Frequentist properties of Bayesian procedures for infinite-dimensional parameters

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Contents

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Recap: frequentist Bayesian theory

Frequentist Bayesian

Given a collection of densities $\{p_w : w \in \mathcal{W}\}$ indexed by a parameter w, and a prior Π on $\mathcal{W}$, the posterior is defined by

$$d\Pi(w|\,X) \propto p_w(X)\,d\Pi(w).$$

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Assume that the data X is generated according to a given parameter w_0 and consider the posterior $\Pi(w \in \cdot|\, X)$ as a random measure on the parameter set $\mathcal{W}$.

We like the posterior to put “most” of its mass near w_0 for “most” X.

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We like the posterior to put "most" of its mass near w_0 for "most" X.

Asymptotic setting: data X^n where the information increases as $n \to \infty$. Three desirable properties:

- Contraction to $\{w_0\}$ at a fast rate
- Adaptation
- (Distributional convergence)

Rate of contraction

Assume X^n is generated according to a given parameter w_0 where the information increases as $n \to \infty$.

- Posterior is consistent if $\mathrm{E}_{w_0} \Pi_n \big(w\colon d(w, w_0) < \varepsilon | \, X^n\big) \to 1$ for every $\varepsilon > 0$.
- Posterior contracts at rate at least ε_n if $\mathrm{E}_{w_0} \Pi_n \big(w\colon d(w, w_0) < \varepsilon_n | \, X^n\big) \to 1$.

Adaptation

To a given class of parameters is attached an optimal rate of convergence defined by the minimax criterion.

We like the posterior to contract at this rate.

Given a scale of regularity classes, indexed by a parameter α, we like the posterior to adapt: if the true parameter has regularity α, then we like the contraction rate to be the minimax rate for the α-class.

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For instance, in typical examples $n^{-\alpha/(2\alpha+d)}$ if w_0 is a function of d arguments with partial derivatives of order α bounded by a constant.

General findings

If w is infinite-dimensional the prior is important.

- The posterior may be inconsistent.
- The rate of contraction often depends on the prior.
- For estimating a functional the prior is less critical, but still plays a role.

The prior does not (completely) wash out as $n \to \infty$.

Examples

Gaussian process

The law of a stochastic process $(W_t: t \in T)$ is a prior distribution on the space of functions $w: T \to \mathbb{R}$.

Gaussian processes have been found useful, because

- they offer great variety;
- they have a general index set T;
- they are easy (?) to understand through their covariance function

$$(s, t) \mapsto \mathrm{E} W_s W_t;$$

- they can be computationally attractive .

Brownian density estimation

For W Brownian motion use as prior on a density p on $[0,1]$:

$$x \mapsto \frac{e^{W_x}}{\int_0^1 e^{W_y}\,dy}.$$

[Leonard, Lenk, Tokdar & Ghosh]

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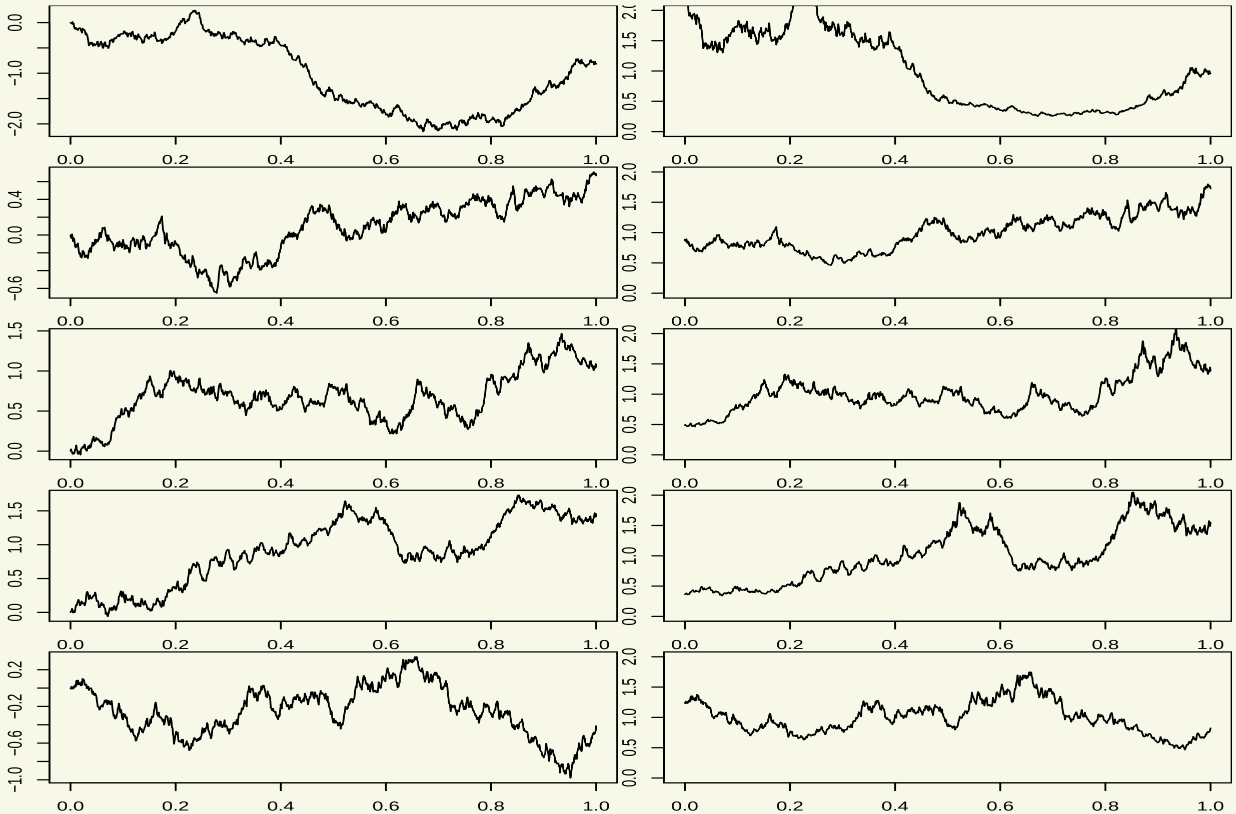

Brownian motion $t \mapsto W_t$ — Prior density $t \mapsto c\exp(W_t)$

Brownian density estimation

Let $X_1, \ldots, X_n$ be iid p_0 on $[0,1]$ and let W Brownian motion. Let the prior be

$$x \mapsto \frac{e^{W_x}}{\int_0^1 e^{W_y}\,dy}$$

THEOREM

If $w_0 := \log p_0 \in C^\alpha[0,1]$, then L_2-rate is: $n^{-1/4}$ if $\alpha \geq 1/2$;
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$n^{-\alpha/2}$ if $\alpha \leq 1/2$.

- This is optimal if and only if $\alpha = 1/2$.
- Rate does not improve if α increases from $1/2$.
- Consistency for any $\alpha > 0$.

(The same result is true for w_0 a regression or classification function.)
[vZanten, Castillo (2008)].

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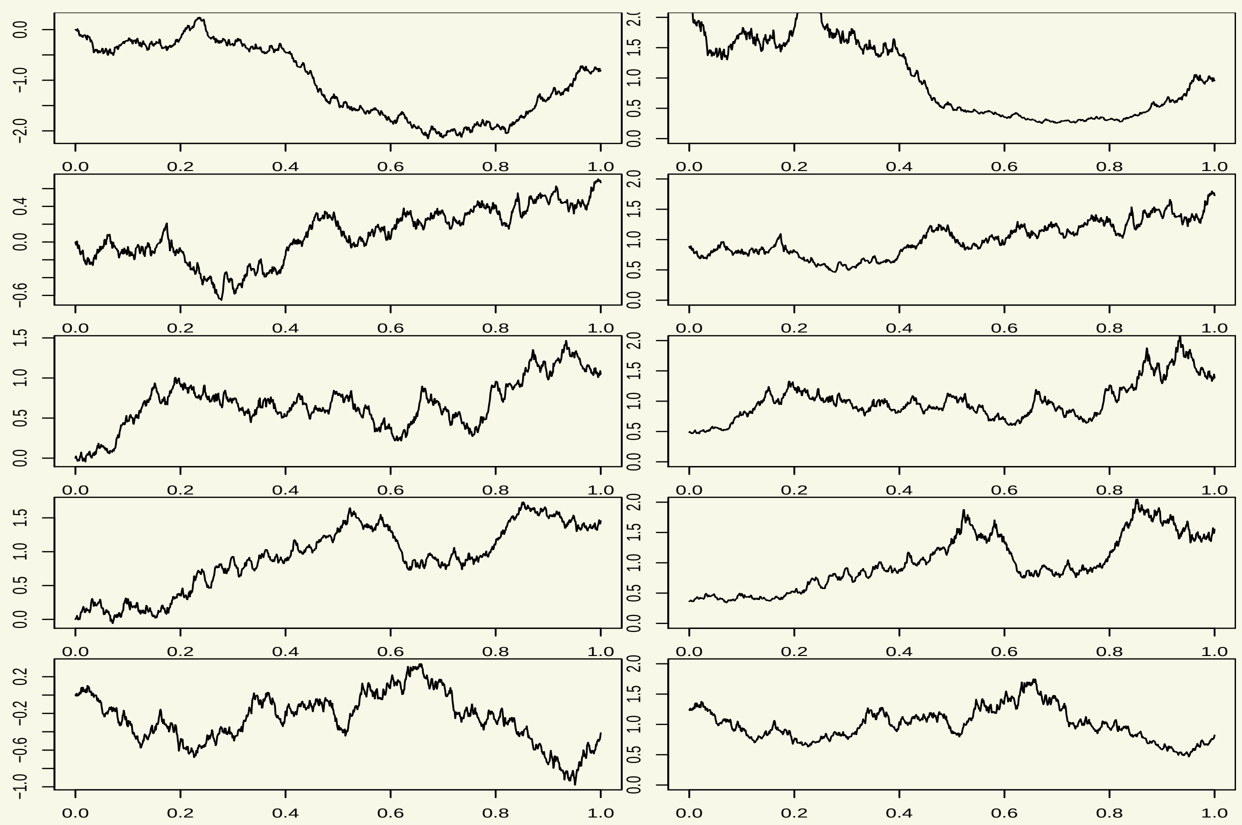

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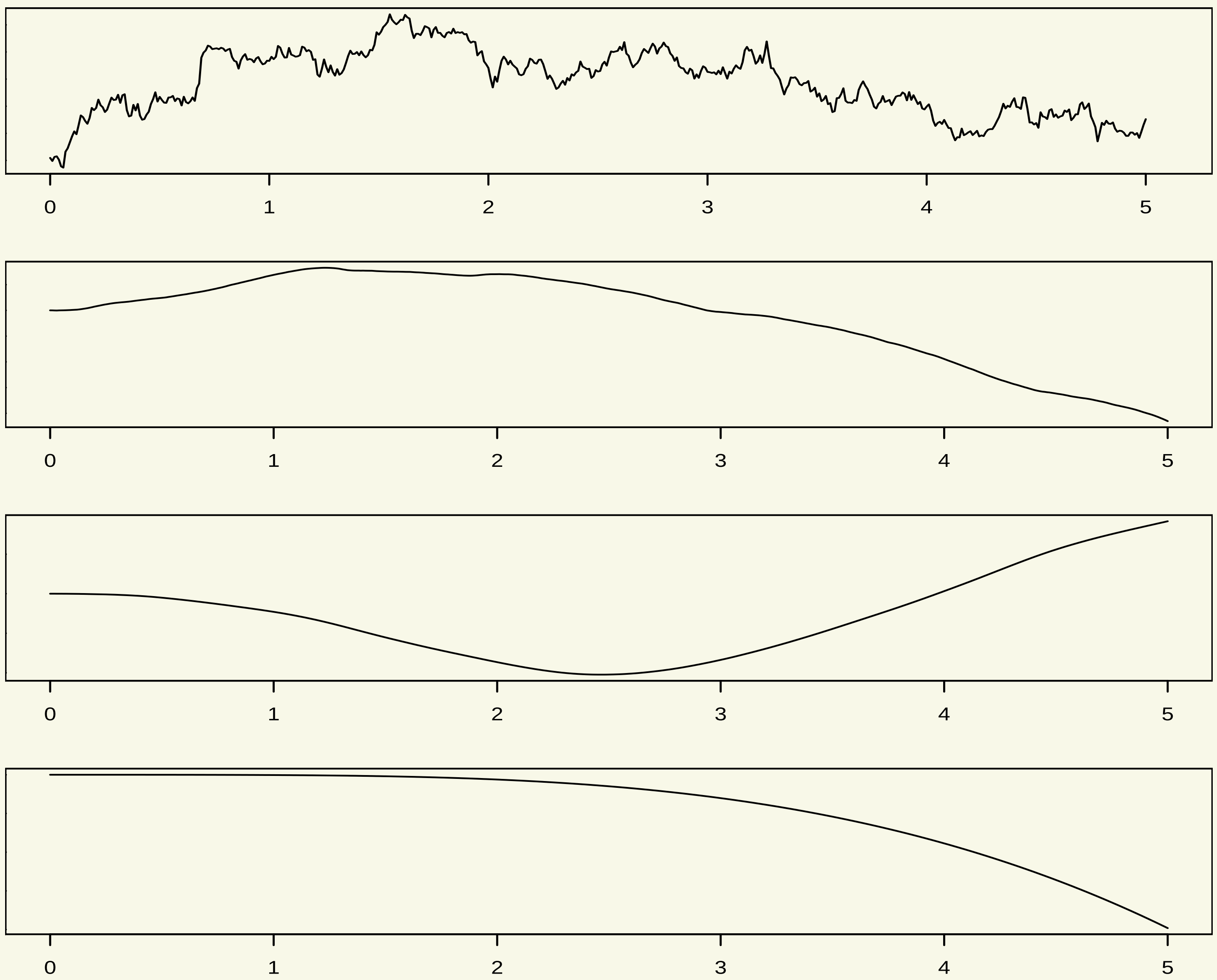
Integrated Brownian motion



0, 1, 2, 3 and 4 times integrated Brownian motion

Integrated Brownian motion: Riemann-Liouville process

$(\alpha - 1/2)$-times integrated Brownian motion, released at 0

$$W_t = \int_0^t (t-s)^{\alpha-1/2}\, dB_s + \sum_{k=0}^{[\alpha]+1} Z_k t^k.$$

[B Brownian motion, $\alpha > 0$, (Z_k) iid $N(0,1)$, “fractional integral”]

THEOREM
IBM gives appropriate model for α-smooth functions: consistency for any true smoothness $\beta > 0$, but the optimal $n^{-\beta/(2\beta+1)}$ if and only if $\alpha = \beta$.

Integrated Brownian motion — spline smoothing

Consider nonparametric regression $Y_i = w(x_i) + e_i$ with Gaussian errors, and prior

$$W_t = \sqrt{b}\int_0^t (t-s)^k\,dB_s + \sqrt{a}\sum_{j=0}^k Z_j t^j.$$

THEOREM [Kimeldorf & Wahba (1970s)]
If $a \to \infty$ and b, n are fixed, then the posterior mean tends to the minimizer of

$$w \mapsto \frac{1}{n}\sum_{i=1}^n \big(Y_i - w(x_i)\big)^2 + \frac{1}{nb}\int_0^1 w^{(k)}(t)^2\,dt.$$

If $w_0 \in C^k[0,1]$ and $b \sim n^{-1/(2k+1)}$, then the penalized least squares estimator is rate optimal.

Brownian sheet

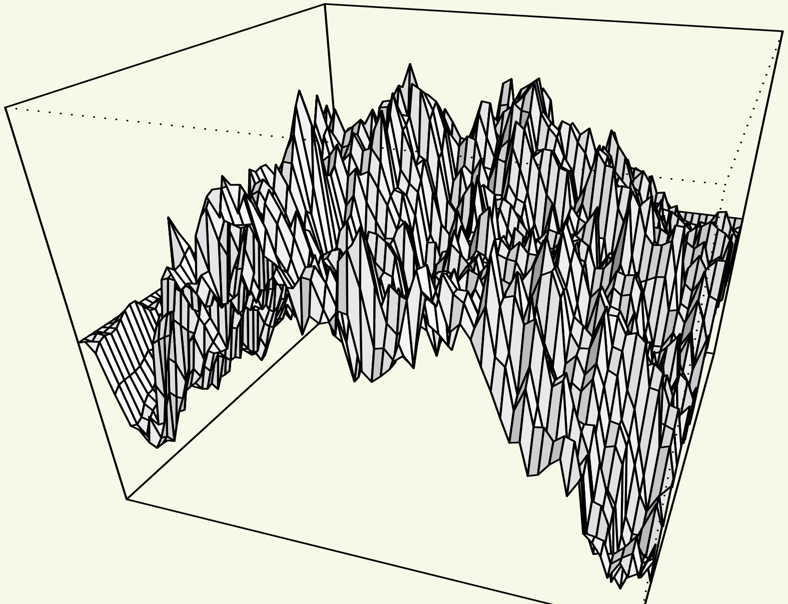
Brownian sheet $(W_t : t \in [0,1]^d)$ has covariance function

$$\mathrm{cov}(W_s, W_t) = (s_1 \wedge t_1) \cdots (s_d \wedge t_d).$$

BS gives rates of the order

$$n^{-1/4} (\log n)^{(2d-1)/4}$$

for sufficiently smooth w_0 $(\alpha \geq d/2)$.

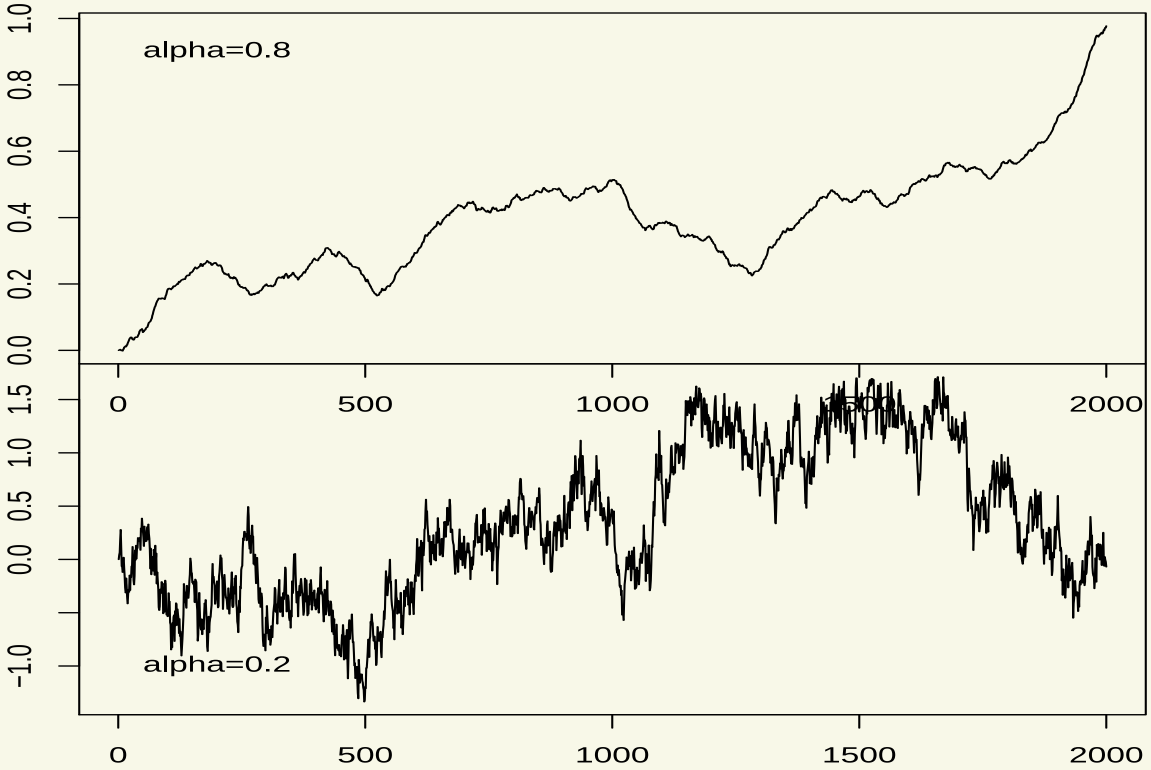


Fractional Brownian motion

W zero-mean Gaussian with (Hurst index $0 < \alpha < 1$)

$$\mathrm{cov}(W_s, W_t) = s^{2\alpha} + t^{2\alpha} - |t-s|^{2\alpha}.$$

fBM is appropriate model for α-smooth functions. Integrate to cover $\alpha > 1$.



Series priors

Given a basis $e_1, e_2, \ldots$ put a Gaussian prior on the coefficients $(\theta_1, \theta_2, \ldots)$ in an expansion

$$\theta = \sum_i \theta_i e_i.$$

For instance: $\theta_1, \theta_2, \ldots$ independent with $\theta_i \sim N(0, \sigma_i^2)$.

Appropriate decay of σ_i gives proper model for α-smooth functions.

Series priors — wavelets

For a wavelet basis $(\psi_{j,k})$ with good approximation properties for $B^{\beta}_{\infty,\infty}[0,1]^d$, and $Z_{j,k}$ iid standard normal variables,

$$W = \sum_{j=1}^{J_\alpha} \sum_{k=1}^{2^{jd}} 2^{-jc}\, 2^{jd/2} Z_{j,k} \psi_{j,k}, \qquad 2^{J_\alpha d} = n^{d/(2\alpha+d)}.$$

THEOREM

If $w_0 \in B^{\beta}_{\infty,\infty}[0,1]^d$, the rate is

$$\varepsilon_n = \begin{cases} n^{-\beta/(2\alpha+d)} \log n & \text{if } c \leq \beta \leq \alpha, \\ n^{-\alpha/(2\alpha+d)} \log n & \text{if } c \leq \alpha \leq \beta, \\ n^{-c/(2c+d)} (\log n)^{d/(2c+d)} & \text{if } \alpha \leq c \leq \beta, \\ n^{-\beta/(2c+d)} (\log n)^{d/(2c+d)} & \text{if } \alpha \leq \beta \leq c. \end{cases}$$

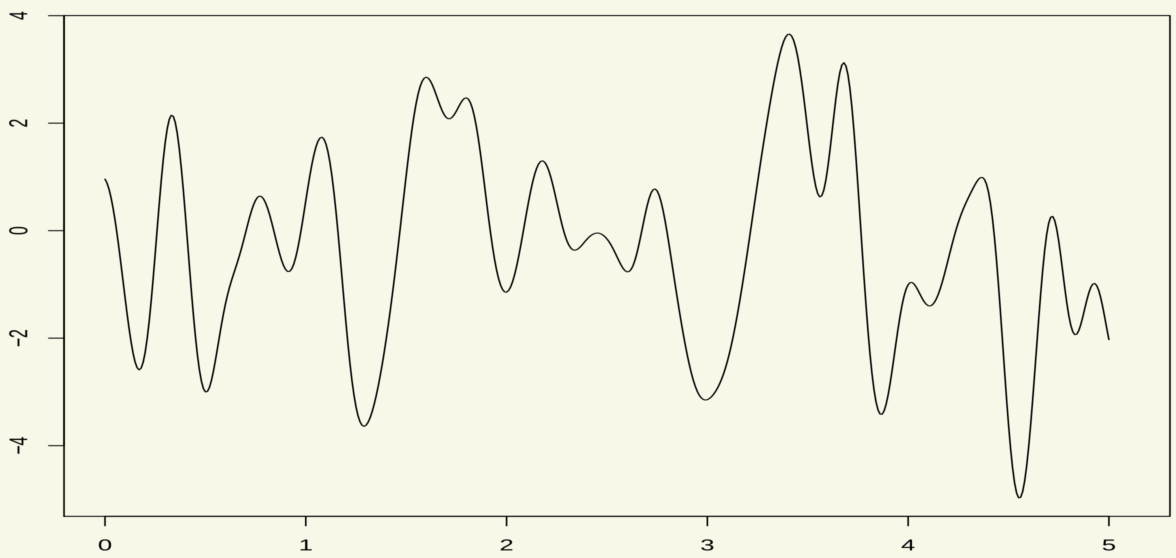
In particular, equal prior weight to all levels ($c = 0$) gives the optimal weight if $\beta = \alpha$ ($c = \beta$ is better).

Stationary processes

A stationary Gaussian field $(W_t: t \in \mathbb{R}^d)$ is characterized through a spectral measure μ, by

$$\operatorname{cov}(W_s, W_t) = \int e^{i\lambda^T(s-t)}\, d\mu(\lambda).$$

Smoothness of $t \mapsto W_t$ is controlled by the tails of μ. For instance, exponentially small tails give infinitely smooth sample paths; Matérn gives α-regular functions.



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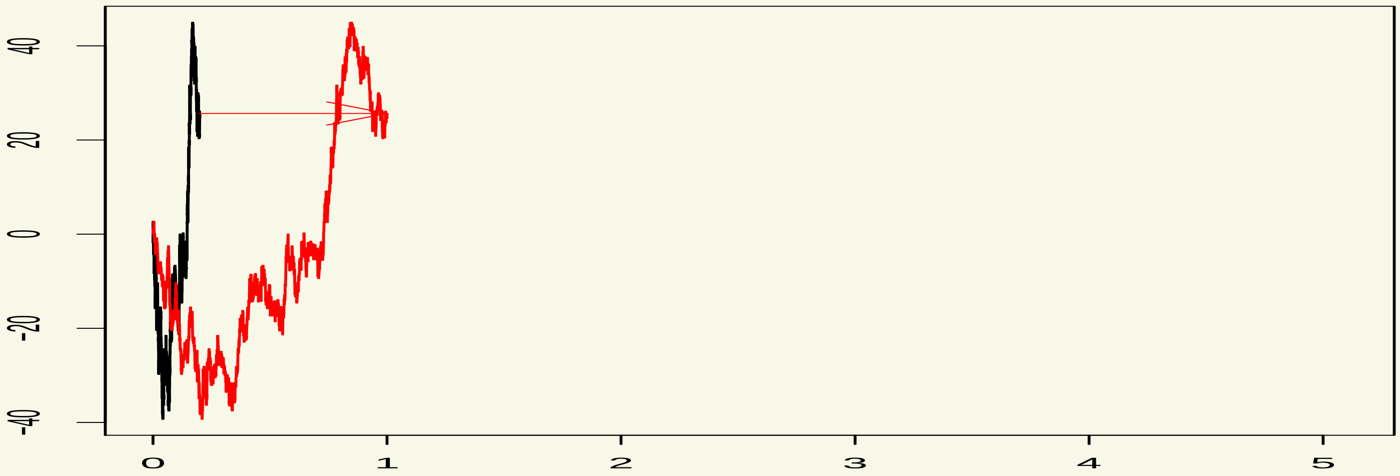
THEOREM If $\int e^{\|\lambda\|} |\hat{w}_0(\lambda)|^2\, d\lambda < \infty$, then the Gaussian spectral measure gives a near $1/\sqrt{n}$-rate of contraction; it gives consistency but suboptimal rates for Hölder smooth functions.

Conjecture: Matérn gives good results for Sobolev spaces.

Rescaling

Stretching or shrinking

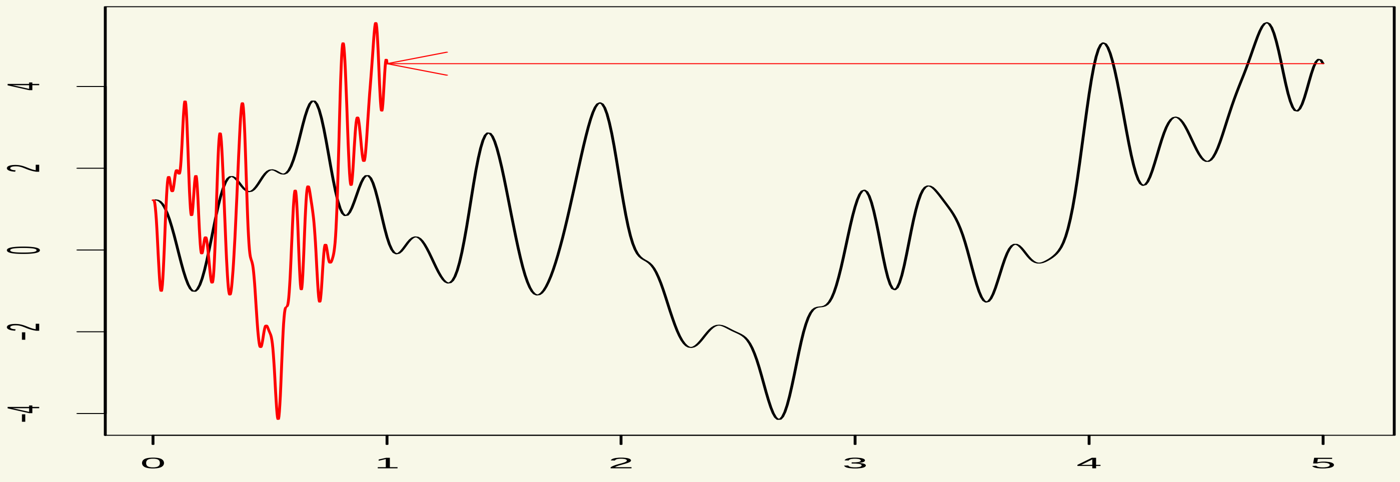
Sample paths can be smoothed by stretching



Stretching or shrinking

Sample paths can be smoothed by stretching

and roughened by shrinking



Rescaled Brownian motion

$W_t = B_{t/c_n}$ for B Brownian motion, and $c_n \sim n^{(2\alpha-1)/(2\alpha+1)}$

- $\alpha < 1/2$: $c_n \to 0$ (shrink).
- $\alpha \in (1/2, 1]$: $c_n \to \infty$ (stretch).

THEOREM
The prior $W_t = B_{t/c_n}$ gives optimal rate for $w_0 \in C^\alpha[0,1]$, $\alpha \in (0,1]$.

Surprising? (Brownian motion is self-similar!.)

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Appropriate rescaling of k times integrated Brownian motion gives optimal prior for every $\alpha \in (0, k+1]$.

For $\alpha = k$ we find the optimal bandwidth for penalized regression as in Kimeldorf and Wahba.

Rescaled smooth stationary process

A Gaussian field with infinitely-smooth sample paths is obtained with

$$\mathrm{E} G_s G_t = \psi(s-t), \qquad \int e^{\|\lambda\|} \hat{\psi}(\lambda)\, d\lambda < \infty.$$

THEOREM
The prior $W_t = G_{t/c_n}$ for $c_n \sim n^{-1/(2\alpha+d)}$ gives nearly optimal rate for $w_0 \in C^\alpha[0,1]$, any $\alpha > 0$.

Messages

- Scaling changes the properties of the prior and hence hyper parameters are important.

A smooth prior process can be scaled to achieve any desired level of “prior roughness”, but a rough process cannot be smoothed much and will necessarily impose its roughness on the data.

Adaptation

Hierarchical priors

For each $\alpha > 0$ there are several priors Π_α (Riemann-Liouville, Fractional, Series, Matern, rescaled processes,...) that are appropriate for estimating α-smooth functions.

We can combine them into a mixture prior:

- Put a prior weight $d\rho(\alpha)$ on α.
- Given α use an optimal prior Π_α for that α.

This works (nearly), provided ρ is chosen with some (but not much) care.

The weights $d\rho(\alpha) \propto e^{-n\varepsilon_{n,\alpha}^2}\, d\alpha$ always work.

[Lember, Szabo]

Adaptation by rescaling

- Choose A^d from a Gamma distribution.
- Choose $(G_t: t > 0)$ centered Gaussian with $\mathrm{E}G_sG_t = \exp\bigl(-\|s-t\|^2\bigr)$.
- Set $W_t \sim G_{At}$.

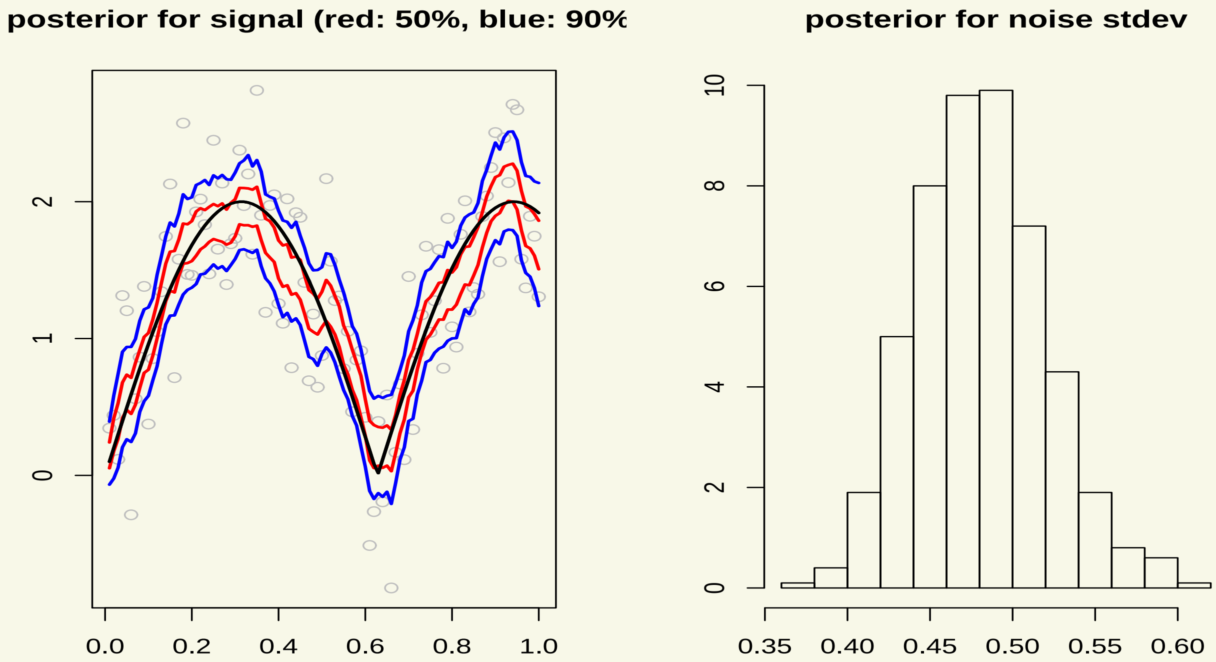
THEOREM

- if $w_0 \in C^\alpha[0,1]^d$, then the rate of contraction is nearly $n^{-\alpha/(2\alpha+d)}$.
- if w_0 is supersmooth, then the rate is nearly $n^{-1/2}$.

Reverend Thomas solved the bandwidth problem!?

Adaptation by rescaling (2)

Gaussian regression with Brownian motion rescaled by a Gamma variable.



Conjecture: this (nearly) gives the optimal rate $n^{-\alpha/(2\alpha+1)}$ if true regression function is in $C^\alpha[0,1]$ for $\alpha \in (0,1]$.
Integrating BM extends this to higher α.

General formulation of rates

Two ingredients

Two ingredients:

- RKHS
- Small ball exponent

Reproducing kernel Hilbert space

Think of the Gaussian process as a random element in a Banach space $(\mathbb{B}, \|\cdot\|)$.

To every such Gaussian random element is attached a certain Hilbert space $(\mathbb{H}, \|\cdot\|_{\mathbb{H}})$, called the RKHS.

$\|\cdot\|_{\mathbb{H}}$ is stronger than $\|\cdot\|$ and hence can consider $\mathbb{H} \subset \mathbb{B}$.

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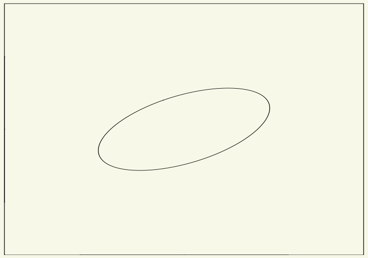
EXAMPLE

If W is multivariate normal $N_d(0, \Sigma)$, then the RKHS is $\mathbb{R}^d$ with norm

$$\|h\|_{\mathbb{H}} = \sqrt{h^t \Sigma^{-1} h}$$



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$\|\cdot\|_{\mathbb{H}}$ is stronger than $\|\cdot\|$ and hence can consider $\mathbb{H} \subset \mathbb{B}$.

EXAMPLE
Brownian motion is a random element in $C[0,1]$.
Its RKHS is $\mathbb{H} = \{h\colon \int h'(t)^2\,dt < \infty\}$ with norm $\|h\|_{\mathbb{H}} = \|h'\|_2$.

Small ball probability

The small ball probability of a Gaussian random element W in $(\mathbb{B}, \|\cdot\|)$ is

$$P(\|W\| < \varepsilon),$$

and the small ball exponent is

$$\phi_0(\varepsilon) = -\log P(\|W\| < \varepsilon).$$

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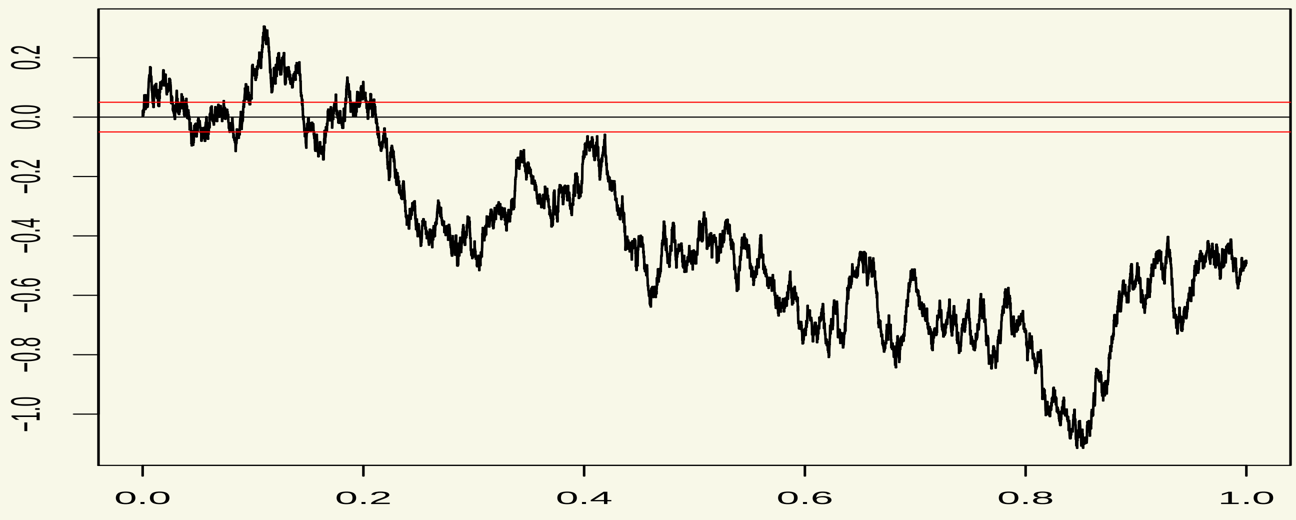
EXAMPLE
For Brownian motion $\phi_0(\varepsilon) \asymp (1/\varepsilon)^2$ as $\varepsilon \downarrow 0$.



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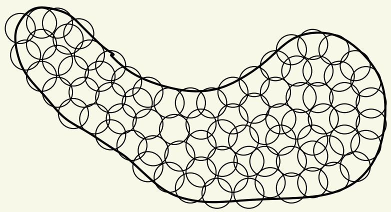

$N(\varepsilon, B, d) = \#\ \varepsilon$-balls

THEOREM [Kuelbs & Li 93]
For $\mathbb{H}_1$ the unit ball of the RKHS (up to constants),

$$\phi_0(\varepsilon) \asymp \log N\Big(\frac{\varepsilon}{\sqrt{\phi_0(\varepsilon)}}, \mathbb{H}_1, \|\cdot\|\Big).$$

There is a big literature on small ball probabilities. (In July 2009 243 entries in database maintained by Michael Lifshits.)

Basic rate result

Prior W is Gaussian map in $(\mathbb{B}, \|\cdot\|)$ with RKHS $(\mathbb{H}, \|\cdot\|_{\mathbb{H}})$ and small ball exponent $\phi_0(\varepsilon) = -\log \mathrm{P}(\|W\| < \varepsilon)$.

THEOREM

If statistical distances on the model combine appropriately with the norm $\|\cdot\|$ of $\mathbb{B}$, then the posterior rate is ε_n if

$$\phi_0(\varepsilon_n) \leq n{\varepsilon_n}^2 \qquad \text{AND} \qquad \inf_{h \in \mathbb{H}: \|h - w_0\| < \varepsilon_n} \|h\|_{\mathbb{H}}^2 \leq n{\varepsilon_n}^2.$$

- Both inequalities give lower bound on ε_n.
- The first depends on W and not on w_0.
- If $w_0 \in \mathbb{H}$, then second inequality is satisfied.

Example — Brownian motion

W one-dimensional Brownian motion on $[0,1]$.

- RKHS $\mathbb{H} = \{h\colon \int h'(t)^2\,dt < \infty\}, \quad \|h\|_{\mathbb{H}} = \|h'\|_2$.
- Small ball exponent $\phi_0(\varepsilon) \lesssim (1/\varepsilon)^2$.

LEMMA

If $w_0 \in C^\alpha[0,1]$ for $0 < \alpha < 1$, then $\inf_{h\in\mathbb{H}:\|h-w_0\|_\infty<\varepsilon} \|h'\|_2^2 \lesssim \left(\frac{1}{\varepsilon}\right)^{(2-2\alpha)/\alpha}$.

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CONSEQUENCE:

Rate is ε_n if $(1/\varepsilon_n)^2 \le n\varepsilon_n^2$ AND $(1/\varepsilon_n)^{(2-2\alpha)/\alpha} \le n\varepsilon_n^2$.

- First implies $\varepsilon_n \ge n^{-1/4}$ for any w_0.
- Second implies $\varepsilon_n \ge n^{-\alpha/2}$ for $w_0 \in C^\alpha[0,1]$.

Examples of settings

Basic rate result

Prior W is Gaussian map in $(\mathbb{B}, \|\cdot\|)$ with RKHS $(\mathbb{H}, \|\cdot\|_{\mathbb{H}})$ and small ball exponent $\phi_0(\varepsilon)$.

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If statistical distances on the model combine appropriately with the norm $\|\cdot\|$ of $\mathbb{B}$, then the posterior rate is ε_n if

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Density estimation

Data $X_1, \ldots, X_n$ iid from density on $[0,1]$,

$$p_w(x) = \frac{e^{w_x}}{\int_0^1 e^{w_t}\, dt}.$$

- Distance on parameter: Hellinger on p_w.
- Norm on W: uniform.

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LEMMA $\forall v, w$

- $h(p_v, p_w) \leq \|v - w\|_\infty\, e^{\|v-w\|_\infty/2}$.
- $K(p_v, p_w) \lesssim \|v - w\|_\infty^2\, e^{\|v-w\|_\infty}(1 + \|v - w\|_\infty)$.
- $V(p_v, p_w) \lesssim \|v - w\|_\infty^2\, e^{\|v-w\|_\infty}(1 + \|v - w\|_\infty)^2$.

Classification

Data $(X_1, Y_1), \ldots, (X_n, Y_n)$ iid in $[0,1] \times \{0,1\}$

$$\mathrm{P}_w(Y = 1 | X = x) = \Psi(w_x),$$

for Ψ the logistic or probit link function.

- Distance on parameter: L_2-norm on $\Psi(w)$.
- Norm on W for logistic: $L_2(G)$, G marginal of X_i.

  Norm on W for probit: combination of $L_2(G)$ and $L_4(G)$.

Regression

Data $Y_1, \ldots, Y_n$, fixed design points $x_1, \ldots, x_n$

$$Y_i = w(x_i) + e_i,$$

for $e_1, \ldots, e_n$ iid Gaussian mean-zero errors.

- Distance on parameter: empirical L_2-distance on w.
- Norm on W: uniform.

Ergodic diffusions

Data $(X_t\colon t \in [0,n])$

$$dX_t = w(X_t)\,dt + \sigma(X_t)\,dB_t.$$

Ergodic, recurrent on $\mathbb{R}$, stationary measure μ_0, "usual" conditions.

- Distance on parameter: random Hellinger h_n.
- Norm on W: $L_2(\mu_0)$.

$$h_n^2(w_1, w_2) = \int_0^n \Bigl(\frac{w_1(X_t) - w_2(X_t)}{\sigma(X_t)}\Bigr)^2\,dt \approx \|(w_1 - w_2)/\sigma\|_{\mu_0,2}^2.$$

[van der Meulen & vZ & vdV, Panzar & vZ]

Reproducing kernel Hilbert space

Definition

For a zero-mean Gaussian W in Banach space $(\mathbb{B}, \|\cdot\|)$, define $S\colon \mathbb{B}^* \to \mathbb{B}$ by

$$Sb^* = \mathrm{E}Wb^*(W).$$

DEFINITION

The RKHS $(\mathbb{H}, \|\cdot\|_{\mathbb{H}})$ is the completion of $S\mathbb{B}^*$ under

$$\langle Sb_1^*, Sb_2^* \rangle_{\mathbb{H}} = \mathrm{E}b_1^*(W)b_2^*(W).$$

Definition (2)

Let $W = (W_x : x \in \mathcal{X})$ be a Gaussian process with bounded sample paths and covariance function

$$K(x,y) = \mathrm{E} W_x W_y.$$

DEFINITION

The RKHS is the completion of the set of functions

$$x \mapsto \sum_i \alpha_i K(y_i, x),$$

relative to inner product

$$\Big\langle \sum_i \alpha_i K(y_i,\cdot), \sum_j \beta_j K(z_j,\cdot) \Big\rangle_{\mathbb{H}} = \sum_i \sum_j \alpha_i \beta_j K(y_i, z_j).$$

Definition (3)

Any Gaussian random element in a separable Banach space can be represented as

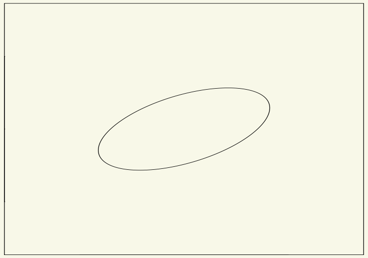
$$W=\sum_{i=1}^{\infty}\mu_i Z_i e_i,$$

for

- $\mu_i \downarrow 0$
- $Z_1, Z_2, \ldots$ iid $N(0,1)$
- $\|e_1\|=\|e_2\|=\cdots=1$

The RKHS consists of all elements $h:=\sum_i h_i e_i$ with

$$\|h\|_{\mathbb{H}}^2:=\sum_i \frac{h_i^2}{\mu_i^2}<\infty.$$



Useful properties

THEOREM
The RKHS of TW for a 1-1 operator $T\colon \mathbb{B} \to \mathbb{B}'$ between Banach spaces is $T\mathbb{H}$, and $T\colon \mathbb{H} \to \mathbb{H}'$ is an isometry.

EXAMPLE
The integration operator

$$T_\alpha w(t) = \int_0^t (t-s)^{\alpha-1} w(s)\, ds$$

applied to Brownian motion gives the $(\alpha + 1/2)$-Riemann-Liouville process $T_\alpha W$. Its RKHS is $\mathbb{H} = T_{\alpha+1}(L_2[0,1])$ with norm

$$\|T_{\alpha+1} h\|_{\mathbb{H}} = \|h\|_2.$$

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THEOREM
The RKHS of the sum $V + W$ of independent Gaussian variables is $\mathbb{H}^V + \mathbb{H}^W$ with norm

$$\|h^V + h^W\|^2_{\mathbb{H}^{V+W}} = \|h^V\|^2_{\mathbb{H}^V} + \|h^W\|^2_{\mathbb{H}^W},$$

whenever the supports of V and W have trivial intersection (and are complemented).

Example — stationary processes

A stationary Gaussian process $(W_t\colon t \in \mathbb{R}^d)$ is characterized through a spectral measure μ, by

$$\mathrm{cov}(W_s, W_t) = \int e^{i\lambda^T(s-t)}\, d\mu(\lambda).$$

LEMMA
The RKHS of $(W_t\colon t \in T)$ is the set of real parts of the functions

$$t \mapsto \int e^{i\lambda^T t}\psi(\lambda)\, d\mu(\lambda), \qquad \psi \in L_2(\mu),$$

with RKHS-norm equal to the infimum of $\|\psi\|_2$ over all ψ. If T has nonempty interior and $\int e^{\|\lambda\|}\, \mu(d\lambda) < \infty$, then ψ is unique.

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To compute rate must approximate w_0 by an element of RKHS. If $d\mu(\lambda) = m(\lambda)d\lambda$, then

$$w_0(t) = \int e^{it^T\lambda}\hat{w}_0(\lambda)\, d\lambda = \int e^{it^T\lambda}\hat{w}_0(\lambda)\frac{1}{m(\lambda)}\, d\mu(\lambda).$$

Proof ingredients

Proof

Given that the relevant statistical distances translate into the Banach space norm, it follows from general results that the posterior rate is ε_n if there exist sets $\mathbb{B}_n$ such that

(1) $\log N(\varepsilon_n, \mathbb{B}_n, d) \leq n\varepsilon_n^2$ and $\Pi_n(\mathbb{B}_n) = 1 - o(e^{-3n\varepsilon_n^2})$. entropy.

(2) $\Pi_n\big(w\colon \|w - w_0\| < \varepsilon_n\big) \geq e^{-n\varepsilon_n^2}$. prior mass.

The second condition actually implies the first.

Prior mass

W a Gaussian map in $(\mathbb{B}, \|\cdot\|)$ with RKHS $(\mathbb{H}, \|\cdot\|_{\mathbb{H}})$ and small ball exponent $\phi_0(\varepsilon)$.

$$\phi_{w_0}(\varepsilon) := \phi_0(\varepsilon) + \inf_{h\in\mathbb{H}:\|h-w_0\|<\varepsilon} \|h\|_{\mathbb{H}}^2.$$

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THEOREM [Kuelbs & Li 93)]
Concentration function measures concentration around w_0:

$$\mathrm{P}(\|W - w_0\| < \varepsilon) \asymp e^{-\phi_{w_0}(\varepsilon)}.$$

up to factors 2

Complexity

RKHS gives the "geometry of the support of W".

THEOREM
The closure of $\mathbb{H}$ in $\mathbb{B}$ is support of the Gaussian measure (and hence posterior inconsistent if $\|w_0 - \mathbb{H}\| > 0$).

THEOREM [Borell 75]
For $\mathbb{H}_1$ and $\mathbb{B}_1$ the unit balls of RKHS and $\mathbb{B}$

$$\mathrm{P}(W \notin M\mathbb{H}_1 + \varepsilon\mathbb{B}_1) \leq 1 - \Phi\Big(\Phi^{-1}(e^{-\phi_0(\varepsilon)}) + M\Big).$$

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Take $\mathbb{B}_n = M_n\mathbb{H}_1 + \varepsilon_n\mathbb{B}_1$ for appropriate M_n.

Conclusion

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Bayesian inference with Gaussian processes is flexible and elegant. However, priors must be chosen with some care: eye-balling pictures of sample paths does not reveal the fine properties that matter for posterior performance.