Projection of Functionals and Fast Pricing of Exotic Options

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Abstract

We investigate the approximation of path functionals. In particular, we advocate the use of the Karhunen-Loève expansion, the continuous analogue of Principal Component Analysis, to extract relevant information from the image of a functional. Having accurate estimate of functionals is of paramount importance in the context of exotic derivatives pricing, as presented in the practical applications. Specifically, we show how a simulation-based procedure, which we call the Karhunen-Loève Monte Carlo (KLMC) algorithm, allows fast and efficient computation of the price of path-dependent options. We also explore the path signature as an alternative tool to project both paths and functionals.

Keywords — Path functional, Karhunen-Loève expansion, signature, derivatives pricing

MSC (2020) Classification — 91G20, 91G60, 41A45

1 Introduction

The pricing of exotic options remains a difficult task in quantitative finance. The main challenge is to find an adequate trade-off between pricing accuracy and fast computation. Efficient techniques such as finite difference [21] or the fast Fourier transform [6] are in general not applicable to path-dependent payoffs. Practitioners are often forced to turn to standard Monte Carlo methods, despite being slow. Therefore, researchers have come up with novel ideas over the years to tackle this issue. Recently, some authors have employed deep learning to price vanilla and exotic options in a non-parametric manner [5] while others showed the benefits of the path signature [2, 17] to project exotic payoffs in a nonlinear way.

In this paper, we move away from prevailing machine learning methods and bring a classical tool back into play: the Karhunen-Loève (KL) expansion [13, 15]. The latter provides an orthogonal decomposition of stochastic processes that is optimal in the $L^2(Q \otimes dt)$ sense. The theory has been applied to Gaussian processes [10, 22], functional quantization [19], and recently to the Brownian Bridge in a weighted Hilbert space [8]. In this paper, the KL expansion takes on a newfound importance when it is applied to the projection of path functionals. We propose a simple simulation-based procedure, which we call the Karhunen-Loève Monte Carlo (KLMC) algorithm, to compute the price of exotic options. The superiority of KL-based Monte Carlo methods compared to the ordinary one was shown numerically in [1] for the Brownian case. Our goal is here to further support these findings and extend this approach. We also discuss alternative methods employing the path signature as basis of the space of functionals.

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1See https://github.com/valentintissot/KLMC for an implementation.
The remainder of this paper is structured as follows. In Section 2, we gather standard results from approximation theory and draw a parallel between Hilbert projection and the à la mode path signature. Section 3 is devoted to the approximation of functionals, where two routes are contrasted as well as a short discussion on the use of the signature for this task. We apply the developed tools and finally present the KLMC algorithm with accompanying numerical evidence in Section 4.

2 Path Approximation

For fixed horizon \( T > 0 \), let \( \Lambda_t = C([0, t], \mathbb{R}) \) and \( \Lambda := \bigcup_{t \in [0, T]} \Lambda_t \). For \( X \in \Lambda_t \) and \( s \leq t \), \( X_s \) denotes the trajectory up to time \( s \), while \( x_s = X(s) \) is the value at time \( s \). We equip \( \Lambda \) with a σ-algebra \( \mathcal{F} \), filtration \( \mathbb{F} \) and probability measure \( \mathbb{Q} \) to form a stochastic basis \((\Lambda, \mathcal{F}, \mathbb{F}, \mathbb{Q})\).

The goal of this paper is to price exotic options with payoff of the form \( f(X_t) \). For fairness sake, however, we always compare projections involving the same number of basis functions.

2.1 Karhunen-Loève Expansion

Let \( \mathcal{H} \) be the Lebesgue space \( L^2([0, T]) \) of square-integrable functions, where we write \((\cdot, \cdot) = (\cdot, \cdot)_{L^2([0, T])}\) for brevity. Among the myriad of bases available, which one should be picked? The answer will depend upon the optimality criterion. One possibility is to minimize the square of the inner product \((\mathcal{H})^\dagger \). A natural way to approximate \( f(X_t) \) is by projecting it onto a Hilbert space. For simplicity, we focus on paths defined on the whole interval \([0, T]\), so working on \( \Lambda_T \) is enough. Also, \( f \) is assumed to preserve continuity, so \( f(X) \in \Lambda_T \) as well. We now present the theory for the original path, although the same would hold for the transformed one; see Section 3. Let \( \mathcal{H} \) be a separable Hilbert space with inner product \((\cdot, \cdot)_\mathcal{H}\). Then any \( X \in \Lambda_T \cap \mathcal{H} \) admits the representation

\[
X_t = \sum_{k} \xi_k F_k(t), \quad \xi_k = (X, F_k)_{\mathcal{H}}, \quad t \in [0, T],
\]

where \( F_k \) is an orthonormal basis (ONB) of \( \mathcal{H} \). An approximation of \( X \) is obtained by truncating the series in (2.1), that is \( X^{K, \mathcal{F}} = \sum_{k \leq K} \xi_k F_k(t) \). Each pair \((K, \mathcal{F})\) thus induces a projection map \( \pi^{K, \mathcal{F}} : \mathcal{H} \to \mathcal{H} \) given by \( \pi^{K, \mathcal{F}}(X) = X^{K, \mathcal{F}} \). Although paths are assumed to be one-dimensional for simplicity, the present framework is easily generalized. Indeed, if \( x_t = (x^{d}_1, \ldots, x^{d}_d) \in \mathbb{R}^d \), it suffices to project each component separately, i.e. \( x^{K, \mathcal{F}}_t = \sum_{k \leq K} \xi_k F_k(t) \) with \( \xi_k = (X^i, F_k)_{\mathcal{H}} \).

2.1.1 Karhunen-Loève Expansion

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\[
\sum_{k \leq K} \xi_k F_k(t)
\]

where \( \mathcal{F} := (F_k) \) is an orthonormal basis (ONB) of \( \mathcal{H} \). An approximation of \( X \) is obtained by truncating the series in (2.1), that is \( X^{K, \mathcal{F}} = \sum_{k \leq K} \xi_k F_k(t) \). Each pair \((K, \mathcal{F})\) thus induces a projection map \( \pi^{K, \mathcal{F}} : \mathcal{H} \to \mathcal{H} \) given by \( \pi^{K, \mathcal{F}}(X) = X^{K, \mathcal{F}} \). Although paths are assumed to be one-dimensional for simplicity, the present framework is easily generalized. Indeed, if \( x_t = (x^{d}_1, \ldots, x^{d}_d) \in \mathbb{R}^d \), it suffices to project each component separately, i.e. \( x^{K, \mathcal{F}}_t = \sum_{k \leq K} \xi_k F_k(t) \) with \( \xi_k = (X^i, F_k)_{\mathcal{H}} \) and \((\mathcal{F})^d_{i=1} \) ONB’s of \( \mathcal{H} \).
Remark 2.2. Brownian motions can be simulated by setting $x_t = x_t^K$.\footnote{denoted by $||.||_*$} between a path and its $K$–order truncation, i.e. 
$$e^{K, \hat{\delta}} := ||X - X^K, \hat{\delta}||^2 = \mathbb{E}^Q \int_0^T |x_t - x_t^K, \hat{\delta}|^2 dt,$$ 
for $X \in \Lambda_T \cap L^2([0, T])$. Thanks to the orthogonality of $\hat{\delta}$, we have
$$e^{K, \hat{\delta}} = \sum_{k,l > K} (\xi_k, \xi_l)_{L^2(Q)} (F_k, F_l)_{L^2([0, T])} = \sum_{k > K} \lambda^2_k, \quad \lambda^2_k := ||\xi_k||^2_{L^2(Q)},$$ 
where it is assumed that $\lambda^2_k \geq \lambda^2_l \quad \forall \ k < l$ without loss of generality. As the mapping $\hat{\delta} \mapsto \sum_k \lambda^2_k$ is constant and equal to the total variance $||X||^2_{L^2(Q \otimes dt)}$, the projection error is solely determined by the speed of decay of $(\lambda^2_k)$. Inversely, the optimal basis will maximize the cumulative sum of variance $\sum_{k \leq K} \lambda^2_k$. This leads us to the Karhunen-Loève expansion \cite{13, 15}, the continuous analogue of Principal Component Analysis. In what follows, assume $\mathbb{E}^Q[x_t] = 0 \ \forall t \in [0, T]$ and define the covariance kernel $\kappa_X(s, t) = (x_s, x_t)_{L^2(Q)}$. As $\kappa_X$ is symmetric, continuous, and non-negative definite, Mercer’s representation theorem \cite{18} ensures the existence of an ONB $\hat{\delta} = (F_k)$ of $L^2([0, T])$ and scalars $\lambda_1^2 \geq \lambda_2^2 \geq \ldots \geq 0$ such that
$$\kappa_X(s, t) = \sum_{k=1}^{\infty} \lambda_k^2 F_k(s)F_k(t). \quad (2.3)$$
Then $\hat{\delta}$ is the Karhunen-Loève (KL) basis associated to $X$ under $Q$. From (2.3), it is immediate that $F_k$ solves the Fredholm integral equation
$$(\kappa_X(t, \cdot), F_k) = \lambda_k^2 F_k(t), \quad t \in [0, T].$$
Accordingly, $\hat{\delta}$ and $(\lambda_k^2)$ are termed eigenfunctions and eigenvalues of $\kappa_X$, respectively. Observe that the squared $L^2(Q)$ norm of the KL coefficient $\xi_k = (X, F_k)$ is precisely $\lambda_k^2$, whence comes the notation in (2.2). The next result reflects the relevance of the KL expansion; see \cite[Theorem 2.1.2.]{10} for a proof.

**Theorem 2.1.** The Karhunen-Loève basis is the unique ONB of $L^2([0, T])$ minimizing $e^{K, \hat{\delta}}$ for every truncation level $K \geq 1$.

**Remark 2.2.** For non-centered trajectories, it suffices to characterize the Karhunen-Loève basis of $x_t - \mathbb{E}^Q[x_t]$. The projected path is then obtained by adding the mean function back to the expansion.

**Example 2.3.** Let $T = 1$ and $Q$ be the Wiener measure, i.e. the coordinate process $X$ is Brownian motion on $[0, 1]$. The covariance kernel is $\kappa_X(s, t) = s \wedge t$, leading to the eigenfunctions $F_k(t) = \sqrt{2} \sin((k - 1/2)\pi t)$ and eigenvalues $\lambda_k^2 = \frac{1}{\pi^2(k - 1/2)^2}, \quad k \geq 1$. The projection error is approximately equal to
$$e^{K, \hat{\delta}} = \frac{1}{\pi^2} \sum_{k > K} \frac{1}{(k - 1/2)^2} \approx \frac{1}{\pi^2} \int_K^\infty \frac{dk}{(k - 1/2)^2} = \frac{1}{\pi^2(K - 1/2)}.$$ 
It is easily seen that $\xi_k = (X, F_k) \sim \mathcal{N}(0, \lambda_k^2)$ so that $\xi_k, \xi_l$ are independent for $k \neq l$. Therefore, ”smooth” Brownian motions can be simulated by setting $x_t^{K, \hat{\delta}} = \sum_{k=1}^{K} \sqrt{\lambda_k^2} z_k F_k(t)$ with $(z_k)_{k=1}^{K} \overset{i.i.d.}{\sim} \mathcal{N}(0, 1), \quad K \geq 1$.

### 2.2 Lévy-Cieselski Construction

Another Hilbert space is the Cameron–Martin space, $\mathcal{R} = \{F \in \Lambda_T | dF \ll dt, \dot{F} \in L^2([0, T])\}$ where $\dot{F}$ denotes the time derivative of $F$. The inner product is $(F, G)_{\mathcal{R}} = (\dot{F}, \dot{G})$, from which $(F_k)$ is an ONB of

...
\[ \mathcal{R} \iff (\hat{F}_k) \text{ is an ONB of } L^2([0,T]) \text{ is immediate. If } X^{\kappa,\delta} \text{ is a projected path with respect to an ONB } \tilde{\mathcal{F}} \text{ of } \mathcal{R}, \text{ then taking derivative gives} \]
\[
\dot{x}_t^{\kappa,\delta} = \sum_{k \leq K} (\dot{X}, \dot{F}_k) \hat{F}_k(t) = \sum_{k \leq K} (X, F_k)_{\mathcal{R}} \dot{F}_k(t). \]

We gather that the projection of a path onto \( \mathcal{R} \) corresponds to an \( L^2([0,T]) \) projection of its (possibly generalized) derivative followed by a time integration. When \( \mathcal{Q} \) is the Wiener measure, this procedure is often called the Lévy-Cieselski construction. With regards to accuracy, we recall the expression for the \( L^2(\mathcal{Q} \otimes dt) \)–error,
\[
\epsilon^{\kappa,\delta} = \| X - X^{\kappa,\delta} \|_2^2 = \sum_{k,l \geq K} (\xi_k, \xi_l)_{L^2(\mathcal{Q})} (F_k, F_l)_{L^2([0,T])}. \]
As orthogonal functions in \( \mathcal{R} \) need not be orthogonal in \( L^2([0,T]) \), we cannot in general get rid of the double sum above. However, if \( \mathcal{Q} \) is the Wiener measure and \( X \) the white noise process, then Fubini’s theorem gives
\[
(\xi_k, \xi_l)_{L^2(\mathcal{Q})} = \int_{[0,T]} \mathbb{E}[\dot{x}_s \dot{x}_t] \hat{F}_k(s) \hat{F}_l(t) ds dt = \int_0^1 \dot{F}_k(t) \dot{F}_l(t) dt = (F_k, F_l)_{\mathcal{R}} = \delta_{kl}. \]
Thus, \( \epsilon^{\kappa,\delta} = \sum_{k > K} \| F_k \|^2 \). The optimal Cameron-Martin basis would therefore have the fastest decay of its squared norms (\( \| F_k \|^2 \)), assuming the latter are sorted in non-increasing order. We illustrate the Lévy-Cieselski construction with two examples, taking \( T = 1 \).

**Example 2.4.** A standard method to prove the existence of Brownian motion follows from the Brownian bridge construction. In short, it consists of a random superposition of triangular functions—the Schauder functions—obtained by integrating the Haar basis on \([0,1]\),
\[
\dot{F}_{k,l}(t) = 2^{k/2} \psi \left( 2^k t - l \right), \quad 0 \leq l < 2^k, \quad t \in [0,1],
\]
with the wavelet \( \psi = (-1)^{[l/2^k]} \), \( \text{supp}(\psi) = [0,1] \). The Schauder and Haar functions are illustrated on the left side of Figure 1. It is easily seen that \( \dot{F}_{k,1} \) as well as \( F_{k,1} \) have support \([l/2^k, (l + 1)/2^k] \), the \( l \)-th subinterval of the dyadic partition \( \Pi_k = [1/2^k, 1] \). The construction is incrementa: First, the terminal value of the path is simulated. Then, for each subinterval of \( \Pi_k, k \geq 0 \), a random value for the mid-point is generated and thereafter connected to the endpoints in a linear fashion (using \( F_{k+1,1} \)). The restriction of \( X \) to \( \Pi_k \) will therefore remain the same when finer characteristics of the path are added.

**Example 2.5.** Let \( \hat{F} \) be the cosine Fourier ONB, i.e. \( \hat{F}_k(t) = \sqrt{2} \sin(\pi k t) / \pi k, \) turns out to correspond—up to a factor—to the Karhunen-Loève basis of the Brownian bridge. Indeed, recalling that \( \kappa_X(s,t) = s \wedge t - st \) if \( X \) is a Brownian bridge, we have for the ONB \( \tilde{\mathcal{F}} = (\hat{F}_k)(\pi k F_k) \),
\[
(\kappa_X(\cdot,t), \hat{F}_k) = \sqrt{2} \left[ (1-t) \int_0^t s \sin(\pi k s) ds + t \int_t^1 (1-s) \sin(\pi k s) ds \right] = \sqrt{2} \frac{\sin(\pi k t)}{\pi k^2},
\]
using integration by parts in the last equality. The eigenvalues are therefore \( \lambda_k^2 = \frac{\sin(\pi k t)}{\pi k^2} \). The first elements of \( \tilde{\mathcal{F}} \) and the Fourier cosine ONB are displayed on the right charts of Figure 1. Following the same argument as in Example 2.3, the (minimal) projection error onto \( K \) basis functions is approximately equal to \( \frac{1}{\sigma^2 \mathcal{R}} \). This is less than Brownian motion (see Example 2.3) as little more is known about a Brownian bridge; \( \mathcal{Q} \)—almost all trajectories return to the origin.
2.3 Signature and Legendre Polynomials

An alternative characterization of a path is available through the so-called signature \[16\]. Roughly speaking, the signature extract from a path an infinite-dimensional skeleton, where each "bone" contains inherent information. We start off with a few definitions. A word is a sequence \(\alpha = \alpha_1...\alpha_k\) of letters from the alphabet \(\{0, 1\}\). The length of \(\alpha\) is denoted by \(l(\alpha)\). Moreover, we augment a path \(X \in \Lambda\) with the time itself \(t\) and write \(x_0 = t, x_1 = x_t\). The words 0, 1 are therefore identified with the time \(t\) and path \(x\), respectively.

Definition 2.6. The signature is a collection of functionals \(S = \{S_\alpha : \Lambda \to \mathbb{R}\}\) given by
\[
S_0 \equiv 1, \quad S_\alpha(X_t) = \int_0^t \int_0^{t_2} \cdots \int_0^{t_k} \circ dx_{t_1}^{\alpha_1} \cdots \circ dx_{t_k}^{\alpha_k}, \quad l(\alpha) = k \geq 1, \quad (2.4)
\]
where \(\circ\) indicates Stratonovich integration.\(^3\)

When referring to a specific path \(X\), we shall call the sequence \((S_\alpha(X))\) the signature of \(X\). This is usually how the signature is defined; see [16]. If \(x_t \in \mathbb{R}^d\) with \(d \geq 2\), then the alphabet becomes \(\{0, 1, \ldots, d\}\) and the signature is obtained analogously. The first signature functionals read
\[
S_0(X_t) = \int_0^t dt = t, \quad S_1(X_t) = \int_0^t \circ dx_{t_1} = x_t - x_0, \\
S_{00}(X_t) = \int_0^t \int_0^{t_2} dt_1 dt_2 = \frac{t^2}{2}, \quad S_{11}(X_t) = \int_0^t \int_0^{t_2} \circ dx_{t_1} \circ dx_{t_2} = \frac{(x_t - x_0)^2}{2}, \\
S_{10}(X_t) = \int_0^t \int_0^{t_2} dx_{t_1} dt_2 = \int_0^t (x_s - x_0)ds, \quad S_{01}(X_t) = \int_0^t \int_0^{t_2} dt_1 dx_{t_2} = \int_0^t s dx_s.
\]

Keeping track of the passage of time is crucial, as the signature would otherwise barely carry information about the path. Indeed, notice that \(S_\alpha(X_t) = (x_t - x_0)^k\) for \(\alpha = 1...1, l(\alpha) = k\) (as seen above for \(k = 1, 2\)) thus only the increment \(x_t - x_0\) is known with the alphabet \(\{1\}\).

\(^3\)The integrals in (2.4) are in the Lebesgue-Stieltjes (respectively Itô) sense when the integrator (respectively integrand) is of bounded variation. In both cases, the symbol \(\circ\) can be omitted.
A property of the signature is that it uniquely characterizes a path, up to a equivalence relation: two paths having same signature differ at most by a tree-like path [11], a specific type of loop. Hence, extending a path with time not only enriches the signature but also ensures injectivity as \( t \to x_t^0 = t \) is increasing. This gives hope to reconstruct the (unique) path associated to a signature sequence. This was investigated in [9], where the author shows a geometric reconstruction using polygonal approximations for Brownian paths. We propose a simple algorithm, in connection with our discussion on Hilbert projections.\(^4\) For ease of presentation, assume \( x_0 = 0 \) and \( T = 1 \). We first make the following observation.

**Lemma 2.7.** Let \( \tilde{X} \) denote the time reversed path, i.e. \( \tilde{x}_t = x_{1-t} \) and introduce the words \( \alpha^{(k)} := 10 \ldots 0 \), \( l(\alpha^{(k)}) = k + 2, k \geq 0 \). Then \( S_{\alpha^{(k)}}(\tilde{X}_1) = \frac{1}{k!}(X, m_k) \) where \( m_k(t) = t^k \).

**Proof.** First, observe that
\[
S_{\alpha^{(k)}}(X_1) = \int_0^t x_s \frac{(t-s)^k}{k!} ds, \quad \forall t \in [0, 1]. \tag{2.5}
\]

Indeed for fixed \( t \in [0, 1] \) and \( k = 0 \), then \( S_{\alpha^{(0)}}(X_t) = S_{10}(X_t) = \int_0^t x_s ds \) which is \( (2.5) \). Now by induction on \( k \geq 1 \), uniformly on \([0, t]\),
\[
S_{\alpha^{(k)}}(X_1) = \int_0^t S_{\alpha^{(k-1)}}(X_u) du = \int_0^t \int_0^u x_s \frac{(u-s)^{k-1}}{(k-1)!} ds du = \int_0^t x_s \frac{(t-s)^k}{k!} ds.
\]

Now taking \( t = 1 \) and \( \tilde{X} \) instead of \( X \), we get \( S_{\alpha^{(k)}}(\tilde{X}_1) = \int_0^1 x_t^{(1-t)^k} dt = \frac{1}{k!}(x, m_k). \)

Essentially, Lemma 2.7 states that the knowledge of \( (S_{\alpha^{(k)}}(\tilde{X}_1))_{k \geq 0} \) is equivalent to the knowledge of the inner products of the path with the monomials. Since also
\[
S_{\alpha^{(k)}}(\tilde{X}_1) = (-1)^k \int_0^1 x_t \frac{(1-t)^k}{k!} dt = \sum_{j=0}^k \frac{(-1)^j}{(k-j)!} S_{\alpha^{(j)}}(X_1),
\]
the coefficients \( (X, m_k)_{k \geq 0} \) can be retrieved from \( (S_{\alpha^{(k)}}(X_1))_{k \geq 0} \) as well. To fall within the context of orthonormal projection, we transform the monomials into the (unique) polynomial ONB of \( L^2([0, 1]) \). Let \( (p_k) \) be the Legendre polynomials [23], forming an orthogonal basis of \( L^2([-1, 1]) \). Then consider the shifted Legendre polynomials, \( q_k(t) = p_k(2t - 1), t \in [0, 1] \). We write
\[
q_k(t) = \sum_{j \leq k} a_{k,j} t^j, \quad a_{k,j} = (-1)^{k+j} \binom{k}{j} \binom{k+j}{j},
\]
with coefficients derived for instance from Rodrigues' formula [23, Section 4.3]. The standardization \( F_k := \frac{a_k}{\|p_k\|} = \sqrt{2k + 1} q_k \) makes \( \mathcal{F} = (F_k) \) an ONB of \( L^2([0, 1]) \). This leads us to the following result.

**Proposition 2.8.** If \( b_{k,j} := \sqrt{2k + 1} j! a_{k,j} \) and \( G_j(t) = \sum_{k \leq j} F_k(t) \), then
\[
x_t^{K,\delta} = \sum_{k \leq K} \xi_k F_k(t) = \sum_{j \leq K} S_{\alpha^{(j)}}(\tilde{X}_1) G_j(t). \tag{2.6}
\]

**Proof.** First, \( (X, F_k) = \sum_{j \leq k} a_{k,j} (X, m_j) \) with \( m_j(t) = t^j \). Using Lemma 2.7, we obtain
\[
\xi_k = \sum_{j \leq k} b_{k,j} S_{\alpha^{(j)}}(\tilde{X}_1).
\]

Thus \( X^{K,\delta} = \sum_{j \leq K} S_{\alpha^{(j)}}(\tilde{X}_1) G_j \) with \( G_j \) as in the statement. \(\square\)

\(^4\)I thank Bruno Dupire for suggesting this interesting parallel.
In summary, the signature elements \((S_{\alpha(k)})_{k \leq K}\) generate the \(L^2([0,1])\) products of the path with the monomials—and in turn, with the Legendre polynomials—from which the projected path \(X^{K,\delta}\) becomes available. We can therefore retrieve \(X\) by letting \(K \to \infty\). Note that this reconstruction works for multidimensional paths as well, as we can apply the procedure to each component \(i = 1, \ldots, d\) with the words \(\alpha_{(i,k)} := i0 \ldots 0, l(\alpha_{(i,k)}) = k + 2, k \geq 0\). We finish this section by computing the projection error of (2.6) when \(X\) is Brownian motion. Recalling that \(\kappa_{X}(s,t) = s \wedge t\), a simple calculation gives

\[
\lambda_{F,k} = \mathbb{E}_{Q}[\xi^2_k] = 2 \int_0^t \int_0^s F_k(s)ds F_k(t)dt = 2(2k + 1) \sum_{i,j \leq k} \frac{a_{k,j} a_{k,i}}{(j+2)(i+j+3)}.
\]

The first values are given by \((\lambda_{F,k}^3)_{k=0} = (\frac{1}{3}, \frac{1}{10}, \frac{1}{42}, \frac{1}{90})\) from which we conjecture that \(\lambda_{F,k}^3 = \frac{1}{(2k+3)(4k+2)}\) for all \(k \geq 1\). This is supported by the fact that \(\lambda_{F,k}^3\) must be rational numbers as \(a_{k,j} \in \mathbb{Z}\) for all \(k, j\) and

\[
\sum_{k=0}^{K} \lambda_{F,k}^3 = \frac{1}{3} + \frac{1}{8} \sum_{k=1}^{K} \left( \frac{1}{2k-1} - \frac{1}{2k+3} \right) = \frac{1}{2} - \frac{K+1}{(2K+3)(4K+2)} \xrightarrow{K \to \infty} \frac{1}{2},
\]

coinciding with the total variance of Brownian motion on \([0,1]\). Thus, the approximation error reads

\[
e^{K,\delta} = \frac{K+1}{(2K+3)(4K+2)} = O\left(\frac{1}{K}\right),
\]

which is of course larger than the Karhunen-Loève basis but smaller than the Brownian Bridge construction (Example 2.4). Note that polynomial ONB’s may well be optimal if the approximation criterion is modified. In [8], the authors show that in the weighted Hilbert space \(L^2([0,1], \mu, \mu(dt) = dt(t(1-t)))\), the Karhunen-Loève basis of the Brownian bridge is formed by the anti-derivatives of the Legendre polynomials. Although the construction is different, it is also curiously related to the signature elements \((S_{\alpha(k)})\); see Theorem 2.3 and 2.4 in [8].

**Remark 2.9.** Note that the approximation in (2.6) may be improved by adding other elements of the signature, especially those that are nonlinear in \(X\), e.g. \(S_{110}(X_t) = \frac{1}{2} \int_0^t x_s^2 ds\). We postpone this discussion to Section 3.3 when projecting running functionals.

### 2.4 Numerical Results

We concentrate our experiments on Brownian trajectories. First, we illustrate the path approximations seen earlier (Karhunen-Loève, Lévy-Cieselski, Signature). Figure 2 displays the projections using \(K = 8\) basis elements. We naturally notice similarities between the Karhunen-Loève transform and the Lévy-Cieselski construction with Fourier cosines, both obtained by superposing trigonometric functions.

![Figure 2: Projected paths with \(K = 8\) basis elements.](image)
Let us gauge the accuracy of the above approximations for Brownian trajectories, in terms of (i) $\epsilon_{K,F}$ and (ii) variance explained $\vartheta_{K,F} := \|X_{K,F}\|_2^2 / \|X\|_2^2$. To compute (i), (ii) and the coefficients $(X,F)_K$, we discretize the interval $[0,1]$ a regular partition made of $N = 10^4$ subintervals. Figure 3 displays the evolution of $\epsilon_{K,F}$, $\vartheta_{K,F}$ for $K \in \{1, \ldots, 128\}$. The Karhunen-Loève expansion clearly dominates the other projections, although being asymptotically equivalent to the Lévy-Cieselski construction with Fourier cosine basis. Besides, the $L^2(Q \otimes dt)$ convergence of the Brownian bridge construction (Lévy-Cieselski with Haar basis) is non-monotonic. Indeed, a bump appears until a full cycle of the dyadic partition is completed. Lastly, the slopes in the log-log convergence plot (left chart of Figure 3) are roughly equal to $-1$. Put differently, the squared approximation error is of order $O(1/K)$, confirming our findings from the above examples.

Figure 3: $L^2(Q \otimes dt)$ error and variance explained.

3 Projection of Functionals

In Section 2, we unveiled two ways to approximate exotic payoffs $\varphi = h \circ f$, namely by projecting the original path $X$ or $Y = f(X)$ directly. If $\pi_{K,F}$ denotes as before the projection map onto a Hilbert space $H$, we can therefore write $\varphi_{K,F} := h \circ f_{K,F}$, where either $f_{K,F} = f \circ \pi_{K,F}$ (functional of projected path) or $f_{K,F} = \pi_{K,F} \circ f$ (projected functional). We shall see in Section 3.2 that the former is suboptimal. Although not so problematic for functionals capturing global features of a path, local path characteristics (e.g. running maximum) will typically be grossly estimated. Indeed, projecting a path first erases most of its microstructure. We thus favor the second option ($f_{K,F} = \pi_{K,F} \circ f$), which consists of replacing $X$ by $Y$ in (2.1). Let us now focus on $H = L^2([0,T])$ and demonstrate how to compute the Karhunen-Loève basis of $Y$.

3.1 Karhunen-Loève Expansion of Functionals

Assume that $Y \in L^2([0,T]) \cap \Lambda_T$ has zero mean (otherwise, see Remark 2.2). Theorem 2.1 suggests to set $\tilde{\alpha}$ equal to the eigenfunctions of $\kappa_Y(s,t) = (y_s,y_t)_{L^2(Q)}$. Optimality comes, however, at the cost of explicitizing $\tilde{\alpha}$. We proceed as follows: take a regular partition $\Pi_N = \{t_n = n \delta t | n = 0, \ldots, N\}$, $\delta t = T/N$ and compute the kernel matrix $\kappa_Y^N = (\kappa_Y(t_n,t_m))_{0 \leq n,m \leq N}$. When $\kappa_Y$ does not admit a closed-form expression, $\kappa_Y^N$ is replaced by the sample covariance matrix using simulated paths for $Y$. The
eigenfunctions thus become eigenvectors and solve the systems

\[
\sum_{t_n \in \Pi_N} \kappa_Y(t_n, t_m) F_k(t_n) \delta t = \lambda_k^2 F_k(t_m), \quad t_m \in \Pi_N, \quad k = 0, \ldots, N. \tag{3.1}
\]

This is a simple eigenvalue problem so all pairs \((F_k, \lambda_k^2)\) can be computed in one go. Let us proceed with two examples where \(T = 1\) and \(Q = \) Wiener measure throughout.

**Example 3.1.** Consider the time integral and average of a Brownian path, \(y_t = f(X_t) = \int_0^t x_s \, ds\), \(\bar{y}_t = f(X_t) = \frac{1}{t} f(X_t)\). These are clearly centered processes and their covariance kernels of can be found explicitly. Starting with \(Y\),

\[
\kappa_Y(s, t) = \left( \int_0^s x_r \, dr, \int_0^t x_u \, du \right)_{L^2(Q)} \int_0^s \int_0^t \kappa_X(r, u) \, dr \, du.
\]

A straightforward calculation gives \(\kappa_Y(s, t) = s^2 t - s^3/6\) and \(\kappa_{\bar{Y}}(s, t) = s^2 - s^3/6t, \quad s \leq t\), where \(Y = f(X)\). We display in Figures 4a and 4b the covariance kernel (top) and first eigenfunctions (bottom) of \(f\) and \(\bar{f}\), respectively. The dashed lines in the top panels are the eigenfunctions of the original (Brownian) path. Note the wider range in the eigenfunctions \(F_1, F_2\) for \(\bar{f}(X)\) compared to the integrated path for small \(t\). This might come from the greater fluctuations of the time average at inception.

Figure 4: Covariance kernels (top) and eigenfunctions (bottom).

(a) Time average
(b) Time integral
(c) Running maximum

Solid lines: transformed path. Dashed lines: Brownian motion.

**Example 3.2.** Consider the running maximum functional \(y_t = f(X_t) = \max_{0 \leq s \leq t} x_s\). Figure 5 provides an illustration in the \((t, X, Y)\) plane. The mean function is in this case non-zero and—using, e.g., the reflection

\[\sum_{t_n \in \Pi_N} \kappa_Y(t_n, t_m) F_k(t_n) \delta t = \lambda_k^2 F_k(t_m), \quad t_m \in \Pi_N, \quad k = 0, \ldots, N. \tag{3.1}\]

In (3.1), \(\sum_{n}^{\pi} \kappa_Y(t_n, t_m) F_k(t_n) \delta t = \lambda_k^2 F_k(t_m)\) means that the first and last summand are halved, i.e. the trapezoidal rule is used to compute \((\kappa_Y(\cdot, t), F_k)\). Another approach, known as Nyström’s method [20] consists of employing a Gaussian quadrature scheme instead. However, for large \(N\), we haven’t observed any improvement and thus favor the more convenient discretization in (3.1).
principle—given by $E_Q[y_t] = \sqrt{\frac{2}{\pi} t}$. The covariance kernel admits an explicit yet complicated expression [3],

$$\kappa_{Y}(s, t) = \frac{s}{2} + \frac{\sqrt{s(t-s)} - 2\sqrt{st} + t \arcsin(\sqrt{s/t})}{\pi}, \quad s \leq t.$$  

Figure 4c displays the covariance kernel (top) and first eigenfunctions (bottom). The latter turns out to be quite close to the eigenfunctions of Brownian motion.

Figure 5: Running maximum functional for two trajectories.

3.2 Numerical Results

Let us compare the $L^2(\mathbb{Q} \otimes dt)$ error $\|Y^{K, \delta} - Y\|^2$ in the Brownian case for the two avenues discussed at the beginning of this section. When $Y^{K, \delta} = (f \circ \pi^{K, \delta})(X)$, the error is calculated using Monte Carlo simulations. As in Section 2.4, we choose $T = 1$, $N = 10^4$ and $K \in \{1, \ldots, 128\}$. Figure 6 displays the result for the running maximum, integral and average functionals. We also add the Brownian motion itself, corresponding to the identity functional $f(X) = X$. We observe a clear improvement when projecting the transformed path. Moreover, it comes as no surprise that smooth functionals (integral, average) exhibits a faster rate of convergence than the running maximum, highly sensitive to local behaviours of a path.

Figure 6: $L^2(\mathbb{Q} \otimes dt)$ approximation errors.

Dashed lines: functionals of projected paths.
Solid lines: projected functionals.
3.3 Discussion: Projection of Functionals using the Signature

Another approximation of \( Y = f(X) \) can be obtained by combining signature functionals in a linear fashion. For instance, one can consider all the words of length less than \( \bar{K} \in \mathbb{N} \), giving the approximation

\[
y^K,S = \sum_{l(\alpha) \leq \bar{K}} \xi^{l(\alpha)} S_\alpha(X_t),
\]

with \( K = \{ \alpha \mid l(\alpha) \leq \bar{K} \} = 2^{\bar{K}+1} - 1 \). The coefficients \( \xi^{l(\alpha)} \) may depend on \( X_0 \) only and can be calculated by either regressing \( Y \) against the signature elements or using a Taylor formula for functionals \([14]\) when \( f \) is smooth (in the Dupire sense) and \( X \) is a diffusion. In the literature, (3.2) is referred to as polynomial functional \([14]\) or signature payoff \([2, 17]\) in finance.

The appeal of such projection comes from the fact that polynomial functionals are dense in the space of continuous functionals restricted to paths of bounded variation; see Theorem 5 in \([14]\). On the other hand, despite the existence of packages to calculate the signature of discrete time paths (e.g., \texttt{iisignature} and \texttt{esig} in Python), the projection in (3.2) is still challenging from a computational perspective. Indeed, contrary to the reconstruction in Section 2.3, the signature functionals have to be known at every intermediate time. Also, as there is a priori no recipe to select words up to a given length, we must retain all of them so the number of elements doubles every time a layer is added.

4 Applications

We now illustrate the benefits of the Karhunen-Loève expansion on functionals for the pricing of exotic derivatives. We slightly change notations and write \( W \) for the coordinate process. The path \( X \) now represents the stock price where for simplicity, we employ the Black-Scholes model with zero interest rate. That is, \( Q \) is the Wiener measure and \( x_t = x_0 \mathcal{E}_t(\sigma W) \), where \( x_0 > 0 \) is fixed and \( \mathcal{E} \) denotes the stochastic exponential. Notice, however, that our method applies to any dynamics of the underlying, possibly multidimensional or involving jumps. As we shall see below, what matters is whether the functional in the payoff, say, \( f \), generates square-integrable paths \( Y = f(X) \) for the covariance kernel to be well-defined.\(^6\)

Let \( \mathcal{M} \subseteq \mathbb{R} \), \( \mathcal{T} \subseteq [0, T] \) be a finite set of option parameters and maturities, respectively. We seek to approximate the price surface \( p : \mathcal{M} \times \mathcal{T} \to \mathbb{R} \), \( p(m, \tau) = \mathbb{E}_Q[\varphi_m(X_{\tau})] \), where the payoffs \( \varphi_m(X_{\tau}) = (h_m \circ f)(X_{\tau}) \) depends on a parameter \( m \in \mathcal{M} \). For example, a call option on \( Y = f(X) \) is obtained with \( h_{\text{Call}}(y) := (y - mx_0)^+ \) and \( m \) is the moneyness of the option.

The standard Monte Carlo approach (MC) consists of simulating the underlying path on a partition \( \Pi_N = \{ 0 = t_0 < t_1 < \ldots < t_N = T \} \) that contains \( \mathcal{T} \) and compute the price as \( p_{N,J}(m, \tau) = \frac{1}{N} \sum_{j=1}^{J} \varphi_m(X_{N,j})^\tau \), \( J \in \mathbb{N} \). In contrast, the Karhunen-Loève Monte Carlo method (KLMC) samples \( Y = f(X) \) directly and computes the price surface using the representation \( p(m, \tau) = \mathbb{E}_Q[h_{\text{Call}}(Y_{\tau})] \). We now describe the method in more depth.

\(^6\)Further work would include a treatment of exotic payoffs depending on several functionals, although the latter can be usually combined. Take for instance range options that entail the difference between the running maximum \( \mathcal{T}(X_t) = \max_{0 \leq s \leq t} x_s \) and minimum \( \mathcal{L}(X_t) = \min_{0 \leq s \leq t} x_s \). Then one simply sets \( f = \mathcal{T} - \mathcal{L} \).
4.1 The KLMC Algorithm

We assume for simplicity that $Y$ has zero mean, otherwise minor changes must be made for the KL expansion; see Remark 2.2. First, we simulate trajectories $Y^j = (f(X^j_t))_{t_n \in \Pi_{N_{off}}}$, $j = 1, \ldots, J_{off}$ with $J_{off}, N_{off} \in \mathbb{N}$, and compute the eigenfunctions of $\kappa_{Y}^{N_{off}}$ as in (3.1). Next, for $k = 1, \ldots, K$, we estimate the sample quantile function $\Phi_k^{-1} : [0, 1] \to \mathbb{R}$ of $\xi_k = (Y, F_k)$ by employing method No 7 in [12]. The coefficients $(\xi_k)$ can thereafter be simulated using inverse transform sampling [7]. Notice that these steps can be done in an offline phase so $(\Phi_k^{-1})$ can be reused for other options contingent upon the functional $f$; see Section 2.4.

In the online phase, we simulate $J \in \mathbb{N}$ transformed paths using inverse transform sampling for $\xi_k$. Finally, the price surface is calculated using Monte Carlo. The procedure is summarized in Algorithm 4.1. It should be noted that although the coefficients $(\xi_k)$ are orthogonal in $L^2(\Omega)$, they may well be dependent when $Y$ is non-Gaussian. While the marginals of $(\xi_k)_{k \leq K}$ are fitted properly, the dependence is omitted as generating dependent random vectors with unknown joint distribution is highly non-trivial. Nevertheless, this simplification doesn’t induce a bias in the obtained prices as we shall see in the numerical experiments.

Algorithm 4.1 (KLMC)

- **Offline:** Given $f, K, J_{off}, N_{off}$
  1. Simulate trajectories $Y^j = (f(X^j_t))_{t_n \in \Pi_{N_{off}}}$ $j = 1, \ldots, J_{off}$
  2. Compute $\kappa_{Y}^{N_{off}}$ (closed-form or from the sample $(Y^j)$)
  3. Solve the eigenvalue problem (3.1) to obtain $(\lambda_k^\delta, F_k)$
  4. Using $(Y^j)$, estimate the quantile functions $\Phi_k^{-1}$

- **Online:** Given $J, M, T$
  1. Simulate $\xi_k^j = \Phi_k^{-1}(u_k^j)$, $(u_k^j) \sim i.i.d. U(0, 1)$, $j \leq J$, $k \leq K$
  2. Compute $y_{k}^{K, \delta, j} = \sum_{k=1}^{K} \xi_k^j F_k(\tau), \tau \in T, j \leq J$
  3. Estimate the price surface $p^{K, \delta, j}(m, \tau) := \frac{1}{J} \sum_{j=1}^{J} h_m(y_{k}^{K, \delta, j})$.

4.2 Numerical Results

First, we build the price surface for Asian and lookback call options, i.e. by choosing $h_m = h_m^{Call}$ and the running maximum and time average as underlying functional, respectively. Of course, the put option price surface can be retrieved thanks to put-call parity. We also consider Up & Out digital options, that is $f(X_t) = \max_{0 \leq s \leq t} x_s$ and $h_m^{UO}(y) := 1_{\{y \leq m_{x_0}\}}$. The parameter $m \geq 1$ thus represents the barrier of the option relative to the spot price. We can therefore reuse the quantile functions computed for the lookback call options.

The parameters are $(x_0, \sigma, N_{off}, J_{off}, J) = (100, 0.2, 10^3, 2^{17}, 2^{19})$, $T = 1$ year and $\mathcal{T} = \{\frac{1}{52}, \frac{2}{52}, \ldots, 1\}$ (weekly maturities). The moneyness and barrier levels are respectively $\mathcal{M}^{Call} = \{0.75, 0.80, \ldots, 1.25\}$ and $\mathcal{M}^{UO} = \{1.05, 1.10, \ldots, 1.50\}$. We assess accuracy in the mean square sense, namely by computing

$$\text{MSE} = \frac{1}{|\mathcal{M}||\mathcal{T}|} \sum_{(m, \tau) \in \mathcal{M} \times \mathcal{T}} |p^{(B)}(m, \tau) - \hat{p}(m, \tau)|^2.$$
The function $\hat{p}$ is the approximated price and $p^{(B)}$ a benchmark obtained using a standard Monte Carlo with $40 \cdot |\mathcal{T}| = 2080$ time steps and same number of simulations. Table 1 displays the MSE, runtime (online phase) and number of variates per simulated path ($K$ and $N$ for the KLMC and MC method, respectively). Notice that we increase $K, N$ for the lookback call and Up & Out digital option as the running maximum has a slower rate of $L^2(Q \otimes dt)$ convergence as seen in Figure 6 for the Brownian case. The KLMC method constantly yields a lower MSE and runtime. For the Asian call option, note that the number of variates per path is less than the number of maturity points and KLMC method, which couldn’t be done with the MC method.

| Option               | K   | MSE    | Time | N   | MSE    | Time |
|----------------------|-----|--------|------|-----|--------|------|
| Asian Call           | 40  | 1.50e-04 | 2.26 | 52  | 3.10e-04 | 2.40 |
| Lookback Call        | 100 | 1.15e-02 | 4.47 | $4 \cdot 52$ | 1.92e-01 | 7.05 |
| Up & Out Digital     | 100 | 1.80e-04 | 4.40 | $4 \cdot 52$ | 1.90e-04 | 6.88 |

## Conclusion

This paper sheds further light on the approximation of path functionals. After a thorough review of Hilbert projections and a connection with the path signature, we show the power of the Karhunen-Loève expansion to parsimoniously simulate path-dependent payoffs. Further work would include the use of copulas in the KLMC algorithm to capture the dependence between the $L^2([0,T])$ coefficients of the Karhunen-Loève expansion and a performance comparison with signature-based methods.

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The experiments have been made on a personal computer; see https://github.com/valentintissot/KLMC for an implementation. The offline phase takes about 10 seconds per functional.
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