An introduction to the Hilbert-Schmidt SVD using iterated Brownian bridge kernels

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Abstract Kernel-based approximation methods—often in the form of radial basis functions—have been used for many years now and usually involve setting up a kernel matrix which may be ill-conditioned when the shape parameter of the kernel takes on extreme values, i.e., makes the kernel “flat”. In this paper we present an algorithm we refer to as the Hilbert-Schmidt SVD and use it to emphasize two important points which—while not entirely new—present a paradigm shift under way in the practical application of kernel-based approximation methods: (i) it is not necessary to form the kernel matrix (in fact, it might even be a bad idea to do so), and (ii) it is not necessary to know the kernel in closed form. While the Hilbert-Schmidt SVD and its two implications apply to general positive definite kernels, we introduce in this paper a class of so-called iterated Brownian bridge kernels which allow us to keep the discussion as simple and accessible as possible.

Keywords Hilbert-Schmidt SVD · Iterated Brownian bridge kernels · Positive definite kernels · Stable interpolation · Splines

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1 Introduction

Kernel-based methods are popular tools for problems of interpolation and differential equations [8, 12], statistics [40], machine learning [30, 41], and other fields. Their popularity stems from their inherently meshfree nature, providing an avenue to potentially avoid the “curse of dimensionality” [13, 27]. Many different kernels exist, and several factors may be considered when choosing the appropriate kernel for a given application, including the numerical stability of computations involving that kernel.

The presence of free parameters influencing the shape and smoothness of kernels allows for high levels of accuracy, but may also introduce ill-conditioning into the standard problem formulation. For many very smooth kernels, or kernels with an increasingly flat parametrization, the computational error may prevent realization of the theoretically optimal accuracy. This problem was analyzed in, e.g., [5, 11, 23, 33, 39] and techniques to circumvent this in certain circumstances were discussed in, e.g., [15–17].

In [14], a technique was developed using Hilbert-Schmidt theory [35] to create a new basis for the Gaussian interpolant derived from the eigenfunction expansion of the Gaussian in \( \mathbb{R}^d \); the new basis is devoid of the standard ill-conditioning. This change of basis approach was first used in the pioneering work [16]. Once increasingly flat Gaussian interpolants could be stably computed, the polynomial limit, as predicted in [11, 22, 23, 33], could be numerically confirmed in arbitrary dimensions. Therefore, Gaussians can always produce at least the same accuracy as polynomials because the polynomial result can be obtained in the limit.

Since the eigenfunction expansion associated with the Gaussian kernel is rather complex and its implementation (which can be found in the MATLAB library http://math.iit.edu/~mccomic/gaussqr/) is non-trivial we have decided to present in this paper a completely transparent implementation of the Hilbert-Schmidt SVD which uses so-called iterated Brownian bridge kernels. The advantage of introducing this new class of kernels, defined on the interval \([0, 1]\) with very specific boundary conditions, lies in the fact that the resulting MATLAB code is almost trivial and can be included in this paper (see Appendix). Moreover, iterated Brownian bridge kernels generalize the Brownian bridge kernel which plays an important role in many applications in statistics or finance (see, e.g., [4, Section 2.2.1], [18, Section 3.1], [32, Section 3.7], [38, Section 4.7.4], and our explanation in Remark 1).

The two main messages we would like to communicate with this paper are

1. The kernel-based solution of interpolation, approximation or differential equations problems can—and perhaps frequently should—be achieved without ever forming the so-called kernel matrix \( K \) (sometimes also referred to as Gram or collocation matrix). This, in particular, implies that the Hilbert-Schmidt SVD (see (3.6)) is not obtained by factoring the kernel matrix. However, the Hilbert-Schmidt SVD does represent a factorization of the kernel matrix. In other words, we can—if needed—obtain \( K \) from the Hilbert-Schmidt SVD, but not vice versa (as is done with the traditional SVD in linear algebra).