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A Kernel-Independent Sum-of-Gaussians Method by de la Vallée-Poussin Sums

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Abstract. Approximation of interacting kernels by sum of Gaussians (SOG) is frequently required in many applications of scientific and engineering computing in order to construct efficient algorithms for kernel summation or convolution problems. In this paper, we propose a kernel-independent SOG method by introducing the de la Vallée-Poussin sum and Chebyshev polynomials. The SOG works for general interacting kernels and the lower bound of Gaussian bandwidths is tunable and thus the Gaussians can be easily summed by fast Gaussian algorithms. The number of Gaussians can be further reduced via the model reduction based on the balanced truncation based on the square root method. Numerical results on the accuracy and model reduction efficiency show attractive performance of the proposed method.

AMS subject classifications: 65D15, 42A16, 70F10

Key words: Sum-of-Gaussians approximation, interaction kernels, de la Vallée-Poussin sums, model reduction.

1 Introduction

For a given smooth function $f(x)$ for $x\in D$ with D a finite interval and an error tolerance ε, we consider the approximation of this function by the sum of Gaussians (SOG),

$$\max_{x\in D}\Big|f(x)-\sum_j w_j e^{-t_j x^2}\Big|<\varepsilon\max_{x\in D}|f(x)|, \tag{1.1}$$

where w_j and $1/\sqrt{t_j}$ are the weight and the bandwidth of the jth Gaussian, respectively. Over the past decades, the SOG approximation has attracted wide interest since it can be

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useful in many applications of scientific computing such as convolution integral in physical space [1–4], the kernel summation problem [5,6] and efficient nonreflecting boundary conditions for wave equations [7–11]. Many kernel functions in these problems have the form of the radial function $f(x)=f(\|\boldsymbol{x}\|)$ for $\boldsymbol{x}\in\mathbb{R}^d$, such as the power kernel $\|\boldsymbol{x}\|^{-s}$ with $s>0$, the Hardy multiquadratic $\sqrt{\|\boldsymbol{x}\|^2+s^2}$, the Matérn kernel [12] and the thin-plate spline $\|\boldsymbol{x}\|^2\log\|\boldsymbol{x}\|$. An SOG approximation to these kernels is particularly useful because a Gaussian kernel can simply achieve the separation of variables such that a convolution of $f(x)$ with it can be computed as the summation of products of d one-dimensional integrals, dramatically reducing the cost.

The solution of (1.1) has been an extensively studied subject in literature [13–23]. One way to construct the SOG expansion is via the best rational approximation or the sum-of-poles approximation, which is based on the fact that the rational approximation for the Laplace transform of function $f(x)$ has explicit expression, and the inverse transform gives the sum-of-exponentials approximation. When the kernel is radially symmetric, the SOG approximation is equivalent to the SOE approximation by a simple change of variable $y=\sqrt{x}$. If one does not restrict the bound of the Gaussian bandwidths, the integral representation of the kernel can be a significant tool. For example, the power function x^{-s} has the following inverse Laplace transform expression [14],

$$x^{-s}=\frac{1}{\Gamma(s)}\int_{-\infty}^{\infty}e^{-e^t x+st}dt, \tag{1.2}$$

with $\Gamma(\cdot)$ being the Gamma function. A suitable quadrature rule to Eq. (1.2) yields an explicit discretization to obtain a sum of exponentials. Constructing the SOG approximation from integral representation is superficially attractive due to the controllable high accuracy with the number of Gaussians. The integral form for general kernels by the inverse Laplace transform can be found in Dietrich and Hackbusch [16].

Another important approach for the SOG is the least squares approximation. A straightforward use of the least squares method will be less accurate due to the difficulty of solving the ill-conditioned matrix. The least squares problem can be solved by employing the divided-difference factorization and the modified Gram-Schmidt method to significantly improve the accuracy [23]. Greengard et al. [3] developed a black-box approach for the SOG of radially symmetric kernels. This approach allocates a set of logarithmically equally spaced points t_j lying on the positive real axis, then a set of sampling points x_i is constructed via adaptive bisections. Then the fitting matrix A with entry $A_{ij}=e^{-t_j x_i}$ and the right hand vector b with $b_i=f(x_i)$ are constructed. After one obtains the weights by solving the least squares problem, the square root method in model reduction [24] is introduced to reduce the number of exponentials and achieve a near-optimal SOE approximation.

Function approximation using Gaussians is a highly nonlinear problem and the design of such approximations for t_j such that it is bounded by a positive number (i.e., the lower bound of bandwidths is independent of the number of Gaussians) is nontrivial. In applications with fast Gauss transform (FGT) [25,26] to calculate the kernel summa-