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Faster fast evaluation of thin plate splines in two dimensions

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ABSTRACT

A new method for fast evaluation of thin plate splines in two dimensions is presented. The paper first develops exponential approximations to thin plate splines. These are the analytical basis for an improved fast multipole evaluator. Analytic error bounds are supplemented by offline parallel numerical computation of the underlying error constants. These error constants enable adaptive selection of series lengths as a function of the weights associated with a source panel, and the desired accuracy. Numerical comparisons with a competing algorithm show that the new method is significantly faster when moderate to high precision is required.

1. Introduction

Radial basis functions (RBFs) on $\mathbb{R}^d$ are functions of the form

$$s(\cdot) = p(\cdot) + \sum_{i=1}^{N} \lambda_i \Phi(\cdot - x_i). \tag{1}$$

Here, Φ, the basic function, is a fixed function mapping $\mathbb{R}^d \to \mathbb{R}$, and p is a low degree polynomial. The points $\{x_i\}$ are called the centers. Initially these functions were studied for their beautiful theory. More recently they have become a standard tool in many applications. Examples are surface reconstruction, uses in medicine such as in the custom manufacture of artificial limbs and of cranial prostheses, use in modeling aquifers, and use in mineral exploration software such as the Leapfrog package. For all these applications there is one immediate drawback in the form given in Eq. (1). Namely, algorithms directly based on this expression for an RBF will require $\mathcal{O}(N)$ arithmetic operations for evaluation of s at a single extra point x. Further, non-specialized methods for fitting such an RBF s to N pieces of data, for example by interpolation, will require $\mathcal{O}(N^3)$ arithmetic operations. Fortunately, the use of fast algorithms, see for example [1], or of compactly supported kernels, see Wendland [2], dramatically reduces the incremental cost of a single extra evaluation, for example to $\mathcal{O}(1)$ operations, ignoring the cost of finding the panel containing the evaluation point. Also, numerical experiments show that iterative fitting methods employing these fast algorithms to compute matrix–vector products, typically solve interpolation problems with N nodes in $\mathcal{O}(N(\log N)^2)$ operations, rather than $\mathcal{O}(N^3)$.

This paper concerns an improved fast evaluation method for thin plate splines in two dimensions. The algorithm and code considered approximates the values of an N center RBF at m evaluation points. The paper develops exponential

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approximations to thin plate splines. These exponential approximations are used in an improved fast multipole (FM) method as an intermediate step in obtaining local polynomial approximations. This intermediate exponential approximation idea was first used by Hrycak and Rokhlin [3] in their method for fast evaluation of two dimensional potentials. Another feature of the current work is that tight estimates of error constants determining the accuracy of the approximation procedure involved have been obtained via large scale offline parallel computation. These constants enable adaptive selection of series lengths depending on the weights associated with a source panel, and the required accuracy. This makes it easy to approximately minimize the amount of work done in order to obtain something very close to the desired accuracy. In contrast, with other algorithms, such as [1], it is somewhat difficult to minimize the work by selecting the parameters to give just the required precision. Numerical experiments show that the method performs very well in practice with the execution time for the task of evaluating an RBF based on N centers at slightly more than N points scaling approximately linearly with N. Theoretically the operation count can be bounded by $AN\log N + B\log N$, with the $N\log N$ part coming from sorting centers into panels. However, A is so small compared with B that the timings, even for N in the millions, are dominated by the BN part.

Recently a non uniform FFT based fast summation code, NFFT code for short, has been demonstrated to be competitive with a fast multipole method for the potential with a desired 10^{-6} relative error (see Tables 3.1, 4.1 in [4,5] respectively). In numerical comparisons our updated FM algorithm for the thin plate spline is significantly faster than the NFFT code when mid to high precision is required. It is only slightly faster than the NFFT code when the required precision is small.

The paper is laid out as follows. Section 2 discusses the idea of an intermediate exponential approximation originally due to Hrycak and Rokhlin [3]. It also sets out an outline of a general fast multipole algorithm. Section 3 discusses multipole expansions for thin plate splines. Section 4 develops exponential approximations for thin plate splines, for source and target panels in a standard scaling and geometry. Section 5 considers such approximations when the panels are scaled and rotated. Section 6 considers the process of forming, and error bounds for, the final piecewise polynomial approximation. Section 7 presents numerical results comparing the performance of direct evaluation, our current implementation, and an NFFT code downloaded from [6].

2. Hrycak and Rokhlin's improved fast multipole method for potentials $1/(z-t)$

This section briefly discusses Hrycak and Rokhlin [3] improved fast multipole method for fast evaluation of a potential $\sum \lambda_i/(z-z_i)$.

In outline, and ignoring many subtleties, a fast multipole procedure for evaluation of a sum $s(x) = \sum_{i=1}^{N} \lambda_i \Phi(x-x_i)$ consists of the following steps.

Algorithm 1. SETUP: Given the centers and weights $\{(x_i, \lambda_i)\}$ and a basic function Φ

- Step 1: Construct a tree which at each new level creates child panels by splitting parent panels, assigning the centers x_i belonging to the parent to the appropriate children. In $\mathbb{R}^2$ the tree is often chosen to be a quadtree.
- Step 2: Starting at the leaf nodes work up the tree constructing for each panel, $\mathcal{T}$, a truncated far field expansion which approximates the influence of the panel, at points far from the panel.
- Step 3: Work down the tree level by level. At level ℓ, and working on panel $\mathcal{T}$, first recenter the polynomial approximation associated with the parent of $\mathcal{T}$. Then considering each panel $\mathcal{S}$ as a source construct polynomials approximating its influence in each nearby target panel $\mathcal{T}$. Sum these polynomials to construct for each panel $\mathcal{T}$ a polynomial approximating the influence of all panels well separated from $\mathcal{T}$.

EVALUATION: Given a point x at which to evaluate $s(x)$.

- Step 1: Find the panel $\mathcal{T}$ containing x.
- Step 2: Evaluate $s(x)$ by using the local polynomial approximation summarizing the influence of all the panels far away from $\mathcal{T}$ to approximate the far field, and evaluating the near field directly.

The reader who is not familiar with these algorithms will find more detailed descriptions in [1,7].

In the case of the potential $\Phi(z-t) = 1/(z-t)$ Hrycak and Rokhlin [3] use exponential approximations to improve step 3 of the setup stage of Algorithm 1. They do this by first converting far field approximations to exponential approximations, and then approximating these exponential approximations by local Taylor polynomials. Their exponential approximations are of the form

$$\sum_{\ell=1}^{L} w_\ell \, e^{-x_\ell(z-t)} \approx \frac{1}{z-t}, \tag{2}$$

where w_ℓ and x_ℓ are specified coefficients, $t \in Q$, $z \in R_0$, and Q and R_0 are sets specified in Section 4 below. These approximations give impressively high accuracy for the number of terms L. The apparatus for finding the exponential approximation formulas, also known as quadrature formulas, was developed by Yarvin and Rokhlin [8]. Tables of nodes and weights can be found at [9].

The procedure can be anticipated to be an improvement for at least three reasons. First, the exponential approximations have relatively few terms for the given accuracy. Second, recentering exponentials $e^{-x_\ell z}$ to the center, t, of a target panel is a