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A NEW ERROR ESTIMATE OF THE FAST GAUSS TRANSFORM*

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Abstract. The fast Gauss transform of L. Greengard and J. Strain [*SIAM J. Sci. Statist. Comput.*, 12 (1991), pp. 79–94] reduces the computational complexity of the evaluation of the sum of N Gaussians at M points in d-dimensional space from $\mathcal{O}(MN)$ to $\mathcal{O}(M+N)$ floating-point operations. In this note, we provide numerical evidence that the error estimate of Lemma 2.1 in [*SIAM J. Sci. Statist. Comput.*, 12 (1991), pp. 79–94] is erroneous and then proceed to calculate a replacement error estimate for the fast Gauss transform, incorporating an improved upper bound for Hermite functions.

Key words. fast Gauss transform, fast algorithms

AMS subject classifications. 65R10, 33A65, 35K05, 62G20, 65P05

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The direct computation of the discrete Gauss transform in d-dimensions, that is, the evaluation of the sum of N Gaussians at M points, requires $\mathcal{O}(MN)$ operations. The computational complexity of this task has been reduced by Greengard and Strain [2] to $\mathcal{O}(M+N)$ by means of the fast Gauss transform algorithm. Without loss of generality, the algorithm assumes that all the points involved in the computation are contained within the unit hypercube $[0,1]^d$.

At the heart of this algorithm lies the following result [3, Lemma 2.1].

Let N points s_j lie in a box $B = \{s \in [0,1]^d : ||s-c||_\infty < \sqrt{\delta}/2\}$ with center c and side length $\sqrt{\delta}$. Then, the Gaussian field

$$G(x) = \sum_{j=1}^{N} q_j e^{-||x-s_j||_2^2/\delta} \tag{1}$$

is equal to a single Hermite expansion about c:

$$G(x) = \sum_{\alpha \geq 0} A_\alpha h_\alpha \left(\frac{x-c}{\sqrt{\delta}} \right). \tag{2}$$

The coefficients A_α are given by

$$A_\alpha = \frac{1}{\alpha!} \sum_{j=1}^{N} q_j \left(\frac{s_j - c}{\sqrt{\delta}} \right)^\alpha. \tag{3}$$

Here α is a multi-index and the notation $\alpha > p$ implies $\alpha_i > p$ for $i = 1, \ldots, d$. The Hermite functions h_n (with nonclassical normalization parameter) are defined by $h_n(x) = e^{-x^2} H_n(x)$, where H_n are the Hermite polynomials [1]. Further, Lemma 2.1 of [3] claims that the error E_p due to the truncation of the series (2) after p^d terms

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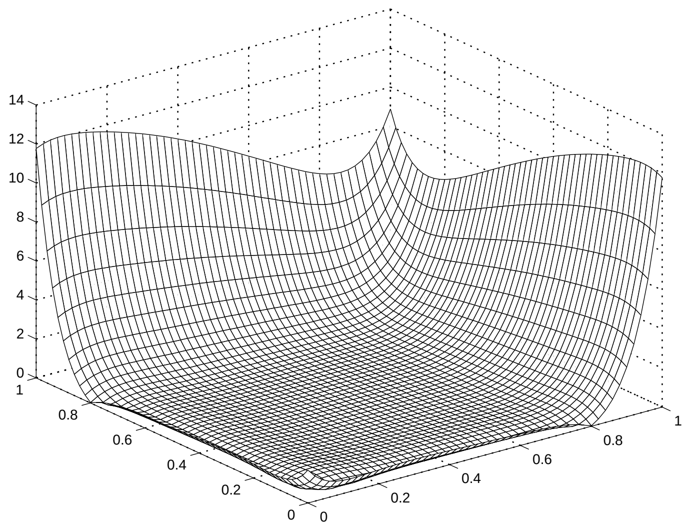

FIG. 1. *Quotient of the actual error divided by the error estimate of* [3, Lemma 2.1].

satisfies the bound

$$\left| e^{-||x-s_j||_2^2/\delta} - \sum_{\alpha<p} A_\alpha h_\alpha \left(\frac{x-c}{\sqrt{\delta}} \right) \right| \leq Q\, 2.75^d (p!)^{-d/2}\, 2^{-(p+1)d/2}, \tag{4}$$

where $Q = \sum |q_j|$.

However, the error estimate (4) is erroneous and underestimates the actual error introduced after the truncation of the series. For example, consider the two-dimensional case of a single Gaussian with parameter $\delta = 1$ at source point $s \equiv (0, 0)$ and weight $q = 1$. Indeed, Figure 1 shows the quotient of the actual error divided by the estimate (4) evaluated on a 50×50 grid on the unit square. The series are truncated after the first 25 terms.

We now construct a replacement error estimate for the fast Gauss transform. For a source point s, an evaluation point x and the center c of a box B we introduce the following componentwise notation:

$$u_p(x_i, s_i, c_i) = \sum_{n_i=0}^{p-1} \frac{1}{n_i!} \left(\frac{x_i - c_i}{\sqrt{\delta}} \right)^{n_i} h_{n_i} \left(\frac{y_i - c_i}{\sqrt{\delta}} \right), \qquad 1 \leq i \leq d, \tag{5}$$

$$v_p(x_i, s_i, c_i) = \sum_{n_i=p}^{\infty} \frac{1}{n_i!} \left(\frac{x_i - c_i}{\sqrt{\delta}} \right)^{n_i} h_{n_i} \left(\frac{y_i - c_i}{\sqrt{\delta}} \right), \qquad 1 \leq i \leq d, \tag{6}$$

which we can use to write the corresponding Gaussian as

$$e^{-||x-s||_2^2/\delta} = \prod_{j=1}^{d} \left(u_p(x_i, s_i, c_i) + v_p(x_i, s_i, c_i) \right). \tag{7}$$

Assuming that the point s is contained in the box $B = \{s \in [0,1]^d : ||s - c||_\infty < r\sqrt{\delta/2}\}$ of side length $r\sqrt{2\delta}$ for some $r < 1$ [2, cf. Lemma 2.1] centered at c, and using the inequality for Hermite functions by Szász [4]

$$\frac{1}{n!}|h_n(x)| \le \frac{2^{n/2}}{\sqrt{n!}}\, e^{-x^2/2}, \qquad n \ge 0 \text{ and } x \in \mathcal{R}, \tag{8}$$

and the properties of the geometric series, we have

$$u_p(x_i, s_i, c_i) \le \frac{1 - r^p}{1 - r}, \qquad 1 \le i \le d, \tag{9}$$

$$v_p(x_i, s_i, c_i) \le \frac{1}{\sqrt{p!}} \frac{r^p}{1 - r}, \qquad 1 \le i \le d, \tag{10}$$

and thus, from (7), we have

$$\left| e^{-||x-s||_2^2/\delta} - \prod_{j=1}^{d} u_p(x_i, s_i, c_i) \right| \le (1 - r)^{-d} \sum_{k=0}^{d-1} \binom{d}{k} (1 - r^p)^k \left(\frac{r^p}{\sqrt{p!}} \right)^{d-k}. \tag{11}$$

Finally we can calculate an error estimate for the fast Gauss transform

$$\left| e^{-||x-s_j||_2^2/\delta} - \sum_{\alpha < p} A_\alpha h_\alpha \left(\frac{x - c}{\sqrt{\delta}} \right) \right| \le \frac{Q}{(1 - r)^d} \sum_{k=0}^{d-1} \binom{d}{k} (1 - r^p)^k \left(\frac{r^p}{\sqrt{p!}} \right)^{d-k}.$$

Note that this error estimate and the error estimate of [2, Lemma 2.1] coincide when $d = 1$, but they are distinct in higher dimensions. Of course, similar reasoning can be directly applied to Lemmas 2.2 and 2.3 of [2] to obtain corresponding error estimates.

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