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A black-box Fast Multipole Method

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ABSTRACT

The fast multipole method (FMM) is an $O(N)$ method to calculate sums involving the kernel $1/r$:

$$\phi_i = \sum_{j \neq i} \frac{\sigma_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

This is a very popular method with applications in many fields such as the N body problem, molecular dynamics, boundary integral equations... The FMM relies on analytical formulae to approximate (in a suitable sense) the kernel $1/r$ for large r. Even though many such approximations, often involving Legendre polynomials, Spherical Harmonics and Bessel functions, have been derived for many applications, many users find it difficult or cumbersome to derive new expansions for new kernels, assuming such expansions can be found analytically. Even when such expansions can be obtained, the implementation of the method itself is a challenge. It is therefore desirable to derive a "black-box" FMM which is applicable to arbitrary kernels. Applying the method should then simply be a matter of installing a library and providing a user-defined routine to evaluate the kernel at a given point. The complexity of the method would be completely hidden from the end-user. This is the goal of this project.

We are proposing a new $O(N)$ method, bbFMM, applicable to kernels which are smooth for large r. The exact condition will be provided below. Our method has several advantages:

- it is optimal in the sense that the smallest possible number of coefficients are used to represent the kernel for a given error ε.
- the pre-computing cost is $O(1)$ for homogeneous kernels and grows like $O(\ln N)$ in the general case.
- it is applicable to periodic and non-periodic cases.
- it is adaptive in the sense that the tree can be refined locally to account for clusters of points with a higher density.

- it is anisotropic in the sense that the computational cost is reduced if the points lie on a sub-manifold (surface or line).

We briefly describe some of the components of bbFMM. Assume we want to compute the following general sum:

$$\phi_i = \sum_{j \neq i} K(\mathbf{r}_i, \mathbf{r}_j)\, \sigma_j$$

bbFMM is based on approximating the kernel using Chebyshev polynomials. Any smooth function $f(x)$ can be approximated on the interval $[-1, 1]$ using $f(x) \approx \sum_{k=1}^{p} w_k(x) f(X_k)$ with

$$w_k(x) = \frac{2}{p} \sum_{m=1}^{p} T_{m-1}(X_k) T_{m-1}(x) - \frac{1}{p}$$

where $T_m(x)$ is a Chebyshev polynomial of order m and X_k are the zeros of $T_p(x)$. Assume now that we want to approximate $K(x, y)$ for x and y in the interval $[-1, 1]$, the following approximation can be used (assuming K is smooth in this region): $K(x, y) \approx \sum_{k,l} w_k(x) w_l(y) K(X_k, X_l)$. For two clusters of N points x_i and y_j, an $O(N)$ method can then be constructed in 3 steps:

1. Calculate equivalent charges at node X_l: $Q_l = \sum_{j=1}^{N} w_l(y_j)\sigma_j$.
2. Calculate the potential at Chebyshev node X_k: $\phi(X_k) = \sum_{l=1}^{p} K(X_k, X_l) Q_l$.
3. Calculate the potential at the N nodes x_i: $\phi_i = \sum_{k=1}^{p} w_k(x_i)\phi(X_k)$.

Each step has a computational cost of either $O(pN)$ or $O(p^2)$. If a tree data structure is used, as in the FMM, the method can be applied to an arbitrary distribution of points $\mathbf{r}_i$. The condition on kernel K for the method to work is that there should exist an integer $p(\varepsilon)$ such that the error using the Chebyshev interpolation of order p is smaller than ε at all levels in the tree. This is true for most kernels but not for oscillatory kernels such as $\cos(r)/r$.

In addition to the Chebyshev interpolation, the singular value decomposition (SVD) was used to reduce the cost of the second step, $\sum_l K(X_k, X_l) Q_l$. This does not change the scaling $O(N)$ of the method but reduces the "constant" in front of N. This also guarantees the optimality of the algorithm since the SVD can be shown to provide the approximation with smallest rank given an error ε. Other methods have used the SVD previously to obtain a fast $O(N)$ method. Our approach, bbFMM, has the advantage of requiring a small pre-processing time since the SVD is only computed locally at each level (and not globally as is sometimes done).

The method was developed and applied to different kernels including $1/r^p$ and Stokes' kernel. The scaling $O(N)$ and the accuracy of the method was verified numerically. We can prove and observed a spectral convergence, e.g. the error decays exponentially fast with the number of terms used in the expansion (parameter p above).

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