Karhunen-Loève decomposition of Gaussian measures on Banach spaces

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First workshop on Gaussian processes at Saint-Etienne - November 2017, 7th.

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Motivation

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The problem of representation of Gaussian elements in linear series is used in:

1. Simulation (e.g. truncated Karhunen-Loève series),
2. Approximation and Dimension reduction (e.g. PCA or POD),
3. Optimal quantization,
4. Bayesian inverse problems.

If the existence of an optimal basis is well known in Hilbert spaces...

- ... it's not always explicit (eigenvalue problem),
- ... it's not the case in Banach spaces.

What if we are interested in non-Hilbertian norms ?

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Motivation

In the case of a continuous Gaussian process on $[0,1]$ we may inject it in $L^2([0,1],dx)$ and use Hilbertian geometry...

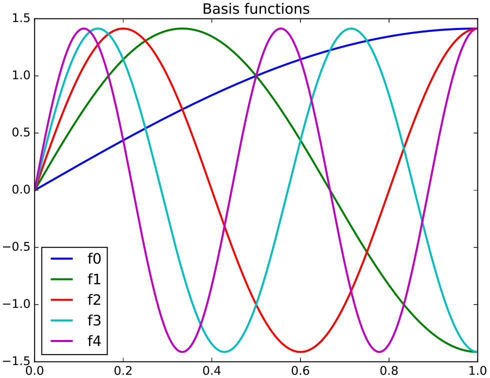

Figure: Karhunen-Loève basis of Brownian motion in $L^2([0,1],dx)$.

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Motivation

or tackle the problem directly in $C([0,1])$...

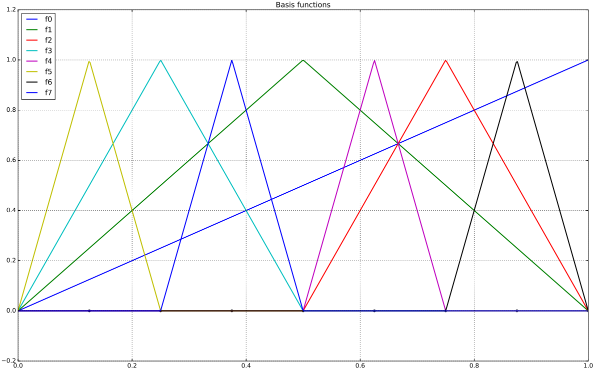

Figure: Brownian motion basis functions in $C([0,1])$ (Paul Levy's construction).

...in the hope of better approximation w.r.t. supremum norm !

Karhunen-Loève decomposition in Hilbert spaces

Gaussian vector in Euclidian spaces

Consider the euclidian space $\mathbb{R}^n$ with canonical inner product $\langle ., . \rangle$.

Gaussian random vector

Let $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space and $X : (\Omega, \mathcal{F}, \mathbb{P}) \to (\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$ a measurable mapping, then X is a Gaussian vector if and only if $\forall y \in \mathbb{R}^n$, $\langle X, y \rangle$ is a Gaussian random variable.

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Covariance

Given a (centered) Gaussian random vector X, define the bilinear form:

$$\forall x, y \in \mathbb{R}^n, \; Cov(x, y) = \mathbb{E}[\langle X, x \rangle \langle X, y \rangle], \tag{1}$$

which uniquely defines $\Sigma : \mathbb{R}^n \to \mathbb{R}^n$ such that:

$$\forall x, y \in \mathbb{R}^n, \; \langle \Sigma x, y \rangle = Cov(x, y). \tag{2}$$

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Considering the Gaussian vector X gives a fundamental structure:

- Gaussian space: $Vect(\langle X, e_k \rangle,\ k \in [1, n]) \subset L^2(\mathbb{P})$
- Cameron-Martin space $H_X = Range(\Sigma)$ equipped with $\langle ., . \rangle_X = \langle \Sigma^{-1} ., . \rangle$

Loève isometry

The following application:

$$\langle X, x \rangle \in L^2(\mathbb{P}) \to \Sigma x \in H_X \tag{3}$$

is an isometry.

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Representation of Gaussian vectors in $\mathbb{R}^n$

- For any orthonormal basis (e_k) in $\mathbb{R}^n$, we can write:

$$X(\omega) = \sum_{k=1}^{n} \langle X(\omega), e_k \rangle e_k \ a.s. \tag{4}$$

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- $\langle X(\omega), e_i \rangle$, $\langle X(\omega), e_j \rangle$ are independent if and only if $Cov(e_i, e_j) = \langle \Sigma e_i, e_j \rangle = \langle \Sigma e_i, \Sigma e_j \rangle_X = 0$.

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- For any orthonormal basis (x_k) in H_X:

$$X(\omega) = \sum_{k=1}^{dim(H_X)} \langle X(\omega), x_k \rangle_X x_k \tag{5}$$

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- The Spectral theorem (on covariance operator) exhibits a particular (Karhunen-Loève) basis (bi-orthogonal and $\Sigma h_k = \lambda_k h_k$):

$$X(\omega) = \sum_{k=1}^{dim(H_X)} \sqrt{\lambda_k} \langle X(\omega), h_k \rangle h_k \tag{6}$$

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Note P^k the linear projector on the k-th biggest eigenvalues, then:

$$\forall k \leq n, \quad \min_{rank(P)=k} \mathbb{E}[\|X - PX\|^2] = \mathbb{E}[\|X - P^k X\|^2] = \lambda_{k+1} + \dots + \lambda_{dim(H_X)}$$

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Representation of Gaussian vectors in $\mathbb{R}^n$

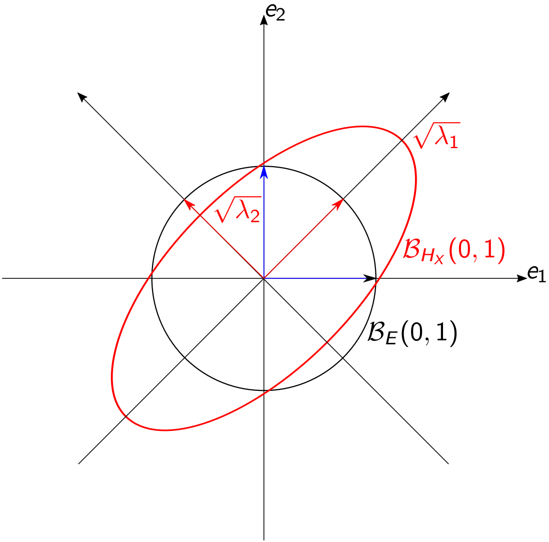

Figure: Karhunen-Loève basis in dimension 2.

Gaussian element in Hilbert spaces

Consider the (real) Hilbert space H with inner product $\langle ., . \rangle$.

Gaussian random element

Let $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space and $X : (\Omega, \mathcal{F}, \mathbb{P}) \rightarrow (H, \mathcal{B}(H))$ a measurable mapping, then X is a Gaussian element if and only if $\forall y \in H$, $\langle X, y \rangle$ is a Gaussian random variable.

Covariance

Given a Gaussian random element X, define the bilinear form:

$$\forall x, y \in H, \; Cov(x, y) = \mathbb{E}[\langle X, x \rangle \langle X, y \rangle], \tag{8}$$

and the associated covariance operator $\mathcal{C} : H \rightarrow H$ such that:

$$\forall x, y \in H, \; \langle \mathcal{C}x, y \rangle = Cov(x, y). \tag{9}$$

Representation of Gaussian elements in Hilbert spaces

- The covariance operator $\mathcal{C} : H \to H$ is positive, symmetric and trace-class (see Vakhania 1987).

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- The covariance operator $\mathcal{C} : H \to H$ is positive, symmetric and trace-class (see Vakhania 1987).
- The Cameron-Martin space H_X is the completion of $Range(\mathcal{C})$ w.r.t. $\langle x, y \rangle_{\mathcal{C}} = \langle \mathcal{C}^{-1} x, y \rangle$ (it's a proper subspace of H, $H_X \hookrightarrow H$, see Vakhania 1987).

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- For any Hilbert basis (e_k) in H we can write:

$$X(\omega) = \sum_{k \geq 0} \langle X(\omega), e_k \rangle e_k \ a.s. \tag{10}$$

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- For any basis (x_k) in H_X and (ξ_k) i.i.d. $\mathcal{N}(0,1)$:

$$X(\omega) \stackrel{d}{=} \sum_{k \geq 0} \xi_k(\omega) x_k \tag{11}$$

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- Spectral theorem applies and exhibits a (Karhunen-Loève) bi-orthogonal basis (h_k): $X(\omega) = \sum_{k \geq 0} \sqrt{\lambda_k} \xi_k(\omega) h_k \ a.s.$

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- Spectral theorem applies and exhibits a (Karhunen-Loève) bi-orthogonal basis (h_k): $X(\omega) = \sum_{k \geq 0} \sqrt{\lambda_k} \xi_k(\omega) h_k \ a.s.$
- Eckart-Young theorem is still valid (functional PCA, ...)

$$\forall k > 0, \quad \min_{rank(P)=k} \mathbb{E}[\|X - PX\|_H^2] = \mathbb{E}[\|X - P^k X\|_H^2] = \sum_{i > k} \lambda_i \tag{12}$$

Karhunen-Loève decomposition in Banach spaces

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Gaussian element in Banach spaces

Consider the (real) Banach space E with duality pairing $\langle ., . \rangle_{E,E^*}$.

Gaussian random element

Let $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space and $X : (\Omega, \mathcal{F}, \mathbb{P}) \to (E, \mathcal{B}(E))$ a measurable mapping, then X is a Gaussian element if and only if $\forall f \in E^*$, $\langle X, f \rangle_{E,E^*}$ is a Gaussian random variable.

Covariance

Given a Gaussian random element X, define the bilinear form:

$$\forall f, g \in E^*,\ Cov(f, g) = \mathbb{E}[\langle X, f \rangle_{E,E^*} \langle X, g \rangle_{E,E^*}], \tag{13}$$

and the associated covariance operator $\mathcal{C} : E^* \to E$ (see Vakhania 1987 or Bogachev 1998) such that:

$$\forall f, g \in E^*,\ \langle \mathcal{C} f, g \rangle_{E,E^*} = Cov(f, g). \tag{14}$$

Representation of Gaussian elements in Banach spaces

- The covariance operator $\mathcal{C} : E^* \to E$ is positive, symmetric and nuclear (see Vakhania 1987).

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- $\mathcal{C} : E^* \to E \Rightarrow$ No Spectral theorem.
- We know that (Bogachev 1998, Vakahnia 1991):
  - $\exists (x_k) \in Range(\mathcal{C})$ Hilbert basis in H_X,
  - $\exists (x_k) \in H_X$ such that $\sum_{k\geq 0} \|h_k\|_E^2 < +\infty$,

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  - $\exists (x_k) \in H_X$ such that $\sum_{k \geq 0} \|h_k\|_E^2 < +\infty$,
- If the basis (x_k) is in $Range(\mathcal{C})$ with $x_k = \mathcal{C} x_k^*$, then:

$$X(\omega) = \sum_{k \geq 0} \langle X(\omega), x_k^* \rangle_{E,E^*} x_k \tag{16}$$

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Factorization of covariance operators (Vakhania 1987, Bogachev 1998).

Let $\mathcal{C}$ be the covariance operator of a Gaussian element, then:

$$\mathcal{C} = SS^*, \tag{17}$$

where $S : H \to E$ is a bounded operator and H a Hilbert space.

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where $S : H \to E$ is a bounded operator and H a Hilbert space.

Examples:

- In the Hilbert case, $S = \mathcal{C}^{\frac{1}{2}}$,
- $S : H_X \to E$ the inclusion map,
- $S : f \in \overline{E^*}^{L^2(\mathbb{P})} \to \mathbb{E}[f(X)X] \in E$ (S^* is the injection from E^* to L^2)

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(Luschgy and Pagès 2009)

Let $\mathcal{C} = SS^*$ with $S : H \to E$. Then for any basis (h_n) in H:

$$X \overset{d}{=} \sum_{k \geq 0} \xi_k S h_k, \tag{18}$$

where (ξ_k) are i.i.d. $\mathcal{N}(0,1)$.

This methodology has been widely used:

- When $E = \mathcal{C}([0,1])$, $S^* : f \in E^* \to L^2([0,1], dx)$...

We will now give a different methodology, mimicking the Hilbert case, to construct a Hilbert basis in H_X. We will proceed as follows:

1. Find "directions" of maximum variance,
2. Choose a right notion of orthogonality to iterate,
3. Study the asymptotics.

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Decomposition of the Cameron-Martin space

1. For any (Gaussian) covariance operator, $f \in E^* \to Cov(f, f) \in \mathbb{R}^+$
   - may be interpreted as a Rayleigh quotient,
   - is weakly sequentially continuous,
   - is quadratic.

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2. $\exists f_0 \in \mathcal{B}_{E^*}(0, 1)$ (non-unique) such that
   $Cov(f_0, f_0) = \max_{\|f\|_{E^*} \leq 1} Cov(f, f) = \lambda_0$ (Banach-Alaoglu),

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3. If $\lambda_0 > 0$, let $x_0 \in E$ such that $\mathcal{C} f_0 = \lambda_0 x_0$, then $P_0 : x \in E \to \langle x, f_0 \rangle_{E, E^*} x_0$ is a projector of unit norm.

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(λ_n) is non-increasing, $\lambda_n \to 0$ and $(\sqrt{\lambda_k} x_k)$ is a Hilbert basis in H_X.

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3. If $\lambda_0 > 0$, let $x_0 \in E$ such that $\mathcal{C}f_0 = \lambda_0 x_0$, then $P_0 : x \in E \to \langle x, f_0\rangle_{E,E^*} x_0$ is a projector of unit norm.
4. $X = (P_0 X, (\mathcal{I} - P_0)X)$.
5. Iterate on $X_1 = (\mathcal{I} - P_0)X$.

Bay & Croix 2017

(λ_n) is non-increasing, $\lambda_n \to 0$ and $(\sqrt{\lambda_k} x_k)$ is a Hilbert basis in H_X.

We will note $x_0^* = f_0$ and $x_n^* = f_n - \sum_{k=0}^{n-1} \langle x_k, f_n\rangle_{E,E^*} x_k^*$ such that $P_n = \sum_{k=0}^{n} x_k^* \otimes x_k$ (similar to Gram-Schmidt).

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Properties of the decomposition

Few comments about the previous construction...

Properties

This construction gives the following properties:

- $X(\omega) = \sum_{k\geq 0} \langle X(\omega), x_k^* \rangle_{E,E^*} x_k$ *a.s.*
- $\mathcal{C} = SS^*$ with $S^* : f \in E^* \to \sum_{k\geq 0} \lambda_k \langle x_k, f \rangle_{E,E^*} x_k$
- Note $\mathcal{C}^n = \sum_{k=0}^n \lambda_k x_k \otimes x_k$ then $\|\mathcal{C} - \mathcal{C}^n\|_{\mathcal{L}(E^*,E)} = \lambda_{n+1}$.
- Recovers Karhunen-Loève basis in the Hilbert case.
- $(x_k, x_k^*) \subset E \times E^*$ is bi-orthogonal.
- $\overline{Vect(x_k, k \geq 0)}^E = \overline{H_X}^E$,
- $\forall k \in \mathbb{N}, \ \|f_k\|_{E^*} = \|x_k\|_E = 1$.

Remarks

- $\sum_{k\geq 0} \lambda_k$ need not be finite (not a nuclear representation of $\mathcal{C}$).
- Optimality seems out of reach (Rate optimality ?).

Particular case of $(\mathbb{R}^n, \|.\|_\infty)$

Application in $\mathbb{R}^n$

Here, $E^* = (\mathbb{R}^n, \|.\|_1)$ and $\forall (x, f) \in E \times E^*$, $\langle x, f \rangle_{E,E^*} = \sum_{i=1}^{n} x_i f_i$.

- Suppose a centered dataset $(y_i)_{i \in [1,p]} \in (\mathbb{R}^n)^p$,
- Form the usual covariance matrix $\Sigma \in \mathcal{M}_n(\mathbb{R})$,
- Find the direction of maximal variance $f_0 \in \mathbb{R}^n$:

$$\lambda_0 = f_0^T \Sigma f_0 = \max_{i \in [1,n]} \Sigma_{(i,i)} \text{ with } f_0 = (0, ..., 0, 1, 0, ..., 0) \qquad (19)$$

- If $\lambda_0 > 0$ then $x_0 = \frac{\Sigma f_0}{\lambda_0}$.
- $\Sigma_1 = \Sigma - \lambda_0 x_0 x_0^T$
- Iterate.

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Application in $\mathbb{R}^n$

- Residuals norm as $r_k = \frac{1}{n}\sum_{i=1}^{n}\|x_i - \sum_{j=0}^{k}\langle x_i, x_j^*\rangle_{E,E^*} x_j\|_\infty$,
- Projections norm as $p_k = \frac{1}{n}\sum_{i=1}^{n}\|\sum_{j=0}^{k}\langle x_i, x_j^*\rangle_{E,E^*} x_j\|_\infty$.

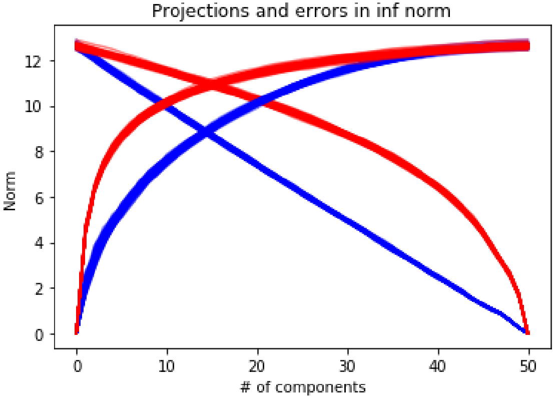

Figure: Residuals (decreasing) and projections (increasing) norm (blue for $L2$-PCA, red for Banach PCA)

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Particular case of $C(K)$, K metric and compact.

$E = C(K)$ with K metric compact.

Let X be a Gaussian element such that $X \in C(K)$ almost-surely and suppose that

$$k : (s,t) \in K^2 \to \langle \mathcal{C}\delta_s, \delta_t \rangle_{E,E^*} = Cov(X_s, X_t) \in \mathbb{R} \qquad (20)$$

is continuous. The Cameron-Martin space H_X coincides here with the Reproducing Kernel Hilbert space (RKHS). The previous decomposition becomes:

1. Set $n = 0$ and $k_n = k$,
2. Find $x_n \in K$ such that $k_n(x_n, x_n) = \max_{x \in K} k_n(x,x)$,
3. If $\lambda_n = k_n(x_n, x_n) > 0$ then $k_{n+1}(s,t) = k_n(s,t) - \frac{k_n(s,x_n)k_n(x_n,t)}{\lambda_n}$,
4. $n \leftarrow n+1$.

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Illustration on Brownian motion: Step 1

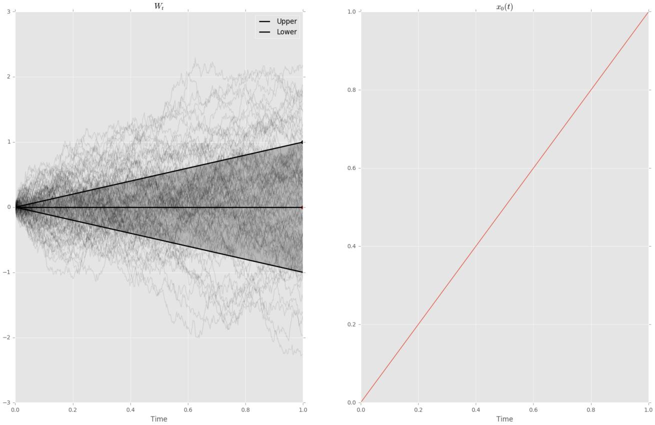

Figure: Left: Brownian motion samples and point-wise (symmetrized) variance. Right: First basis function $x_0(t) = t$ associated to $f_0 = \delta_1$.

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Illustration on Brownian motion: Step 2

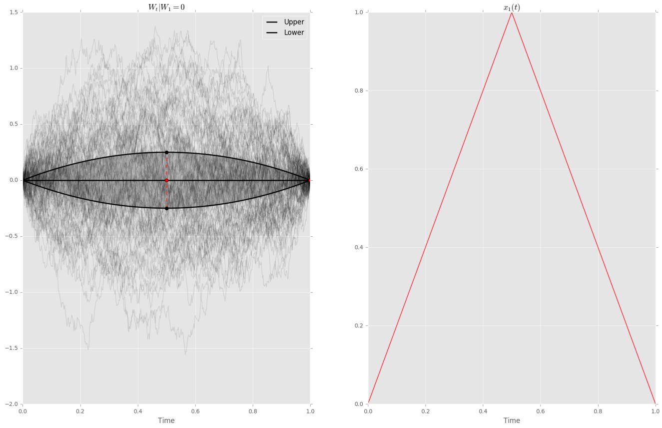

Figure: Left: Brownian bridge samples and point-wise (symmetrized) variance. Right: Second basis function $x_1(t) = \min(t, 0.5) - 0.5t$, associated to $f_1 = \delta_{\frac{1}{2}}$.

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Illustration on Brownian motion: Step 3

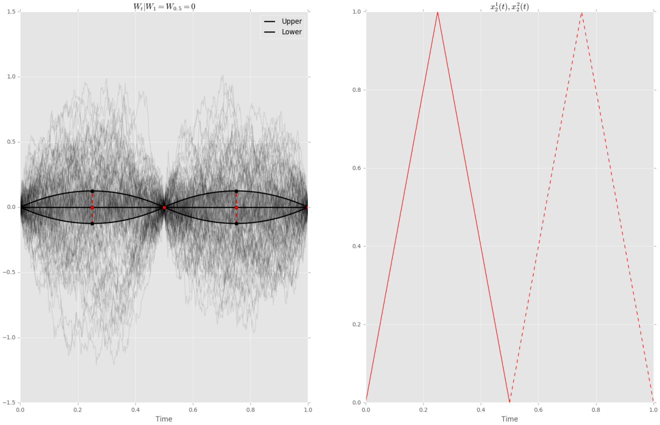

Figure: Left: Conditional Brownian motion samples and point-wise (symmetrized) variance. Right: Third and fourth basis functions.

A word on summability

The proposed decomposition need not be a nuclear representation of $\mathcal{C}$, that is $\sum_{k\geq 0}\lambda_k \in [0, +\infty]$. Indeed, the Brownian case shows us:

$$\sum_{k\geq 0}\lambda_k = 1 + \frac{1}{2} + 2 * \frac{1}{4} + 4 * \frac{1}{16} + 8 * \frac{1}{32} + ... = +\infty \qquad (21)$$

However, a simple transformation gives a nuclear representation in this case:

$$\tilde{f}_2^1 = \frac{f_2^1 - f_2^2}{2} \Rightarrow Cov(\tilde{f}_2^1, \tilde{f}_2^1) = \frac{Cov(f_2^1, f_2^1)}{2} = \frac{1}{8} \qquad (22)$$

$$\tilde{f}_2^2 = \frac{f_2^1 + f_2^2}{2} \Rightarrow Cov(\tilde{f}_2^2, \tilde{f}_2^2) = \frac{Cov(f_2^2, f_2^2)}{2} = \frac{1}{8} \qquad (23)$$

Doing similar transformations at each step gives:

$$\sum_{k\geq 0}\lambda_k = 1 + \frac{1}{2} + 2 * \frac{1}{8} + 4 * \frac{1}{64} + 8 * \frac{1}{256} + ... = 2 \qquad (24)$$

Remark that $\mathbb{E}[\|\sum_{k\geq n}\xi_k h_k\|^2] \leq \sum_{k\geq n}\lambda_k$, thus the approximation error is exponentially decreasing !

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Conclusion and open questions

Conclusion and open questions

Conclusions

- New "practical" method to represent Gaussian elements, based on covariance operator.
- Numerical solution in the case of $E = C(K)$ (K metric and compact).
- Rediscovers Paul Levy's construction of Brownian motion.

Open question & future work

- Other properties of $(x_k, x_k^*) \in E \times E^*$?
- Rate optimality of finite dimensional approximations in $C(K)$?
- Multiplicity of decomposition elements ?
- Links with approximation numbers (ex: $l(X) = \mathbb{E}[\|X\|^2]^{\frac{1}{2}}$) approximation theory ($s$-numbers) ? Properties of Banach spaces ?
- Optimality for projection norm ? Dual problem ?
- Interpretation of $\sum_{k\geq 0} \lambda_k$ when it is finite ?
- Evolution of $\|x_k^*\|_{E^*}$?

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Appendix

Examples with different kernels

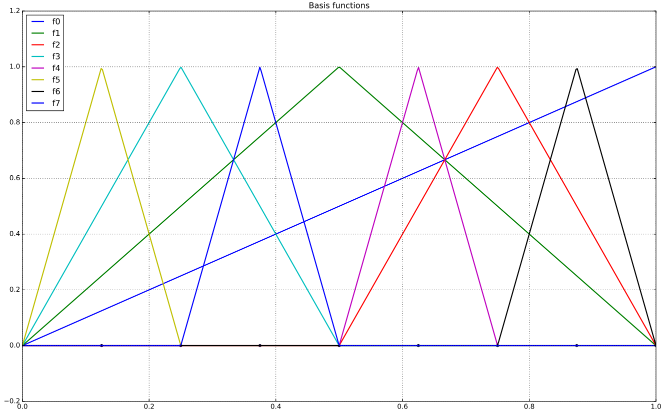

Figure: Wiener measure basis functions.

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Examples with different kernels

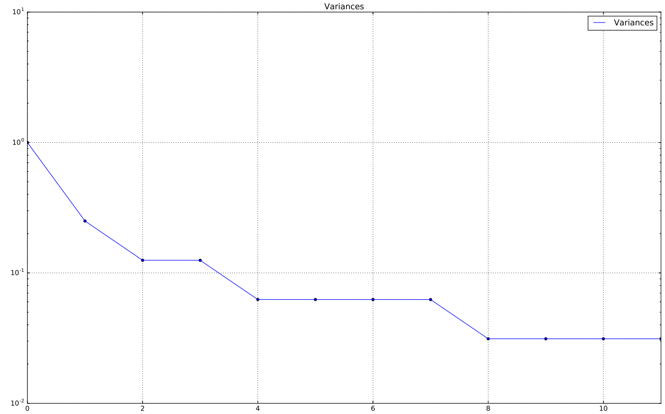

Figure: Wiener measure basis variances.

Examples with different kernels

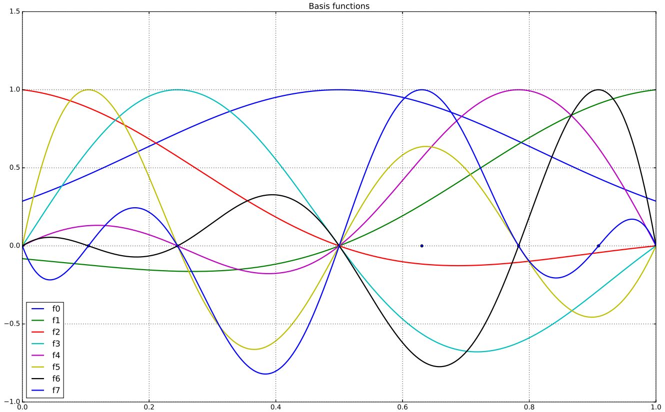

Figure: $k(s,t) = \exp\left(-\frac{(s-t)^2}{2}\right)$ basis functions.

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Examples with different kernels

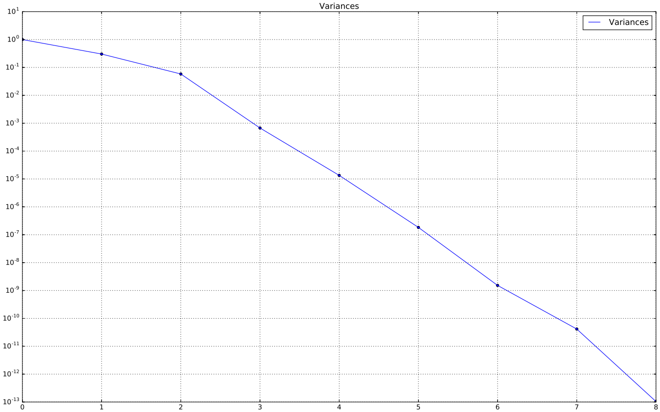

Figure: $k(s,t) = \exp\left(-\frac{(s-t)^2}{2}\right)$ basis variances.

Examples with different kernels

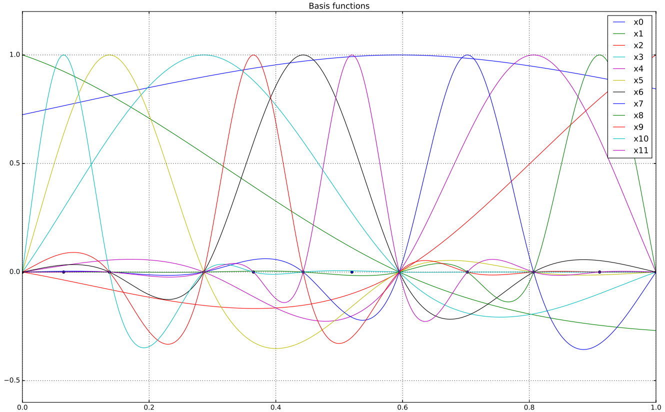

Figure: Matern 3/2 kernel basis functions.

Examples with different kernels

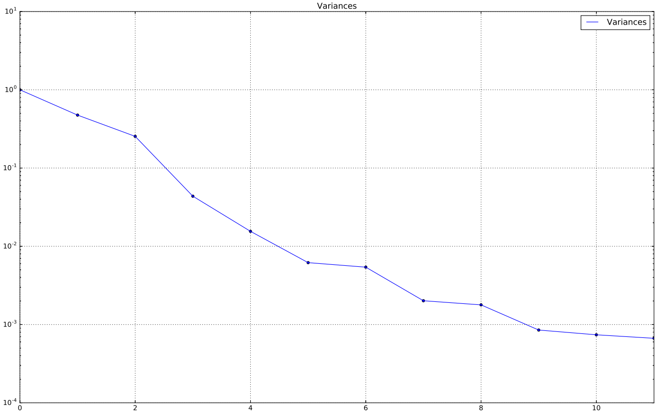

Figure: Matern 3/2 kernel basis variances.

Examples with different kernels

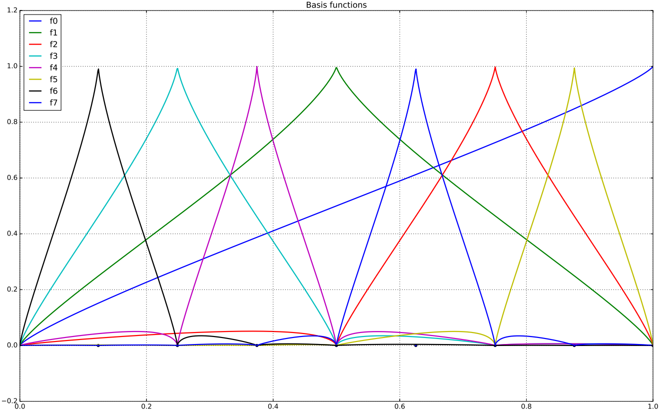

Figure: Fractional brownian motion ($H = 75\%$) basis functions.

Examples with different kernels

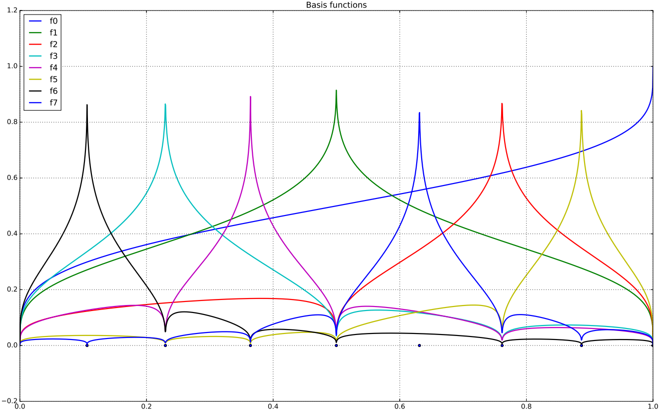

Figure: Fractional brownian motion ($H = 25\%$) basis functions.

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