Faster Gaussian Summation: Theory and Experiment

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Abstract

We provide faster algorithms for the problem of Gaussian summation, which occurs in many machine learning methods. We develop two new extensions - an \(O(D^p)\) Taylor expansion for the Gaussian kernel with rigorous error bounds and a new error control scheme integrating any arbitrary approximation method - within the best discrete-algorithmic framework using adaptive hierarchical data structures. We rigorously evaluate these techniques empirically in the context of optimal bandwidth selection in kernel density estimation, revealing the strengths and weaknesses of current state-of-the-art approaches for the first time. Our results demonstrate that the new error control scheme yields improved performance, whereas the series expansion approach is only effective in low dimensions (five or less).

1 Fast Gaussian Summation

Kernel summations occur ubiquitously in both old and new machine learning algorithms, including kernel density estimation, kernel regression, radial basis function networks, spectral clustering, and kernel PCA (Gray & Moore, 2001; de Freitas et al., 2006). This paper will focus on the most common form

\[
G(x_q) = \sum_{r=1}^{N} w_r K(\delta_{qr})
\]

in which we desire the sum for \(M\) different query points \(x_r\)’s, each using \(N\) reference points \(x_r\)’s weighted by \(w_r > 0\). \(K(\delta_{qr}) = e^{-\frac{\delta_{qr}^2}{2h^2}}\) is the Gaussian kernel, where \(\delta_{qr} = ||x_q - x_r||\) with scaling parameter, or bandwidth \(h\). For concreteness we will take as our main example kernel density estimation (Silverman, 1986), the most widely used distribution-free method for the fundamental task of density estimation. Because the Gaussian kernel has infinite tail, we must pursue approximation in order to achieve runtimes less than that of exhaustive summation. Our goal is to compute each \(G(x_q)\) as quickly as possible while ensuring that \(\forall x_q \frac{|G(x_q) - G(x_q)|}{G(x_q)} \leq \epsilon\) where \(\epsilon\) is a user-supplied error tolerance. In practice we wish to perform this computation for a range of bandwidths, from small to large, for example in order to do optimal bandwidth selection by cross-validation.

The basic idea in kernel summation is to approximate the kernel sum contribution \(G_R(x_q)\) of some subset of the reference points \(X_R\) of size \(N_R\), lying in some small region of space \(R\) with centroid \(x_R\), to a query point. In more efficient schemes the approximate contribution is made to an entire subset of the query points \(X_Q\) of size \(N_Q\) lying in some region of space \(Q\), with centroid \(x_Q\).

Methods from computational physics. The successful Fast Multipole Method (FMM) (Greengard & Rokhlin, 1987) developed for the Coulombic kernel, used multipole expansions for the continuous approximation, octrees (a form of hierarchical grid) for the discrete data structure, and an explicit level-by-level enumeration of the node-node comparisons. Since the expansions only hold locally, (Greengard & Rokhlin, 1987) developed a set of three ‘translation operators’ for converting between expansions centered at different points in order to create their hierarchical algorithm.

The original Fast Gauss Transform (FGT) (Greengard & Strain, 1991) was developed in the same style, but for the Gaussian kernel using two different expansions. The first one is the multivariate Hermite expansion which expresses a sum as an expansion about a representative centroid \(x_R\) in the reference region \(R\): \(^1\)

\[^1\)In this paper we use the multi-index notation (Greengard & Strain, 1991; Yang et al., 2003). A multi-index \(\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_D)\) is a \(D\)-tuple of integers. For any multi-index \(\alpha, \beta\) and any \(x \in \mathbb{R}^D\), (1) \(|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_D\), (2) \(\alpha! = \alpha_1! \alpha_2! \cdots \alpha_D!\), (3) \(x^\alpha = x_{\alpha_1} x_{\alpha_2} \cdots x_{\alpha_D}\), (4) \(D^\alpha = \partial_{\alpha_1}^2 \partial_{\alpha_2}^2 \cdots \partial_{\alpha_D}^2\), (5) \(\alpha + \beta = (\alpha_1 + \)
\[ G(x_q) = \sum_{x_r \in R} w_r \sum_{|\alpha| \geq 0} \frac{1}{\sqrt{2\pi^{d/2} h_\alpha^{2d}}} (x_r - x_q)^\alpha h_\alpha \left( \frac{x_r - x_q}{\sqrt{2h}} \right) \]

This can be re-written as:

\[ G(x_q) = \sum_{x_r \in R} w_r \sum_{|\alpha| \geq 0} \frac{1}{h_\alpha} (x_r - x_q)^\alpha h_\alpha \left( \frac{x_r - x_q}{\sqrt{2h}} \right) \]

as a Taylor (local) expansion about a representative centroid \( x_Q \) in the query region. 

**Dual-tree recursion.** In terms of discrete algorithmic structure, the dual-tree framework of (Gray & Moore, 2001), in the context of kernel summation, generalizes all of the well-known algorithms, including the Barnes-Hut algorithm (Barnes & Hut, 1986), the Fast Multipole Method (Greengard & Rokhlin, 1987), Appel’s algorithm (Appel, 1985), and the WSPD (Callahan & Kosaraju, 1995): it is a node-node algorithm (considers query regions rather than points), is fully recursive, can use adaptive data structures such as kd-trees, and is bichromatic (can specialize for differing query and reference sets). The idea is to represent both the query points and the reference points respectively with a tree and recurse on a pair of query and reference node. This is shown in depth-first form in Figure 1 though it can also be performed using a priority queue (Gray & Moore, 2003a). It was applied to the problem of kernel density estimation in (Gray & Moore, 2003b) using a finite-difference approximation, a variant of a monopole approximation. Partially by avoiding series expansions, which depend explicitly on the dimension, the result was the fastest such algorithm for general dimension, when operating at the optimal bandwidth. However, when performing cross-validation to determine the (initially unknown) optimal bandwidth, both suboptimally small and large bandwidths must be evaluated. This finite-difference-based method tends to be efficient around or below the optimal bandwidth, and at very large bandwidths, but for intermediate-large bandwidths it suffers.

\( \beta_1, \cdots, \alpha_D + \beta_D, (\alpha_0 - \beta) = (\alpha_1 - \beta_1, \cdots, \alpha_D - \beta_D) \), where \( \alpha_i \) is an \( i \)-th directional partial derivative. We define \( \alpha > \beta \) if \( \alpha_i > \beta_i \) and \( \alpha \geq p \) for \( p \in \mathbb{Z} \) if \( \alpha_i > p \) for \( 1 \leq i \leq D \).

2 We define the Hermite functions \( h_n(t) \) by \( h_n(t) = e^{-t^2} H_n(t) \), where the Hermite polynomials \( H_n(t) \) are defined by the Rodrigues formula: \( H_n(t) = (-1)^n e^{t^2} D^n e^{-t^2}, t \in \mathbb{R}^d \). The multivariate Hermite function is then defined as a product of its univariate versions: \( h_n(t) = \prod_{d=1}^D h_{n_d}(t_d) \).

**Automatic error control.** Among the existing methods, dual-tree method is the only one to automatically achieve the user’s error tolerance \( \epsilon \). Other methods are overridden with many \textit{tweak parameters} whose values have to be changed simultaneously with little or no guidance. These parameters waste human time and offer no error tolerance guarantee (unless verified by a procedure that computes density estimate exhaustively). This issue is discussed in Section 7.

**Series expansion.** Expansions in (Greengard & Strain, 1991) require the computation of \( O(p^D) \) sub-terms. While effective in the context of computational physics problems, this is problematic in statistical/data mining applications, in which \( D \) may be larger than 2 or 3. (Lee et al., 2006) developed the translation operators and error bounds necessary to perform the original FGT-style \( O(p^D) \) approximation within the context of the dual-tree framework, demonstrating the first hierarchical fast Gauss transform. However, the new algorithm showed efficiency over any of the aforementioned methods over the entire range of bandwidths necessary in cross-validation, only in very low dimensions (3 or less). The Improved Fast Gauss Transform (IFGT) (Yang et al., 2003) introduced a rearranged series approximation requiring \( O(D^p) \) sub-terms, which seemed promising for higher dimensions with an associated error bound, which was unfortunately incorrect. The IFGT was based on a flat set of clusters and did not provide any translation operators.

**This paper.** We demonstrate for the first time the \( O(D^p) \) (rather than \( O(p^D) \)) expansion of the Gaussian kernel (different from that of the IFGT) within a hierarchical (dual-tree) algorithm. We also introduce a more efficient mechanism for automatically achieving the user’s error tolerance which works with both discrete and continuous approximation schemes. We evaluate these new techniques empirically on real datasets, revealing the strengths and weaknesses of the main current approaches for the first time.

### 2 \( O(D^p) \) and \( O(p^D) \) Expansions

For conciseness, we first discuss the difference between \( O(p^D) \) and \( O(D^p) \) expansion by approximating the 2-D Gaussian kernel using its Hermite expansion at order \( p = 2 \). Its \( O(p^D) \) expansion is:

\[
e^{-\frac{||x_q-x_r||^2}{2h^2}} = \sum_{d=1}^2 \left( h_0 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) h_1 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) + \cdots \right) \approx 1 \cdot h_0 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) h_0 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) + (\frac{x_{qd} - x_{rd}}{\sqrt{2h^2}}) h_1 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) h_0 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) + \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) h_1 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) h_1 \left( \frac{x_{qd} - x_{rd}}{\sqrt{2h^2}} \right) \right)
\]
In both cases, \( D \) expansions are used in the corresponding reference node. \( O(p^D) \) expansion requires exactly \( p^D \) coefficients, while \( O(D^p) \) one requires \( (D^p - D) \). If we iterate over all reference points in the reference node with their weights taken into account, we store:

\[
\sum_{r=1}^{N_R} w_r \left( \frac{x_{r1} - x_{q1}}{\sqrt{2h^2}} \right), \quad \sum_{r=1}^{N_R} w_r \left( \frac{x_{r1} - x_{q1}}{\sqrt{2h^2}} \right) \quad \text{and} \quad \sum_{r=1}^{N_R} w_r \left( \frac{x_{r2} - x_{q2}}{\sqrt{2h^2}} \right) \quad \text{for} \quad O(p^D), \quad \text{and} \quad \sum_{r=1}^{N_R} w_r \left( \frac{x_{r2} - x_{q2}}{\sqrt{2h^2}} \right) \quad \text{for} \quad O(D^p),
\]

The Taylor expansion works similarly, except that the coefficients are stored in the corresponding query node.

## 3 Translation Operators

Since the properties of the Gaussian kernel do not require that approximation be made in the local fashion, the original FGT used a flat grid with only \( H2L \) operator whose associated incorrect error was corrected by (Baxter \\& Roussos, 2002). (Lee et al., 2006) derived two additional translation operators necessary for a hierarchical FGT and the associated error bounds for \( O(p^D) \) expansion of Hermite/Taylor coefficients. We briefly review all three translation operators.

The first translation operator transfers the contribution of a reference node \( R \) into the Taylor series centered about \( x_R \) in a query node \( Q \).

**Lemma 1.** Hermite-to-local (H2L) translation operator (in Lemma 2.2 in (Greengard \\& Strain, 1991)): Given a reference node \( R \), a query node \( Q \), and the Hermite expansion centered at a centroid \( x_R \) of \( R \):

\[
G(x_q) = \sum_{|\alpha| \geq 0} A_{\alpha} h_{\alpha}(\frac{x_q - x_R}{\sqrt{2h^2}}) \quad \text{where} \quad A_{\alpha} = \sum_{\beta | |\beta| \geq 0} w_{\beta} (\frac{x_q - x_R}{\sqrt{2h^2}})^\beta \quad \text{and} \quad B_{\beta} = (-1)^{\beta} \sum_{|\alpha| \geq 0} A_{\alpha} h_{\alpha + \beta}(\frac{x_q - x_R}{\sqrt{2h^2}}).
\]

The next operator allows efficient precomputation of the Hermite moments in the reference tree in a bottom-up fashion from its children.

**Lemma 2.** Hermite-to-Hermite (H2H) translation operator: Given the Hermite expansion centered at a centroid \( x_R \) in a reference node \( R' \):

\[
G(x_q) = \sum_{|\alpha| \geq 0} A'_{\alpha} h_{\alpha}(\frac{x_q - x_R}{\sqrt{2h^2}}) \quad \text{this same Hermite expansion shifted to a new location} \quad x_R \quad \text{of the parent node} \quad R \quad \text{is given by:} \quad G(x_q) = \sum_{|\gamma| \geq 0} A_{\gamma} h_{\gamma}(\frac{x_q - x_R}{\sqrt{2h^2}}) \quad \text{where} \quad A_{\gamma} = \sum_{0 \leq \alpha \leq \gamma} \frac{1}{(\gamma - \alpha)!} A'_{\alpha} (\frac{x_q - x_R}{\sqrt{2h^2}})^{\gamma - \alpha}.
\]

The final operator combines the approximations at different scales through one breadth-first traversal.

**Lemma 3.** Local-to-local (L2L) translation operator: Given a Taylor expansion centered at a centroid \( x' \) of a query node \( Q' \):

\[
G(x_q) = \sum_{|\beta| \geq 0} B_{\beta}(\frac{x_q - x'_Q}{\sqrt{2h^2}})^\beta \quad \text{the Taylor expansion obtained by shifting this expansion to the new centroid} \quad x_Q \quad \text{of the child node} \quad Q \quad \text{is:} \quad G(x_q) = \sum_{|\alpha| \geq 0} \sum_{\beta | |\beta| \geq \alpha} B_{\beta} (\frac{x_q - x'_Q}{\sqrt{2h^2}})^{\beta - \alpha} (\frac{x_q - x_Q}{\sqrt{2h^2}})^\alpha.
\]

## 4 Error Bounds for \( O(D^p) \) Expansions

Because Hermite/Taylor expansions are truncated after a finite number of terms, we incur an error in approximation. In order to bound the total approximation error, we need one error bound for each translation operator. In (Lee et al., 2006), the Hermite and
the Taylor expansion were treated as products of $D$ univariate Hermite/Taylor expansions. The trailing sum in each univariate expansion was bounded using the property of infinite geometric series, which in turn limited the size of the query/reference node for pruning to be valid. Here, we use the same translation operators, but instead view each expansion as a vector function and use the $O(D^p)$ expansion advocated in (Yang et al., 2003). The new error bounds based on this new expansion scheme depend on the multidimensional Taylor’s Theorem, and effectively eliminate the node size restriction imposed by the $O(p^D)$ expansion (Greengard & Strain, 1991; Lee et al., 2006).

**Theorem 1.** Multidimensional Taylor’s Theorem: Let $O \subseteq \mathbb{R}^D$ be an open set. Let $x_0 \in O$ and $f$ be a function which is $n$ times differentiable in $O$. For any $x \in O$, there exists $\theta \in \mathbb{R}$ with $0 < \theta < 1$ such that $f(x) = \sum_{|\alpha| = p} \frac{1}{\alpha!} D^\alpha f(x_0)(x - x_0)^\alpha + \sum_{|\alpha| = p+1} \frac{1}{\alpha!} D^\alpha f(x_0 + \theta(x - x_0))(x - x_0)^\alpha$. The last term $R_n = \sum_{|\alpha| = p+1} \frac{1}{\alpha!} D^\alpha f(x_0 + \theta(x - x_0))(x - x_0)^\alpha$ is called the Lagrange remainder and $|R_n| \leq \frac{1}{p!} \sup_{|\alpha| \leq p \in (0,1)} |D^\alpha f(x_0 + \theta(x - x_0))(x - x_0)^\alpha| \prod_{d=1}^D |x_d - x_d|^{\alpha_d}$.

The first lemma gives an upper bound on the absolute error on estimating a reference node contribution by evaluating a truncated Hermite expansion. The second lemma gives an upper bound on the absolute error incurred from approximating the contribution of a reference node by evaluating the Taylor series formed via direct local accumulation of each reference point.

**Lemma 4.** Given a query node $Q$, a reference node $R$ with an Hermite expansion about its centroid $x_R$: $G(x_R) = \sum_{|\alpha| \leq 0} A_\alpha h_\alpha \frac{(x_q - x_R)}{\sqrt{2\pi} h} ^\alpha$, with $x_q \in Q$, the absolute truncating error after taking the $O(D^p)$ term is bounded by: $E_{DH}(p) = W_R \frac{e^{-\frac{(p+1)^2}{4h^2}}}{\sqrt{2\pi} \sqrt{h^p}}$ where $r_R = \max_{x \in R} \frac{||x - x_R||}{h}$ and $p'= p \mod D$.

**Proof.** By Theorem 1 and the triangle inequality,

$$\left|G(x_q) - \sum_{|\alpha| \leq 0} A_\alpha h_\alpha \frac{(x_q - x_R)}{\sqrt{2\pi} h} ^\alpha\right| \leq \sum_{x \in R} w_x K(\delta_R') - \sum_{|\alpha| \leq 0} \frac{1}{\alpha!} h_\alpha \frac{(x_q - x_R)}{\sqrt{2\pi} h} ^\alpha |x_q - x_R|^{\alpha_0} \leq W_R \sum_{|\alpha| = p} \frac{1}{\alpha!} \max_{x \in Q, x \in R} h_\alpha \frac{|x_q - x_R|}{\sqrt{2\pi} h} ^\alpha \prod_{d=1}^D \frac{|x_d - x_{d_R}|}{\sqrt{2\pi} h} ^{\alpha_d} \leq W_R e^{-\frac{(p+1)^2}{4h^2}} \frac{e^{-\frac{(p+1)^2}{4h^2}}}{\sqrt{2\pi} \sqrt{h^p}}$$

The final lemma gives an upper bound on the absolute error incurred by approximating the reference node contribution by the Taylor expansion converted from the truncated Hermite expansion.

**Lemma 5.** Given the following expansion about the centroid $x_Q$ of a query node $Q$:

$$G(x_Q) = \sum_{|\beta| \geq 0} B_\beta \frac{(x_q - x_Q)^\beta}{\sqrt{2\pi} h}$$

where $B_\beta = \frac{(-1)^{|\beta|}}{\beta!} \sum_{|\alpha| \leq 0} A_\alpha h_\alpha + \beta \frac{(x_q - x_Q)^\beta}{\sqrt{2\pi} h}$, for any $x_Q \in Q$, the absolute error due to truncating the series after $O(D^p)$ terms is bounded by: $E_{DL}(p) = W_R e^{-\frac{(p+1)^2}{4h^2}} \frac{e^{-\frac{(p+1)^2}{4h^2}}}{\sqrt{2\pi} \sqrt{h^p}}$ where $r_Q = \max_{x \in Q} \frac{||x_q - x_Q||}{h}$ and $p'= p \mod D$.

**Proof.** The derivation is similar to one in Lemma 4.

The derivation is similar to one in Lemma 4.
Clearly, $|E_2| \leq \frac{e^{-\frac{q_{min}^2}{4h^2}}(\frac{D^p + p - 1}{D^p - 1})^p}{\sqrt{\left(\frac{4}{h}\right)!}}$. In addition, $|E_1| \leq \sum_{|\beta| < p} \frac{1}{\sqrt{|\beta|!}} \sum_{|\alpha| = p} \frac{1}{\sqrt{|\alpha|!}} \left(\sum_{d=1}^{D} \frac{Q_d}{\sqrt{2h^2}} \right)^\beta \left(\sum_{d=1}^{D} \frac{R_d}{\sqrt{2h^2}} \right)^\alpha \max_{x_q \in Q, x_r \in R} |h_{\alpha + \beta}(\frac{x_q - x_r}{\sqrt{2h^2}})|$

$$\leq e^{-\frac{q_{min}^2}{4h^2}} \sum_{|\beta| < p} \frac{1}{\sqrt{|\beta|!}} \sum_{|\alpha| = p} \left(\frac{4}{h}\right)^\beta \left(\frac{4}{h}\right)^\alpha$$

$$\leq e^{-\frac{q_{min}^2}{4h^2}} \sum_{|\beta| < p} \frac{1}{\sqrt{|\beta|!}} \sum_{|\alpha| = p} D^\beta \left(\frac{2(x_q - x_r)}{h}\right)^\alpha$$

$$\leq e^{-\frac{q_{min}^2}{4h^2}} \sum_{|\beta| < p} \frac{1}{\sqrt{|\beta|!}} \sum_{|\alpha| = p} D^\beta \left(\frac{2(x_q - x_r)}{h}\right)^\alpha$$

Figure 4: Four ways a reference node can send its contributions to a query node using the original FGT style pruning. In the clockwise order starting from the top left, exhaustive computation (few reference/query points), multipole evaluation (many reference/few query points), direct Taylor accumulation (few reference/many query points), $H2L$-translation (many reference/query points).

5 New Error Guarantee Rule

Let us first revisit our method of automatically guaranteeing the user’s error tolerance $\epsilon$ defined in Section 1. We now specify the function $\text{Can-approximate}(Q,R,\epsilon)$, which only has local information (contained in the query node $Q$ and the reference node $R$) available to it, but must guarantee a global error criterion.

In the dual-tree finite-difference algorithm (DFD) (Gray & Moore, 2003b), the function $\text{Approximate}(Q,R)$ approximates the contribution of $R$ to each query point $x_q$ in $Q$, $G_R(x_q)$, by $G_R(x_q) = W_R K = W_R \frac{K(q_{min}^R) + K(q_{max}^R)}{2}$, where $W_R = \sum_{x_r \in R} w_r$ and $q_{min}^R$ and $q_{max}^R$ are lower and upper bounds on the distance between $x_q \in Q$ and $x_r \in R$, respectively. These distances are easily obtained using the bounding boxes of the nodes. By using these bounds DFD algorithm maintains a running lower bound $G_{min}^R$ on $G_R(x_q)$ which holds for all $x_q \in Q$. In Section 4, we laid out more approximation methods in addition to finite-difference approximation (FD): evaluating a truncated Hermite expansion centered at $x_R$ (DDH), forming a truncated Taylor expansion centered at $x_q$ using each reference point (DL), and forming an approximated truncated Taylor expansion centered at $x_q$ by converting the truncated Hermite expansion centered at $x_R$ (H2L). The following specifies $\text{Can-approximate}(Q,R,\epsilon)$, which incorporates the new approximation methods.

Theorem 2. Given the following methods for approximating the contribution of a reference node $R$: $\mathcal{A} = \{EX, DH, DL, H2L, FD\}$ where DH, DL, H2L, and FD are denoted as above, and EX for exhaustive computation, $A \in \mathcal{A}$ with a maximum absolute error of $E_A$ can be used to guarantee the global error tolerance $\epsilon$ if: $E_A \leq \frac{W_R \epsilon}{W} G_{min}^Q$ where $W = \sum_{r=1} W_r$.

Proof. Given $x_q \in Q$, suppose $\tilde{G}(x_q)$ was computed using $k$ reference nodes $R_i$’s, whose contribution was approximated using $A_i$. By the triangle inequality:

$$|G(x_q) - \tilde{G}(x_q)| = \sum_{i=1}^k |G_{R_i}(x_q) - \tilde{G}_{R_i}(x_q)| \leq \sum_{i=1}^k |G_{R_i}(x_q) - \tilde{G}_{R_i}(x_q)| \leq \sum_{i=1}^k E_{A_i} \leq \sum_{i=1}^k \frac{W_{R_i} G_{min}^Q}{W} \leq \epsilon G_{min}^Q \leq \epsilon G(x_q) \quad \square$$

This new rule generalizes the previous local approximation condition (Gray & Moore, 2003b): $|K(q_{min}^R) - K(q_{max}^R)|/G_{min}^Q \leq 2\epsilon$, where $E_{DFD} = \frac{W_R (K(q_{min}^R) - K(q_{max}^R))}{2}$. Clearly, $E_{EX} = 0$, and $E_{DDH}$, $E_{DL}$, and $E_{H2L}$ are given as Lemma 4, 5, 6 respectively. The approximation rule above essentially gives each reference node $R$ a maximum relative error proportional to the sum of the weights of reference points it contains. In considering the $i$-th reference node contribution, when $A_i = EX$, the maximum allowable
relative error of \( \frac{W_{E_a}}{E_{Q_{min}}} \) is not used up; Otherwise, if \( G_{Q_{min}}^{min} > 0 \), pruning requires only a relative error of \( \frac{W_{E_a}}{E_{Q_{min}}} \) where \( W_{E_a} \). Our new approximation rule notes that the portion of the weights not used to cover the incurred pruning error can be stored into a field \( W_T \) (initialized to zero before the computation and denoted \( Q,W_T \) hereon) in each query node \( Q \) to use them in future pruning opportunities. The first case yields \( W_{R_i} \) as the leftover, while the second case (pruned case) yields \( W_{R_i} - W_{R_i}' \).

Given \( A \in A \) with the maximum absolute error of \( E_A \), we now modify the approximation condition to:

\[
\frac{E_A}{G_{Q_{min}}^{min}} \leq \frac{e(W_{R_i} + W_T)}{W_T}. \]

Solving for \( W_T \) yields:

\[
W_T \geq W_R \left( \frac{W_{E_a}}{G_{Q_{min}}^{min}} - 1 \right). \]

Whenever a pruning is attempted, the modified algorithm will evaluate the right handside of the inequality. If the evaluated value is negative, it represents the leftover “token” after pruning is performed and \( Q,W_T \) of the current query node will be incremented by \( W_R \left( 1 - \frac{W_{E_a}}{G_{Q_{min}}^{min}} \right) \). If positive, it represents the required extra “token” from the \( Q,W_T \) slot of the current query node, in order to prune the given query and reference node pair. If \( Q,W_T \geq W_T \), pruning succeeds and \( Q,W_T \) is decremented by \( W_R \left( \frac{W_{E_a}}{G_{Q_{min}}^{min}} - 1 \right) \).

6 New Dual-tree Algorithm

We first introduce an extra field in each query node \( G_{Q_{est}}^{est} \) storing contributions from reference nodes obtained by finite-difference approximation and direct Hermite evaluations. The contributions from Taylor coefficients obtained via direct local accumulation and \( H2L \) translation operator will be accounted for during the post-processing step.

In preprocessing, we construct two trees, one for the query dataset and one for the reference dataset. In this paper an efficient form of sphere-rectangle trees (Katayama & Satoh, 1997) is used, with idea of cached sufficient statistics as in mrkd-trees (Deng & Moore, 1995). The Hermite moments of order \( PLIMIT \) is pre-computed for the reference tree. For the experimental results, we have fixed \( PLIMIT = 8 \) for \( D = 2 \), \( PLIMIT = 6 \) for \( D = 3 \), \( PLIMIT = 4 \) for \( D = 5 \), \( PLIMIT = 2 \) for \( D = 6 \). We presume that \( PLIMIT = 1 \) for \( D > 6 \).

During the recursive function call \( DITO \), an optimized version of finite-difference pruning is first attempted. In case of failure, we attempt FMM-type pruning in which we choose the cheapest operation given a query node \( Q \) and a reference node \( R \) from the followings: direct Hermite evaluation (\( DIRECTM(Hermite \ coefficients, \ truncation \ order, \ query \ point) \)), direct local accumulation (\( DI-

![](image)

Figure 5: Building the tree from the reference dataset.

7 Experiments and Conclusions

We empirically evaluated the runtime performance of six algorithms on six real-world datasets (astronomy (2-D), physical simulation (3-D), pharmaceutical (5-D), biology (7-D), forestry (10-D), image textures (16-D)) scaled to fit in \( [0,1]^D \) hypercube, for kernel density estimation at every query point with a range of bandwidths, from 3 orders of magnitude smaller than optimal to three orders larger than optimal, according to the standard least-squares cross-validation scores (Silverman, 1986). In our case, the set of reference points...
is the same as the set of query points. All datasets have 50K points so that the exact exhaustive method can be tractably computed. We set the tolerance \( c = 0.01 \). We compare: FGT (Fast Gauss Transform (Greengard & Strain, 1991)), IFGT (Improved Fast Gauss Transform (Yang et al., 2003)), DFD (dual-tree with finite-difference (Gray & Moore, 2003b)), DFDO (dual-tree with finite-difference and improved error control (Section 3.2)), DFTO (dual-tree with \( O(p^D) \) expansion (Lee et al., 2006) and improved error control), and DITO (dual-tree with \( O(D^p) \) expansion and improved error control).

All times (which include preprocessing but exclude parameter selection time) are in CPU seconds on a dual Intel Xeon 3 GHz with 2 Gb of main memory/1 Mb of CPU cache. Codes are in C/C++, compiled under –O6 –funroll –loops flags on Linux kernel 2.6.9-11. The measurements in columns two to eight are obtained by running the algorithms at the bandwidth \( kh^* \) where \( 10^{-3} \leq k \leq 10^3 \) is the constant in the corresponding column. The dual-tree algorithms all achieve the error tolerance automatically. We also note that the FGT uses a different error tolerance definition: 
\[
|\hat{G}(x_q) - G(x_q)| \leq W\tau.
\]
We first set \( \tau = \epsilon \), halving it until the error tolerance \( \epsilon \) was met. For the IFGT, we created an automatic scheme to tweak its multiple parameters based on recommendations given in the paper and software documentation: For \( D = 2 \), use \( p = 8 \); for \( D = 3 \), use \( p = 6 \); set \( \rho_s = 2.5 \); start with \( K = \sqrt{N} \) and double \( K \) until the error tolerance is met. When this failed to meet the tolerance, we resorted to additional trial and error by hand. We are primarily concerned with the sum of the times over all the bandwidths, shown in the last column of the table. Entries in the tables of ‘X’ denote cases where the algorithm exhausted RAM and caused a segmentation fault. Entries of \( \infty \) denote cases where no setting of the algorithm’s parameters was able to satisfy the parameters

**Figure 6:** Choosing the FMM-type approximation with the least cost for a query and reference node pair.

**Figure 7:** The main procedure implementing a new error-control and \( O(D^p) \) expansion.

**Figure 8:** Combining different types of approximations on different scales, using a breadth-traversal.

error tolerance.

Our results demonstrate that the \( O(D^p) \) expansion helps reduce the computational time on datasets of dimensionality up to 5. For example, on the 2-D dataset, the new algorithm DITO performed about 12 times as fast as the original DFD algorithm, which is in it-
self an improvement over the naive algorithm. The datasets above five dimensions, however, present difficulty for the series expansion idea to be effective, and the new algorithm is slower than DFDO algorithm. Yet the algorithm with the optimized pruning rule (DFDO) consistently yields about 10% to 15% improvement over DFDO algorithm in higher dimensions.

\[
\begin{array}{cccccccc}
\text{Alg} & 10^{-6} & 10^{-5} & 10^{-4} & 1 & 10^1 & 10^2 & 10^3 & \Sigma \\
\text{Naive} & 5472 & 6554 & 613 & 472 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\text{DFDO} & 5472 & 6554 & 613 & 472 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\text{IFGT} & 5472 & 6554 & 613 & 472 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\text{DFD} & 889 & 1393 & 130 & 92.8 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\end{array}
\]

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\[
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\text{IFGT} & 5472 & 6554 & 613 & 472 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\text{DFD} & 889 & 1393 & 130 & 92.8 & 0.58 & 52.8 & 3386 & 703 & 515 & 1 & 461 & 461 & 1 & 3227 \\
\end{array}
\]