A note on the Karhunen-Loève expansions for infinite-dimensional Bayesian inverse problems

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Abstract

In this note, we consider the truncated Karhunen-Loève expansion for approximating solutions to infinite dimensional inverse problems. We show that, under certain conditions, the bound of the error between a solution and its finite-dimensional approximation can be estimated without the knowledge of the solution.

1 Introduction

Nonparametric inverse problems have applications in many scientific or engineering problems, ranging from geophysical tomography [2] to medical imaging [6]. In such problems the unknown that we want to determine is of infinite-dimension, for example, a function of space or time.

Identifying the unknown is usually cast as an optimization problem that needs to be solved numerically. Infinite-dimensional problems can not be solved directly with standard numerical techniques. A common practice is to first approximate the unknown with a finite-dimensional parameter, and then solve the resulting finite-dimensional problem numerically. In particular, when the inverse problem is treated in a Bayesian framework, the Karhunen-Loève (K-L) expansion ([10], Chapter 11) can be used to construct such a finite-dimensional approximation.
approximation. In the K-L method, the unknown is represented by a finite expansion of the eigenfunctions of the covariance operator of the prior measure.

The K-L method has been long used to reduce the dimensionality in practical problems [9,7,8]; however, the use of it is never rigorously justified to the best of my knowledge. To be specific, it is unclear whether a fixed-dimensional representation can well approximate the solutions of the problem. In this note, we address the problem by proving that, if \( u \) is a solution to the inverse problem defined as a minimizer to Eq (2), the error bound between \( u \) and its finite K-L approximation can be estimated without the knowledge of \( u \).

2 Problem setup

We consider the inverse problems in a Bayesian framework (see [11] for a comprehensive overview of the Bayesian methods for infinite-dimensional inverse problems). We assume the state space \( X \) is a separable Hilbert space with inner product \( \langle \cdot, \cdot \rangle_X \). Our goal is to estimate \( u \in X \) from some data \( y \). The Bayes’ formula in this setting should be interpreted as providing the Radon-Nikodym derivative between the posterior measure \( \mu \) and the prior measure \( \mu_0 \) [3,5]:

\[
\frac{d\mu}{d\mu_0}(u) = \exp(-\Phi(u)),
\]

where \( \exp(-\Phi(u)) \) is the likelihood function. A typical example is to assume that the unknown \( u \) is mapped to the data \( y \) via a forward model \( y = G(u) + \zeta \), where \( G: X \rightarrow \mathbb{R}^d \) and \( \zeta \) is a \( d \)-dimensional Gaussian noise with mean zero and covariance \( C \). In this case \( \Phi(u) = |C^{-\frac{1}{2}}(Gu - y)|_2^2 \).

Next we assume a Gaussian prior is used. Namely we let \( \mu_0 \) be a zero-mean Gaussian measure defined on \( X \) with covariance operator \( Q \). Note that \( Q \) is symmetric positive and of trace class. \( E = Q^{\frac{1}{2}}(X) \) is a Hilbert space with inner product

\[
\langle \cdot, \cdot \rangle_E = \langle Q^{-\frac{1}{2}} \cdot, Q^{-\frac{1}{2}} \cdot \rangle_X,
\]

which is known as the Cameron-Martin space associated with measure \( \mu_0 \). Often we are only interested in a point estimate of \( u \), rather than the posterior measure \( \mu \) itself. To this end, as is shown in [3,5], the maximum a posterior (MAP) estimator of \( u \) can be defined as the minimizers of the Onsager-Machlup functional over \( E \):

\[
\min_{u \in E} I(u) := \Phi(u) + \|u\|_E^2,
\]

where \( \|u\|_E^2 = \langle u, u \rangle_E \). Note that Eq. (2) can also be understood as a classic inverse problem where the cost function \( \Phi(\cdot) \) is minimized with a Tikhonov regularization in the Hilbert space \( E \) [1].
3 Karhunen-Loève representation

Note that solving Eq. (2) directly involves inverting the operator $Q$, which can be rather challenging in practice. Alternatively, one can use substitution $u = Q^{\frac{1}{2}}x$ and rewrite Eq. (2) as

$$
\min_{x \in X} J(x) := \Phi(Q^{\frac{1}{2}}x) + \|x\|^2_X. \tag{3}
$$

The following proposition states the equivalence of the two optimization problems.

**Proposition 3.1** If $x$ minimizes $J(x)$ over $X$, $u = Q^{\frac{1}{2}}x$ minimizes $I(u)$ over $E$, and if $u$ minimizes $I(u)$ over $E$, $x = Q^{-\frac{1}{2}}u \in X$ minimizes $J(x)$ over $X$.

**Proof.** We prove the proposition by contradiction. First it is easy to verify that, for any $x \in X$ and $u \in E$ satisfying $u = Q^{\frac{1}{2}}x$, we have $I(u) = J(x)$. Let $x$ be a minimizer $J(\cdot)$ over $X$, and assume $u = Q^{\frac{1}{2}}x$ is not a minimizer of $I(\cdot)$ over $E$. Namely, there exists an $u' \in E$ such that $I(u') < I(u)$. It follows directly that $x' = Q^{-\frac{1}{2}}u' \in X$ and $J(x') < J(x)$, which contradicts that $x$ is a minimizer of $J$ over $X$. Thus we have proved the first part of the proposition. The second part can be proved by following the same argument. $\square$

Now we introduce the K-L expansion to reduce the dimensionality of Eq. (3). We start with the following lemma ([4], Chapter 1):

**Lemma 3.2** There exists a complete orthonormal basis $\{e_k\}_{k \in \mathbb{N}}$ on $X$ and a sequence of non-negative numbers $\{\lambda_k\}_{k \in \mathbb{N}}$ such that $Qe_k = \lambda_k e_k$ and $\sum_{k=1}^{\infty} \lambda_k < \infty$, i.e., $\{e_k\}_{k \in \mathbb{N}}$ and $\{\lambda_k\}_{k \in \mathbb{N}}$ being the eigenfunctions and eigenvalues of $Q$ respectively.

The basic idea of the K-L method is to solve the optimization problem in a finite-dimensional subspace of $X$:

$$
\min_{x \in X_n} J(x) := \Phi(Q^{\frac{1}{2}}x) + \|x\|^2_X, \tag{4}
$$

where $X_n$ be the space spanned by $\{e_k\}_{k=1}^n$ for a given $n \in \mathbb{N}$. In numerical implementation Eq. (4) can be recast as

$$
\min_{(\xi_1, \ldots, \xi_n) \in \mathbb{R}^n} \Phi\left(\sum_{k=1}^{n} \xi_k \sqrt{\lambda_k} e_k\right) + \sum_{k=1}^{n} \xi_k^2 \tag{5}
$$

which is the usual K-L representation. As is mentioned earlier, a critical question here is whether the finite subspace $X_n$ can provide good approximation to the solutions of Eq. (3). Our main results regarding this problem are presented in the following theorem:
Theorem 3.3 Suppose $\Phi(u)$ is locally Lipschitz continuous, i.e., for every $r > 0$, there exists a constant $L_r > 0$ such that for all $z_1, z_2 \in X$ with $\|z_1\|_X, \|z_2\|_X < r$, we have

$$|\Phi(z_1) - \Phi(z_2)| < L_r \|z_1 - z_2\|_X.$$ 

Let $\{e_k\}_{k \in \mathbb{N}}$ and $\{\lambda_k\}_{k \in \mathbb{N}}$ be the eigenfunctions and eigenvalues of $Q$ as defined in Lemma 3.2. There exists a constant $L > 0$ such that, for any $x \in \arg \min_{x \in X} J(x)$, we have

$$\|x - x_n\|_X < L \sqrt{\lambda^*_n}$$

where $x_n = \sum_{k=1}^{n} \langle x, e_k \rangle_X e_k$, and $\lambda^*_n = \max_{k > n} \lambda_k$.

Proof. Let $x \in X$ be a minimizer of Eq. (3). Since $\{e_k\}$ is a complete orthonormal basis for $X$, $x$ can be written as

$$x = \sum_{k=1}^{\infty} \xi_k e_k,$$

where $\xi_k = \langle x, e_k \rangle_X$. Let

$$x_n = \sum_{k=1}^{n} \xi_k e_k.$$

As $x$ is a minimizer of $J(\cdot)$, take $r = \Phi(0) + 1$ and so we have $J(x) < r$, which implies that $\|x_n\|_X \leq \|x\|_X < r$. $Q^\frac{1}{2}$ is bounded, and so we have $\|Q^\frac{1}{2} x_n\|_X, \|Q^\frac{1}{2} x\|_X < \|Q^\frac{1}{2}\| r$. Now recall that $\Phi(\cdot)$ is locally Lipschitz continuous, and so there exists a constant $L > 0$ such that

$$|\Phi(Q^\frac{1}{2} x) - \Phi(Q^\frac{1}{2} x_n)| < L \|Q^\frac{1}{2} x - Q^\frac{1}{2} x_n\|_X.$$ 

Since $x$ minimizes $J(\cdot)$, we have $J(x) \leq J(x_n)$ which implies

$$\|x - x_n\|_X^2 \leq |\Phi(Q^\frac{1}{2} x) - \Phi(Q^\frac{1}{2} x_n)| < L \|Q^\frac{1}{2} x - Q^\frac{1}{2} x_n\|_X$$

$$= L \langle x - x_n, Q(x - x_n) \rangle_\frac{1}{2} = \sum_{k=n+1}^{\infty} \xi_k e_k, \sum_{k=n+1}^{\infty} \xi_k \lambda_k e_k \rangle_\frac{1}{2}$$

$$= L \sum_{k=n+1}^{\infty} \lambda_k \xi_k^2 \leq L \sqrt{\lambda^*_n} \|x - x_n\|_X.$$ 

It then follows immediately that

$$\|x - x_n\|_X \leq L \sqrt{\lambda^*_n}.$$ 

$\square$
Certainly we also want to know if the minimizer of the original problem (2) is well approximated by the K-L expansion. To this end, we have the following corollary, which is a direct consequence of Theorem 3.3:

**Corollary 3.4** Let \( u = Q^\frac{1}{2} x \) and \( u_n = Q^\frac{1}{2} x_n \), and we have \( \| u - u_n \|_X < L\lambda^*_n \).

Another important question is that whether a solution to finite-dimensional problem (4) is a good approximation to that of the infinite-dimensional problem (3). We have the following results regarding this issue:

**Corollary 3.5** Let \( x'_n \in \arg \min_{x \in X_n} J(x) \) and we have

\[
\min_{x \in X} J(x) \leq J(x'_n) \leq \min_{x \in X} J(x) + L^2\lambda^*_n
\]

The corollary follows directly from Theorem 3.3 and so proof is omitted.

## 4 Concluding remarks

We theoretically study the truncated K-L expansions for approximating the solutions of infinite-dimensional Bayesian inverse problems. We show that the error between a solution to the inverse problem and its projection on the chosen finite-dimensional space is bounded by the eigenvalues of the covariance operator of the prior.

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