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Approximating the Gaussian as a Sum of Exponentials and its Applications to the Fast Gauss Transform

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Abstract. We develop efficient and accurate sum-of-exponential (SOE) approximations for the Gaussian using rational approximation of the exponential function on the negative real axis. Six digit accuracy can be obtained with eight terms and ten digit accuracy can be obtained with twelve terms. This representation is of potential interest in approximation theory but we focus here on its use in accelerating the fast Gauss transform (FGT) in one and two dimensions. The one-dimensional scheme is particularly straightforward and easy to implement, requiring only twenty-four lines of MATLAB code. The two-dimensional version requires some care with data structures, but is significantly more efficient than existing FGTs. Following a detailed presentation of the theoretical foundations, we demonstrate the performance of the fast transforms with several numerical experiments.

AMS subject classifications: 31A10, 65F30, 65E05, 65Y20

Key words: Fast Gauss transform, sum-of-exponential approximation, best rational approximation, model reduction.

1 Introduction

In this paper, we consider the approximation of the Gaussian kernel

$$G(x;\delta)=e^{-\frac{x^2}{4\delta}}, \tag{1.1}$$

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using a sum-of-exponential (SOE) representation:

$$G(x;\delta) \approx S_{K_e}(x;\delta) := \sum_{k=1}^{K_e} w_k e^{-t_k \frac{|x|}{\sqrt{\delta}}}, \tag{1.2}$$

where w_k and t_k are complex weights and nodes and K_e is the number of such terms. We show numerically that the SOE approximation converges geometrically, with maximum error of the order $\mathcal{O}\left(c^{-K_e}\right)$. The optimal value for c is difficult to determine, but using ideas from rational approximation (see, for example, [7,11,36]), we show that only twelve terms are needed for ten-digit accuracy. Moreover, when K_e is even, the weights and nodes are constructed in complex conjugate pairs so that (with a suitable ordering) we may write

$$S_{K_e}(x;\delta) = \Re\mathrm{e}\left(\sum_{k=1}^{K_e/2} w_k e^{-t_k \frac{|x|}{\sqrt{\delta}}}\right). \tag{1.3}$$

Thus, in one dimension, only six terms are needed for ten-digit accuracy.

Remark 1.1. Unfortunately, the factor of two reduction in (1.3) can only be used in one dimension. When approximating the two dimensional Gaussian, we will make use of the separable approximation

$$G(x,y;\delta) = e^{-\frac{x^2+y^2}{4\delta}} \approx \Re\mathrm{e}\left(\sum_{k=1}^{K_e/2} w_k e^{-t_k \frac{|x|}{\sqrt{\delta}}} \sum_{l=1}^{K_e} w_l e^{-t_l \frac{|y|}{\sqrt{\delta}}}\right). \tag{1.4}$$

We show here that the SOE approximation of the Gaussian can be used to develop a new version of the fast Gauss transform (FGT), which computes sums of the form

$$u_i = \sum_{j=1}^{N} G(x_i - y_j;\delta) q_j, \quad i = 1,\cdots M, \tag{1.5}$$

in $\mathcal{O}(N+M)$ time. The main advantage of exponential functions in this context follows from the fact that they are eigenfunctions of the translation operator, which leads to a simple "sweeping" algorithm in one dimension, whose performance is entirely independent of the variance δ. In higher dimensions, the SOE approximation can be used to accelerate existing FGTs [13,14,29,38]. The SOE-based scheme shares some feature with the "plane wave" versions of the FGT [14,29,38], with an important difference. The earlier plane-wave schemes use the Fourier transform to develop an approximation of the Gaussian in terms of oscillatory exponentials with a restricted range of validity. The SOE approximation uses the Laplace transform, involves many fewer terms, and is uniformly accurate in the ambient space. It outperforms existing FGTs in the literature. A slight difficulty arises from the fact that the argument in the SOE approximation involves the