INSA – Gaussian processes

Continuity and differentiability of sample functions

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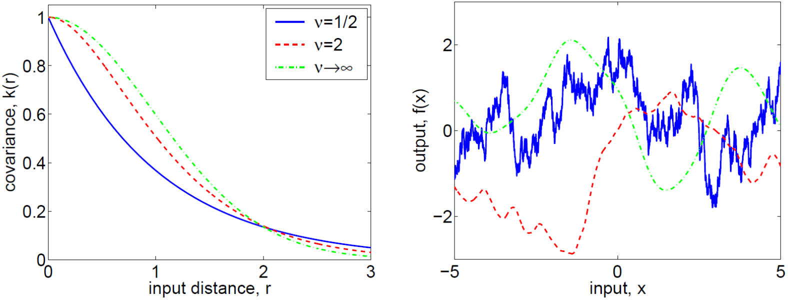
Introduction

- Regularity assumptions can be encoded in kernel functions:
  - periodicity, **smoothness**, stationarity, isotropy, ...



(left) Matérn covariance functions, (right) GP samples [Rasmussen and Williams, 2005]

Notation and preliminary remarks

- Let Y_t be a stochastic process (e.g. a GP): $\{Y(t), t \in \mathbb{R}\}$
- In the following, we assume that Y_t is centred, i.e. $\mathbb{E}\{Y_t\} = 0$
  - Otherwise, we consider $Z_t = Y_t - \mathbb{E}\{Y_t\}$ instead
- We denote $k(t, t') = \mathsf{cov}\{Y_t, Y_{t'}\}$ the covariance function
  - We assume stationary kernels $k(\tau) := k(t, t + \tau)$ (abuse of notation)

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Definition (Finite 2nd order moments)

A stochastic process Y_t has finite 2nd order moments if for all $t \in \mathbb{R}$:

$$\mathbb{E}\{|Y_t|^2\} < \infty.$$

This implies that $\mathbb{E}\{Y_t\}$ and $\mathbb{E}\{Y_t Y_{t'}\}$ are well defined for all $t, t' \in \mathbb{R}$.

- We denote L^2 the set of r.v's with finite 2nd order moments
- In the following, L^2 is a *Hilbert space* (3rd lecture), with inner product:

$$\langle X, Y \rangle = \mathbb{E}\{XY\}.$$

- We can also denote $k(t, t') = \langle Y_t, Y_{t'} \rangle$ since Y_t is a centred

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Outline

Sample functions properties in quadratic mean

Sample functions properties in quadratic mean

- There is no simple relationship between the covariance function k of a stochastic process Y and the **smoothness** of its realizations
- However, one can relate k to quadratic mean properties of Y:
  - Convergence
  - Continuity
  - Differentiability

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Convergence in quadratic mean

Definition (Convergence in quadratic mean)

Let $\{X_n\}_{n=1}^{\infty}$ be a random sequence, with r.v's $X_1, X_2, \ldots$ defined on the same probability space as a r.v. Y. Define $\mathbb{E}\left\{|X_n|^2\right\} < \infty$ (finite variances). $\{X_n\}$ converges in quadratic mean (q.m.), $X_n \xrightarrow{q.m.} X$, if there exists Y such that:

$$\|X_n - Y\|_{L^2} \to 0 \qquad \left(\text{i.e. } \mathbb{E}\left\{|X_n - Y|^2\right\} \to 0\right)$$

Theorem (Loeve criterion)

$\{X_n\}$ converge in q.m. iif $\mathbb{E}\{X_n X_m\} = \langle X_n, X_m \rangle$ converges to a finite limit c when $n, m \to \infty$ (independently).

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Proof.

· The "if" part follows from

$$\begin{aligned}\mathbb{E}\{|X_n - X_m|^2\} =& \mathbb{E}\left\{[X_n - X_m][X_n - X_m]\right\} \\ =& \mathbb{E}\left\{X_n X_n\right\} + \mathbb{E}\left\{X_m X_m\right\} - 2\mathbb{E}\left\{X_n X_m\right\} \\ =& c + c - 2c = 0\end{aligned}$$

· The "only if" part follows from

$$\mathbb{E}\left\{X_n X_m\right\} \to \mathbb{E}\left\{XX\right\} = \mathbb{E}\{|X|^2\}.$$

$\square$

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Continuity in quadratic mean

Definition (Continuity in quadratic mean)

A stochastic process Y_t is said to be continuous in q.m. at $t = t_0$ if

$$Y_t \xrightarrow{q.m.} Y_{t_0}.$$

Proposition

1. *Y_t is continuous in q.m. at $t = t_0$ iif $k(u, v)$ is continuous at (t_0, t_0)*
2. *If $k(u, v)$ is continuous at every diagonal point (t, t), then Y_t is continuous everywhere.*

Proof hints.

1. - For the "if" part, compute the expression $\mathbb{E}\left\{(Y_{t+\tau} - Y_t)^2\right\}$
   - For the "iff" part, use the equality

$$\begin{aligned} k(t+\tau, t+\nu) - k(t,t) &= \langle Y_{t+\tau} - Y_t, Y_{t+\nu} - Y_t \rangle \\ &+ \langle Y_{t+\tau} - Y_t, Y_t \rangle + \langle Y_{t+\nu} - Y_t, Y_t \rangle \end{aligned}$$

2. Use (1) and continuity of $\langle \cdot, \cdot \rangle$

Differentiability in quadratic mean

Definition (Differentiability in quadratic mean)

Y_t is differentiable in q.m. at t if $\frac{Y_{t+h}-Y_t}{h}$ converge in q.m.

Proposition

1. *If $\frac{\partial^2 k}{\partial u \partial v}$ exists at (t,t), then Y_t is differentiable in q.m. at t.*
2. *If $\frac{\partial^2 k}{\partial u \partial v}$ exists for every (t,t), then $\frac{\partial k}{\partial u}(u,v)$ and $\frac{\partial^2 k}{\partial u \partial v}(u,v)$ exist everywhere and we have:*

$$\operatorname{cov}\left\{Y'_u, Y_v\right\} = \frac{\partial k}{\partial u}(u,v) \quad \textit{and} \quad \operatorname{cov}\left\{Y'_u, Y'_v\right\} = \frac{\partial^2 k}{\partial u \partial v}(u,v)$$

Proof hints.

1. Apply Loeve criterion to $Z_n = \frac{Y_{t+h_n}-Y_t}{h_n}$ for any sequence $h_n \to 0$
2. For the 1st derivative, use (1) and compute $\langle \frac{Y_{u+h}-Y_u}{h}, Y_v \rangle$. Then, develop $\langle \frac{Y_{u+h}-Y_u}{h}, \frac{Y_{v+h}-Y_v}{h} \rangle$

Exercise.

1. Show that if $\frac{\partial^4 k}{\partial^2 u \partial^2 v}$ exist at (t, t), then Y_t is twice diff. in q.m. at t.
2. In addition, if $\frac{\partial^4 k}{\partial^2 u \partial^2 v}$ exists at every (t, t), then all the derivatives written below exist everywhere and we have:

$$\operatorname{cov}\left\{Y''_u, Y_v\right\} = \frac{\partial^2}{\partial u^2} k(u, v)$$

$$\operatorname{cov}\left\{Y''_u, Y'_v\right\} = \frac{\partial^3}{\partial u^2 \partial v} k(u, v)$$

$$\operatorname{cov}\left\{Y''_u, Y''_v\right\} = \frac{\partial^4}{\partial u^2 \partial v^2} k(u, v)$$

2nd order stationary processes

Definition (2nd order stationary processes)

Y_t is 2nd order stationary if for any t, τ, $\mathbb{E}\{Y_t\}$ and $\operatorname{cov}\{Y_t, Y_{t+\tau}\}$ do not depend on t.

· If Y_t is a centred process, then Y_t is stationary if $k(t, t')$ is a function of $t - t'$ (see also the definition from 1st lecture).

Proposition (continuity and differentiability)

Let Y_t be a stationary stochastic process.

1. *Y_t is continuous in q.m. at $t = t_0$ iif $k(\tau)$ is continuous at 0. In this case, Y_t is continuous everywhere.*
2. *If $k^{2p}(\tau)$ exists in an open set containing 0, then Y_t is differentiable in q.m. at order p everywhere.*

Proof hint. Show that the local properties of $k(\tau)$ at 0 imply the same properties to $k(u, v)$ at the diagonal points.

Challenges

· Continuity or differentiability in q.m. do not necessarily imply sample function continuity or differentiability.

· However, they can be easily related to stationary covariance functions

Equivalence

Definition (Equivalence)

We say that Y_t and Z_t are equivalent if they have the same finite-dimensional distributions for all $t \in \mathbb{R}$:

$$P(\{Y_t = Z_t\}) = 1$$

Remarks.

- This implies that two equivalent processes have the same family of finite-dimensional distributions
- Two equivalent processes do NOT have necessarily the same sample functions properties

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Example.

· Let Y_t and Z_t two stochastic processes defined over $[0, 1]$ by:

$$Y(t) = 0 \quad \forall t$$

$$Z(t) = \begin{cases} 1, & \text{if } t = \tau \text{ for } \tau \in [0,1] \\ 0, & \text{otherwise} \end{cases}$$

· Then Y_t and Z_t have the same finite-dimensional distributions but

$$P(\{Y_t \text{ is continuous in } [0,1]\}) = 1$$

$$P(\{Z_t \text{ is continuous in } [0,1]\}) = 0$$

Sample function properties

Sample function continuity

Theorem (Sample function continuity– Kolmogorov's theorem)

Let Y_t be a stochastic process defined over $[0,1]$. Suppose that, for all $t, t+h \in [0,1]$,

$$P(\{|Y_{t+h} - Y_t| \geq g(h)\}) \leq q(h),$$

where g and q are even functions of h, non increasing as $h \downarrow 0$, and such that

$$\sum_{n=1}^{\infty} g(2^{-n}) < \infty \quad \text{and} \quad \sum_{n=1}^{\infty} 2^n q(2^{-n}) < \infty.$$

Then, there exists an equivalent stochastic process Z_t whose sample functions are, with probability one, continuous in $[0,1]$.

Proof. See [Cramér and Leadbetter, 1967]

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Sample function continuity

Corollary

If with the notation above we have

$$\mathbb{E}\left\{|Y_{t+h} - Y_t|^p\right\} \leq c\,\frac{|h|}{|\log|h||^{1+r}},$$

where $p < r$ and c are positive constants, the conclusion of the theorem holds.

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Proof.

· Consider $g(h) := |\log|h||^{-b}$ with $1 < b < r/p$ and the Markov inequality: $P(|X| \geq a) \leq \mathbb{E}\{|X|^p\}/a^p$.

· By applying the Kolmogorov's theorem, we have

$$P(\{|Y_{t+h} - Y_t| \geq g(h)\}) \leq c\frac{|h|}{|\log|h||^{1+r-bp}} = q(h)$$

· Since $b > 1$, then

$$\sum_{n=1}^{\infty} g(2^{-n}) = \sum_{n=1}^{\infty} \frac{1}{|\log(2^{-n})|^b} = \frac{1}{(n\log 2)^b} < \infty$$

· Since $1 + r - bp > 1$, then

$$\sum_{n=1}^{\infty} 2^n q(2^{-n}) = \sum_{n=1}^{\infty} \frac{c}{|\log(2^{-n})|^{1+r-bp}} = \sum_{n=1}^{\infty} \frac{c}{[n\log(2)]^{1+r-bp}} < \infty$$

$\square$

Sample function continuity

Theorem (Stochastic processes with finite 2nd order moments)

Let Y_t be a stochastic process defined with finite second moments. If for all $t, t+h \in [a,b]$ the difference

$$\Delta_h^2 k(t,t) := k(t+h,t+h) - k(t+h,t) - k(t,t+h) - k(t,t)$$

satisfies the inequality $\Delta_h^2 k(t,t) < c\frac{|h|}{|\log|h||^q}$, with $q > 3$ and $c > 0$, then Y_t is equivalent to a stochastic process which, with probability one, is sample continuous.

Theorem (Stationary processes)

Let Y_t be a stationary stochastic process. If $k''(0)$ exists, then Y_t is equivalent to a stochastic process which, with probability one, is sample continuous, i.e. $Y_t \in \mathcal{C}$.

Proof hint. Apply Corollary with $p = 2$.

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Sample function differentiability

Theorem (Sample function differentiability)

Let Y_t be a stochastic process defined over $[0,1]$. Suppose that the hypothesis of Kolmogorov's theorem hold, and that, for all $t-h, t, t+h \in [0,1]$,

$$P(\{|Y_{t+h} + Y_{t-h} - 2Y_t| \geq g_1(h)\}) \leq q_1(h),$$

where g_1 and q_1 are even functions of h, non increasing as $h \downarrow 0$, and such that

$$\sum_{n=1}^{\infty} 2^n g_1(2^{-n}) < \infty \quad \text{and} \quad \sum_{n=1}^{\infty} 2^n q_1(2^{-n}) < \infty.$$

Then, Y_t is equivalent to a process which, with probability one, has continuous sample function derivatives in $[0,1]$.

Proof. See [Cramér and Leadbetter, 1967].

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Sample function differentiability

Corollary

If the conditions of the corollary of the Kolmogorov's theorem are satisfied, and if

$$\mathbb{E}\left\{|Y_{t+h} + Y_{t-h} - 2Y_t|^p\right\} \leq c\frac{|h|^{1+p}}{|\log|h||^{1+r}},$$

where $p < r$ and c are positive constants, the conclusion of the theorem holds.

Proof hint. Apply the Markov inequality.

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Sample function differentiability

Theorem (Stochastic processes with finite 2nd order moments)

Let Y_t be a stochastic process defined with finite second moments. If for all $t, t+h$, the 4th difference $\Delta_h^4 k(t,t)$ satisfies the inequality $\Delta_h^4 k(t,t) < c\frac{|h|^3}{|\log|h||^q}$, with $q > 3$ and $c > 0$, then Y_t is equivalent to a stochastic process which, with probability one, has continuous sample function derivatives.

Theorem (Stationary processes)

Let Y_t be a stationary stochastic process. If $k^{(4)}(0)$ exists, then Y_t is equivalent to a stochastic process which, with probability one, has continuous C^1 sample functions.

Proof hint. Apply Corollary with $p = 2$.

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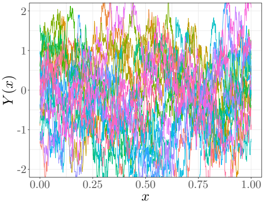
Theorem (Differentiability in high orders)

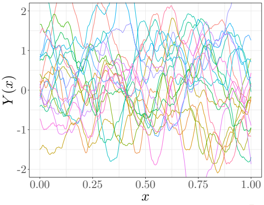
There are analogous results. In particular, if Y_t is a stationary stochastic process and if $k^{(2k+2)}(0)$ exists, then Y_t is equivalent to a process which, with probability one, has C^k sample functions.

Effects of 1D stationary kernels in GP samples

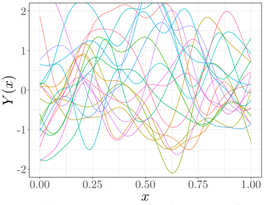
1D stationary kernel	$k_{\sigma^2,\ell}(\tau)$	Class
Exponential	$\sigma^2 \exp\left\{-\frac{\lvert\tau\rvert}{\ell}\right\}$	$\mathcal{C}$
Matérn 3/2	$\sigma^2 \left(1+\sqrt{3}\frac{\lvert\tau\rvert}{\ell}\right) \exp\left\{-\sqrt{3}\frac{\lvert\tau\rvert}{\ell}\right\}$	$\mathcal{C}^1$
Matérn 5/2	$\sigma^2 \left(1+\sqrt{5}\frac{\lvert\tau\rvert}{\ell}+\frac{5}{3}\frac{\tau^2}{\ell^2}\right) \exp\left\{-\sqrt{5}\frac{\lvert\tau\rvert}{\ell}\right\}$	$\mathcal{C}^2$
Squared Exponential (SE)	$\sigma^2 \exp\left\{-\frac{1}{2}\frac{\tau^2}{\ell^2}\right\}$	$\mathcal{C}^\infty$



(a) Exponential



(b) Matérn 3/2



(c) Squared Exponential

GP samples

Conclusions

Conclusions

- Continuity and differentiability in quadratic mean have been studied
  - They do not imply sample function continuity or differentiability
  - They can be related to stationary covariance functions
- Sample function continuity/differentiability can be shown but at the cost of technicality

References

Harald Cramér and M. Ross Leadbetter. *Stationary and Related Stochastic Processes - Sample Function Properties and Their Applications*. Wiley, 1967.

Marc G. Genton. Classes of kernels for machine learning: A statistics perspective. *Journal of Machine Learning Research*, 2001.

Carl E. Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning)*. MIT Press, 2005.

Michael L. Stein. *Interpolation of Spatial Data: Some Theory for Kriging*. Springer, 1999.

A. M. Yaglom. *Correlation Theory of Stationary and Related Random Functions*. Springer, 1987.