U,V)_{\overline{\mathcal{L}}(\Xi)} = E[UV] \qquad U,V \in \overline{\mathcal{L}}(X)$$

(inner product of $L^2(\Xi)$)

RKHS and random process

<u>Theorem</u>

k : positive definite kernel on a set Ω

$\{X_t\}_{t\in\Omega}$: random process with mean 0 and covariance function k

⇨ $$\overline{\mathcal{L}}(X) \cong H_k \quad \text{(isomorphic as Hilbert space)}$$

$$X_t \leftrightarrow k(\cdot,t)$$

$$(U,V)_{\overline{\mathcal{L}}(\Xi)} = \langle f, g\rangle \qquad U \leftrightarrow f,\ V \leftrightarrow g$$

注） $$(X_t, X_s)_{\overline{\mathcal{L}}(\Xi)} = E[X_t X_s] = k(t,s) = \langle k(\cdot,t), k(\cdot,s)\rangle_{H_k}$$

(inner product) (cov) (reproducing)

Stationary process and shift-invariant kernel

- Stationary case

$\{X_t\}_{t\in\mathbb{R}^m}$: random process on $\mathbf{R}^m$

– stationary process

$$E[X_{t+h}X_{s+h}] = E[X_t X_s] \qquad (\forall t, s, h \in \mathbf{R}^m)$$

covariance function is given by

$$R(t,s) \equiv R(t-s)$$

– Positive definite kernel for a stationary process is given by

$$K(t,s) = K(t-s)$$

– Bochner's theorem ⇔ Wiener-Khinchine's theorem (covariance function of a stationary process on $\mathbf{R}^m$ is the inverse Fourier transform of the power spectral.)

Inference with random process

- Estimation of random process
  - Modeling by a random process

    X_t : random process on Ω with mean zero and finite 2nd moments

    $$Y_t = X_t + \varepsilon_t$$

    ε_t : noise indep. with X_t $E[\varepsilon_t] = 0,\ \mathrm{Cov}[\varepsilon_t, \varepsilon_s] = \sigma^2 \delta(t - s)$

    $R(t,s) = \mathrm{Cov}[X_t, X_s]$: known. σ^2 : known

  - Estimation

    Estimate X_{t_0} for t_0 given the observation $Y_{t_1}, \ldots, Y_{t_n}$

Minimizing mean square error

- Linear estimator for random process
  - Linear estimator

$$\hat{X}_{t_0} = \sum_{j=1}^{n} \alpha_j Y_{t_j}$$

  - Mean square error

$$\min E\,|X_{t_0} - \hat{X}_{t_0}|^2 = \min_{\alpha} E\,|X_{t_0} - \sum_{j=1}^{n} \alpha_j Y_{t_j}|^2$$

  - Least square error estimator

$$\hat{X}_{t_0} = \hat{\alpha}^T Y_{\mathbf{t}} = r^T (K + \sigma^2 I_n)^{-1} Y_{\mathbf{t}}$$

$$\because) \quad \min_{\alpha} \; \alpha^T (K + \sigma^2 I_n)\alpha - 2r^T \alpha$$

$$\Rightarrow \quad \hat{\alpha} = (K + \sigma^2 I_n)^{-1} r$$

Bayesian estimation of Gaussian process

– Joint probability

$$\begin{pmatrix} Y_{\mathbf{t}} \\ X_{t_0} \end{pmatrix} \sim N\left(0, \begin{pmatrix} K + \sigma^2 I_n & r \\ r^T & R(t_0, t_0) \end{pmatrix}\right)$$

where $K = (R(t_i, t_j)) \in \mathbf{R}^{n \times n}$ $\quad r = (R(t_i, t_0)) \in \mathbf{R}^{n}$

$\because)$ $E[Y_t, Y_s] = R(t,s) + \sigma^2 \delta(t-s),$ $\quad E[Y_t, X_s] = R(t,s)$

– Bayesian estimation = LSE estimation

$$E[X_{t_0} \mid Y_{\mathbf{t}}] = r^T (K + \sigma^2 I_n)^{-1} Y_{\mathbf{t}}$$

Gaussian process and regularization

- LSE estimation of a process ＝ Regularization with RKHS
  - Linear LSE estimator of a process (Bayesian estimator of Gaussian process)

$$\min E|X_{t_0} - \hat{X}_{t_0}|^2 = \min_{\alpha} E|X_{t_0} - \sum_{j=1}^{n} \alpha_j Y_{t_j}|^2$$

Sol. $$\hat{X}_{t_0} = r^T (K + \sigma^2 I_n)^{-1} Y_{\mathbf{t}}$$

  - Ridge regression on RKHS

$$\min_{f \in H} \sum_{i=1}^{N} (Y_i - f(t_i))^2 + \lambda \| f \|_H^2$$

Sol. $$f(t) = r(t)^T (K + \lambda I_N)^{-1} Y$$

identical

$\sigma^2 \Leftrightarrow \lambda$

Correspondence between RKHS and random process

RKHS	random process
Pos. def. kernel $K(\mathrm{t,s})$	Covariance fun. $K(\mathrm{t,s}) = \mathrm{E}[\mathrm{X_t},\mathrm{X_s}]$
$\sum c_i K(\cdot, t_i)$	$\sum c_i X_{t_i}$
$\lim \sum c_i K(\cdot, t_i)$ (completion)	$\lim \sum c_i X_{t_i}$ (closure)
Regularization (smoothing)	Linear estimation
$\min_{f \in H} \sum_{i=1}^{N} (Y_i - f(t_i))^2 + \lambda \Vert f \Vert_H^2$	$\min_{\alpha} E \lvert X_{t_0} - \sum_{j=1}^{n} \alpha_j Y_{t_j} \rvert^2$
$f(t) = r(t)^T (K + \lambda I_N)^{-1} Y$	$\hat{X}_{t_0} = r^T (K + \sigma^2 I_n)^{-1} Y_{\mathbf{t}}$
Shift-invariant kernel	Cov. fun. of a statinary process
$K(\mathrm{t,s}) = K(\mathrm{t-s})$	$K(\mathrm{t,s}) = K(\mathrm{t-s})$
Bochner's theorem	Wiener-Khinchine's theorem

Iterative random functions

m-IRF

A random process $\{X_t\}_{t\in\Omega}$ is said to be an m-iterative random functions (m-IRF) if for any finite subset $\mathbf{t} = (t_1, \ldots, t_n)$ of Ω and any generalized increment $c_1, \ldots, c_n$ of order m, the process

$$\left\{\sum_{i=1}^{n} c_i X_{t+t_i}\right\}_{t\in\Omega}$$

is second-order stationary.

– A stationary process is called (-1)-IRF in convention.

Modeling by non-stationary process

– Kriging is a modeling by 0-IRF.
The generalized covariance function $G(t\text{-}s)$ is used instead of covariance function $K(t, s)$ for the modeling.

Generalized covariance

<u>Theorem</u> (Matheron 1973)

$\{X_t\}_{t\in\Omega}$: continuous m-IRF.

There is a continuous function G_K such that for any finite subset $\mathbf{t} = (t_1, \ldots, t_n)$ of Ω and any two generalized increments $(c_1,\ldots, c_n)$ and $(d_1,\ldots, d_n)$ of order m,

$$\mathrm{Cov}\left[\sum_{i=1}^n c_i X_{t_i}, \sum_{i=1}^n d_i X_{t_i}\right] = \sum_{i,j=1}^n c_i d_i G_K(t_i - t_j).$$

– The function G_K is called generalized covariance.

– The generalized covariance is conditionally positive definite of order m (obvious by definition and above theorem).

– Matheron (1973) proves the converse, also. There is a correspondence between m-IRF and conditionally positive definite functions of order m.
(Generalization of the correspondence between the stationary processes and positive definite functions.)

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