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An Adaptive Method for Choosing Center Sets of RBF Interpolation

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***Abstract*—Radial basis functions (RBF) provide powerful meshfree methods for multivariate interpolation for scattered data. RBF methods have been praised for their simplicity and ease of implementation in multivariate scattered data approximation. But both the approximation quality and stability depend on the distribution of the center set. It leads immediately to the problem of finding good or even optimal point sets for the reconstruction process. Many methods are constructed for center choosing. In this paper, we give a short overview of these algorithms including thinning algorithm, greedy algorithm, arclength equipartition like algorithm and k-means clustering algorithm. A new adaptive data-dependent method is provided at the end with some numerical examples to show its effectiveness..**

***Index Terms*—radial basis function interpolation, greedy algorithm, Native space, thinning algorithm, adaptive method**

I. Introduction

Interpolation by radial basis functions is a well-established method for reconstructing multivariate functions from scattered data [1, 2]. Radial basis function (RBF) methods have been praised for their simplicity and ease of implementation in multivariate scattered data approximation [3]. Since RBF methods are completely meshfree, requiring only interpolation nodes and a set of points called centers defining the basis functions, it leads immediately to the problem of finding good or even optimal point sets for the reconstruction process. Several researchers have incorporated RBF method in several adaptive schemes. In this paper, we will do a short overview of the adaptive methods concerning the computation of optimal center sets for interpolation by radial basis functions. A new idea and some examples for this goal are presented.

The paper is organized as follows. In section 2 we collect some introductory material and necessary definitions such as power functions, and native Hilbert spaces. In the third section, we summarize some effective center location methods like thinning algorithms, greedy algorithms, arclength equipartition methods and k-mean clustering methods. At the end of this paper, we provide a new adaptive data-dependent method for center selecting. The new algorithm produces the momentarily so called weighted Leja-Bos sequence which performs better in the numerical experiments.

II. Radial Basis Function

Take a set $X = \{x_1, \cdots, x_N\} \subseteq \Omega \subseteq R^d$ of N pairwise distinct points coming from a compact subset Ω of R^d. These points $\{x_i\}$ are referred as data sites (or data locations or centers) and the set X as data set. Suppose further that N data values $f_1, \cdots, f_N$ should be interpolated at the data sites. A simple way is to fix a symmetric kernel function $\Phi : \Omega \times \Omega \to R$ and to form an interpolant

$$s_{f,X} = \sum_{j=1}^{N} a_j \Phi(\|x - x_j\|) \qquad (1)$$

where $\|\cdot\|$ is the Euclidean norm and the coefficients $\{a_j\}$ are uniquely determined by the interpolation conditions $s_{f,X}(x_j) = f_j$ ($1 \le j \le N$) if the

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interpolation matrix $A_{\Phi,X}=(\Phi(\|x_i-x_j\|))_{1\le i,j\le N}$ is invertible. Furthermore, it is sometimes necessary to add the space P_m^d of d -variate polynomials of order not exceeding m to the interpolating function. Call function Φ is conditionally positive definite of order m on R^d, if for all sets X with N distinct points and all vectors $\{a_1,\cdots a_N\}$ satisfying $\sum_{j=1}^N a_j p(x_j)=0$ for all $p\in P_m^d$, the quadratic form $\sum_{i,j=1}^N a_i a_j \Phi(\|x_i-x_j\|)$ attains nonnegative values and vanishes only if $a_j=0$ for all $1\le j\le N$ [4]. Function Φ is called positive definite for the case $m=0$. Interpolation is uniquely possible under the precondition: If $p\in P_m^d$ satisfies $p(x_j)=0$ for all $x_j\in X$, then $p=0$, and Φ is conditionally positive definite of order m [4,5].

In the paper we focus to the case of positive definiteness, since every conditionally positive definite kernel has an associated normalized positive definite kernel [6,7].

The kernel Φ defines on the linear space expanded by $\Phi(x,\cdot)$

$$F_\Phi:=\left\{\sum_{j=1}^M a_j\Phi(x_j-\cdot)\,|\,a_j\in R, M\in \mathrm{N}, x_j\in R^d\right\}$$

an inner product via

$$\left(\Phi(x-\cdot),\Phi(y-\cdot)\right)_\Phi=\Phi(x-y),\quad x,y\in R^d.$$

The closure of F_Φ with reproducing kernel Φ is called the Native Hilbert space, denoted by $\mathsf{N}_\Phi(\Omega)$ [7-11]. Moreover, there is a Lagrange-type representation of interpolant (1)

$$s_{f,X}=\sum_{j=1}^N f(x_j)u_j,\ u_j(x_i)=\delta_{ij},\ 1\le i,j\le N.$$

Then the local error estimates have the form [12]

$$\left|f(x)-s_{f,X}(x)\right|\le P_{\Phi,X}(x)\left\|f\right\|_\Phi$$

Where $P_{\Phi,X}(x)$ is the power function [13, 14] with explicit form

$$P^2_{\Phi,X}(x)=\Phi(x,x)-2\sum_{j=1}^N u_j(x)\Phi(x,x_j)+\sum_{j=1}^N u_j(x)u_k(x)\Phi(x_j,x_k)$$

.

The power function is bounded in term of fill distance

$$h_{X,\Omega}=\sup_{x\in\Omega}\min_{x_j\in X}\left\|x-x_j\right\|_2$$

and for any function $f\in\mathsf{N}_\Phi(\Omega)$, the local error of the interpolant is bounded by

$$\left|f-s_{f,X}\right|\le C\cdot h^k_{X,\Omega}\cdot\left\|f\right\|_\Phi$$

here $C\in R$ is a constant, k is a natural number and $\|f\|_\Phi$ depends on f and Φ only, details in [13]. On the other hand, as the number of centers grow, RBF method needs to solve a large algebraic system and large condition number of interpolation matrix causing instability makes convergence difficult. Denote separation distance by

$$q_X=\frac{1}{2}\min_{1\le i\ne j\le N}\left\|x_i-x_j\right\|.$$

Roughly speaking, for a fixed basis function Φ, good approximation quality needs small $h_{X,\Omega}$ and fine stability require large q_X. However one can't minimize $h_{X,\Omega}$ and maximize q_X at same time which is referred to as uncertainty relation in [15].

There are several factors affecting the performance of the RBF interpolation process including kernel function, center distribution, shape parameter and the unknown function. In this paper, we focus to the problem of finding good or even optimal center sets for RBF interpolation process. Many researchers (e.g., M.S. Floater, A. Iske, S.D. Marchi and R. Schaback [16-30]) have developed several adaptive schemes. All these algorithms can be roughly divided into two categories: data dependent methods and data independent methods. We will summarize these methods in the next section.

III. Adaptive Methods for Center Locations

In this section, we will display some recent results on selecting near-optimal point sets for interpolation by radial basis functions. Almost all the algorithms are based on theoretical results especially on power function, local error bound and the trade off relation about the point distribution.

According to theoretical research on the error estimate and condition number of RBF interpolation and numerical experiments, a balance between the stability and the approximation quality will be achieved when the point sets is evenly distributed in the domain. By taking the ratio of separation distance q_X and fill distance $h_{X,\Omega}$, Iske A. defined a measure of the uniformity of set X with respect to Ω:

$$\rho_{X,\Omega}=\frac{q_X}{h_{X,\Omega}}.$$

Iske and his cooperator have done a lot of fruitful work on thinning algorithm which removes points from X one by one judging by a pre-selected criterion in order to reach a subset of a certain size. According to the selection of criterion determining which points to be removed, there are several different thinning schemes.

3.1. Thinning Algorithm

Using the uniformity of the subsets as the criterion, we say a point x is removable if the remove of x would maximize the uniformity $\rho_{X,\Omega}$. The following algorithm [16] generates a subset sequence $X=X_N\supset X_{N-1}\supset\cdots\supset X_1$ each of which are chosen to

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be as evenly distributed in Ω as possible with cardinality $\#(X_i) = i$.

Thinning Algorithm 1.

(1) Let $X_N = X$.

(2) For decreasing $i = N, N-1, \cdots, 2,$

(a) locate a removable point $x \in X_i$,

(b) let $X_{i-1} = X_i \setminus \{x\}$

(3) Output $X^* = (X_1, X_2, \cdots, X_N)$.

Instead of recursively removing points from $X \subset \Omega$, the inserting algorithm which is the dual of the thinning algorithm recursively iteratively insert points into Ω [24].

Inserting Algorithm.

(1) Let $X_0 = \phi$.

(2) For decreasing $i = 0, 1, \cdots, N-1,$

(a) search for an insertable point $x \in X \setminus X_i$,

(b) let $X_{i+1} = X_i \bigcup \{x\}$

(3) Output $X^* = (X_1, X_2, \cdots, X_N)$.

A swapping algorithm also can be found in [24]. On view of algorithmic complexity, for a scattered data set X of N pairwise different centers from general spaces, implement Algorithm 1 requires $O(N^3)$ steps. In planar case, by the method of successive Delaunay triangulations [33], Algorithm 1 can be improved to be faster requiring only $O(N^2)$ steps.

Thinning Algorithm 2.

(1) Set $X_N = X$ and compute a Delaunay triangulation T_N of X_N.

(2) For decreasing $i = N, N-1, \cdots, k+1,$

(a) locate a removable point $x \in X_i$,

(b) let $X_{i-1} = X_i \setminus \{x\}$,

(c) compute a Delaunay triangulation T_{i-1} from T_i.

(3) Output $X^* = (X_k, X_{k+1}, \cdots, X_N)$

Furthermore, by storing the interior nodes of the Delaunay triangulations in a heap and applying the priority queue skill [16, 20], the computational cost of the thinning algorithm can be reduced to $O(N \log N)$. Algorithm 1 and 2 depends only on the locations of the centers (so it is a non-adaptive thinning) and the numerical result is shown in Fig. 1.a. and Fig. 1.b. from Iske A. [16].

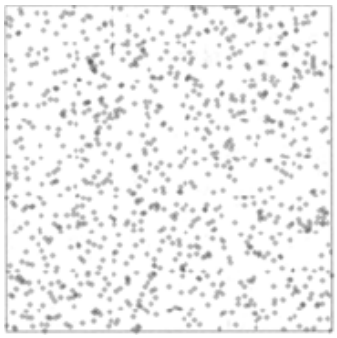

Figure 1.a Original center set X

All such non-adaptive (data-independent) algorithms produce well distributed sets whose uniformity is large. Moreover, the following theorem is proved in [17]

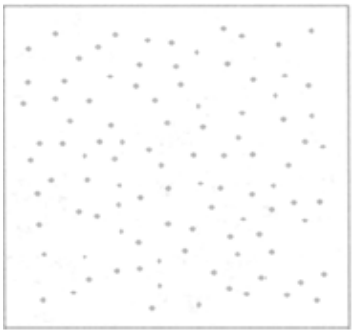

Figure 1.b. Subset X_{100} from X by Algorithm 1

Theorem 1. Let X be a point set in $\Omega \subset R^d$, then the uniformity of X can be bounded over by

$$\rho_{X,\Omega} \le \sqrt{\frac{(d+1)}{2d}},$$

where equality holds if and only if every simplex of its Delaunay triangulation is regular.

When the criterion determining whether a point is removable is chosen to minimize the anticipated error which depends on the function values $\{f(x): x \in X\}$, the algorithm is called adaptive thinning. Different error measures define different removable points, and lead out different algorithm schemes. For the details including complexity analysis we refer to [18, 20, 22].

3.2 Greedy Algorithm

In order to minimizing the power function, Marchi S.D., Schaback R. and Wendland H. constructed a numerical greedy algorithm produces near-optimal point sets by recursively adding one of the maxima points of the power function w.r.t. the preceding set [25,27]. Obviously, greedy algorithm is data-dependent and adaptive algorithm.

Greedy Algorithm.

(1) Let $X_1 = \{x_1\}$ for $x_1 \in \Omega$ arbitrary.

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(2) Do $X_j := X_{j-1} \bigcup \{x_j\}$ with

$$P_{\Phi,X_{j-1}}(x_j) = \left\| P_{\Phi,X_{j-1}} \right\|_{L_\infty(\Omega)}, \quad j \geq 2$$

until $\left\| P_{\Phi,X_j} \right\|_{L_\infty(\Omega)}$ is small enough.

In practice, the maxima is taken over some large discrete set $X \subset \Omega \subset R^d$. The convergence rate of the above Greedy Algorithm is at least like

$$\left\| P_{\Phi,X_j} \right\|_{L_\infty(\Omega)} \leq C \cdot j^{-1/d}$$

where C is a constant.

Based on numerous numerical experiments of Greedy Algorithm, the same authors suggested a geometric greedy algorithm which is data-independent.

Geometric Greedy Algorithm.

(1) Let $\Omega \subset R^d$ be a compact set, and set $X_1 = \{x_1\}$ where x_1 belongs to the boundary of Ω.

(2) For $n \geq 1$, choose $x_{n+1} \in \Omega \setminus X_n$ that its distance to X_n is maximal. Let $X_{n+1} := X_n \bigcup \{x_{n+1}\}$.

For the sets from Geometric Greedy Algorithm, the following inequalities hold

$$h_{X_n,\Omega} \geq q_{X_n} \geq \frac{1}{2} h_{X_{n-1},\Omega} \geq \frac{1}{2} h_{X_n,\Omega}.$$

Let X be 10000 random points picked on square [-1,1]×[-1,1], and the first 65 optimal points for Gaussian and 80 optimal points for Wendland's function by Greedy and Geometric Greedy algorithm are show in Fig. 2.a. and Fig. 2.b. respectively from [25].

3.3 ArcLength Equipartition Like Algorithm

Based on the idea that to display a function with some finite discrete sampling data efficiently, one requires more sampling data where the function is more oscillatory, and less sampling data where the function is more flat, Wu Z.M. [34] and Sarra S.A. [28] both used arclength equipartition algorithm to solve PDEs.

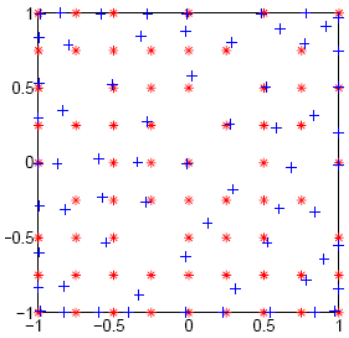

Figure 2.a. Points (*) are from Geometric greedy algorithm, (+) are from greedy algorithm

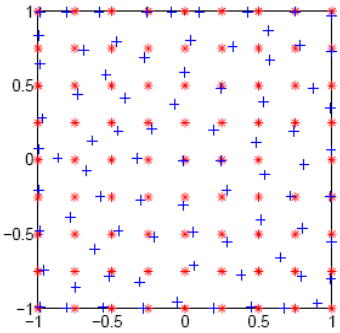

Figure 2.b. Points (*) are from Geometric greedy algorithm, (+) are from greedy algorithm

Driscoll T.A. and Heryudono A.R.H. provide a so called residual subsampling method [29]. Take 1D case for example: First, fit the unknown function using a number of equally spaced centers. Second, compute interpolation error at halfway point between the nodes, add the points where the error exceed an upper threshold to the center set, and the centers whose error is below a lower threshold will be removed. An example of Runge function on interval [-1, 1] is shown in Fig. 3.

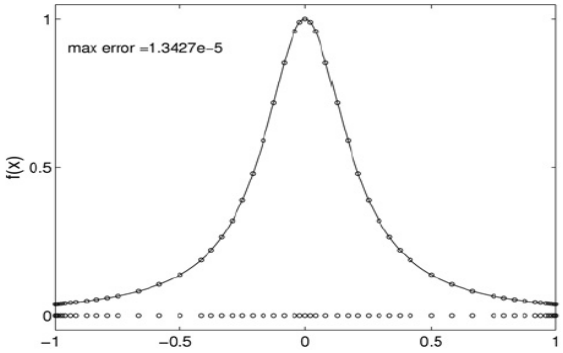

Figure 3. Numerical example for residual subsampling method

3.4 k-Means Clustering Algorithm

Finally, k-means clustering algorithm commonly used in radial basis function neural networks is easy to implement and of high performance [35]. The working process of k-means: first, choose arbitrary k points as the initial cluster centers. For all other points, compute their Euclidean distances to the k cluster centers, and add each to its nearest cluster. Then recalculate the k cluster centers by taking the geometric center of each cluster, and repeat the above process until the center errors go below a given threshold. This is also a data-independent method.

IV. Our Attempts on Data-dependent Adaptive Method

In recent years, we also attempt to design some data-dependent adaptive algorithms, our idea based on the facts that not only center distribution but also the

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unknown function reflected by the scattered data set $\{(x_i, f_i): x_i \in X\}$ will effect the interpolation process.

Definition 1. Let $\Omega \subset R^2$ be a finite compact domain, and let z_1 be arbitrarily chosen in Ω. The points z_n, $n = 2,3,\cdots$

$$z_n := \max_{z \in \Omega_D \setminus \{z_1,\cdots,z_{n-1}\}} \min_{1 \le k \le n-1} \|z - z_k\|_2 .$$

are a set of Leja-Bos points for Ω.

Note: The points selected by Geometric Greedy Algorithm is in fact a Leja-Bos sequence [36, 37].

In order to take the function values into account, we construct a weight function $w(z)$ which is built on the values $\{f_i\}_{i=1}^N$, and define the weighted-Leja-Bos sequence as following:

(1) Choose x_1 such that $w(x_1)\|x_1\| = \max_{x_i \in X} w(x_i)\|x_i\|$.

(2) For $n = 2,3,\cdots$

$$x_n := \max_{x_j \in X \setminus \{x_1,\cdots,x_{n-1}\}} \min_{1 \le k \le n-1} w(x_j)\|x_j - x_k\|_2$$

here, $\|\cdot\|$ is the Euclidean distance.

Figure 4. Distribution of the weighted-Leja-Bos sequence

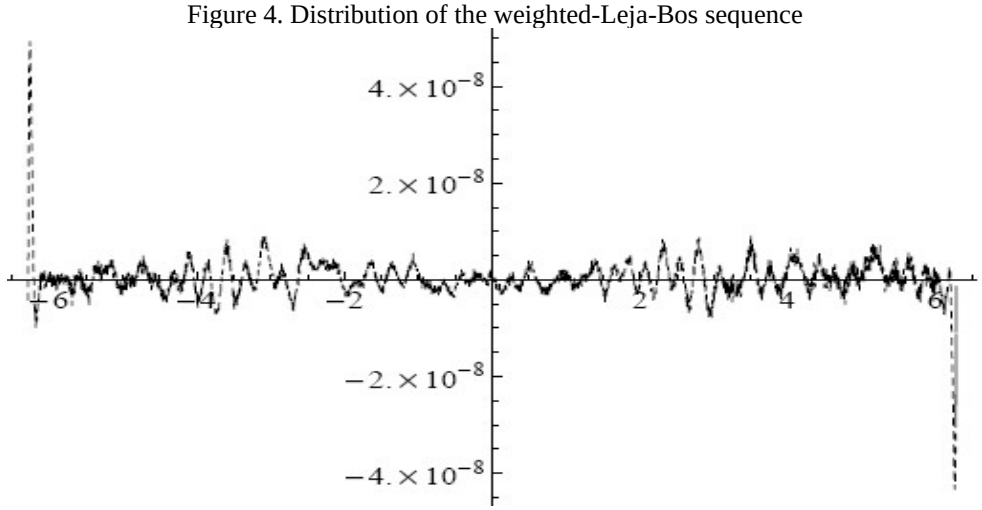

Fig. 5. Error function corresponding to weighted-Leja-Bos sequence

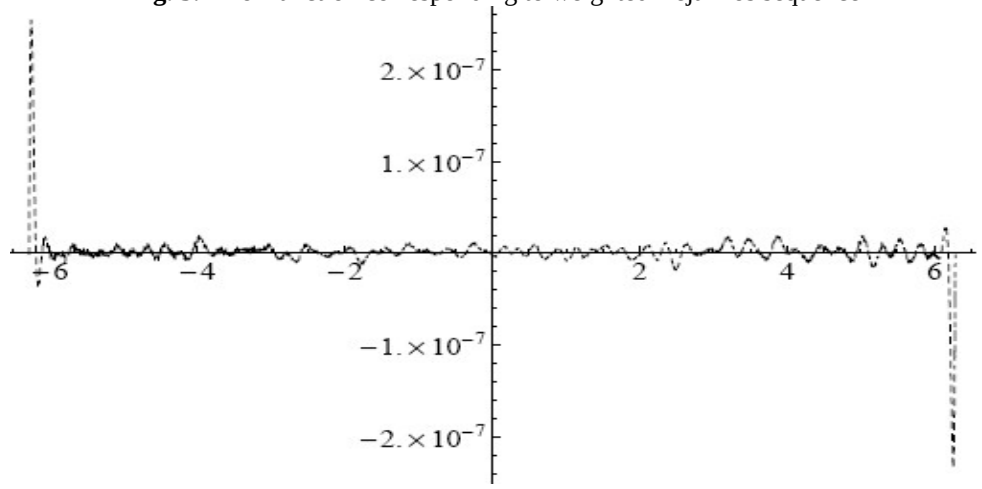

Fig. 6. Error function corresponding to ArcLength Equipartition method

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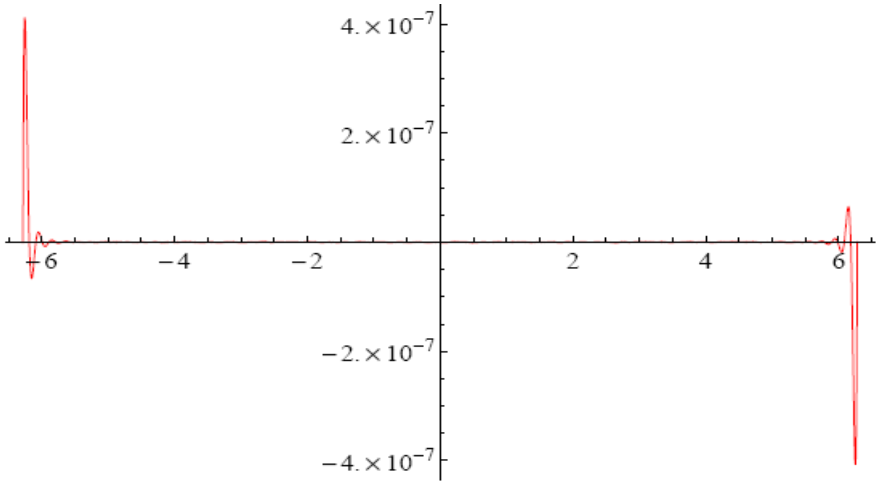

Fig. 7. Error function corresponding to 129 equidistant nodes

Choosing a weighted-Leja-Bos sequence under a certain weight function as the interpolation site set, good results obtained in numerical experiments.

Example: Interpolate function $f(x)=\sin(\frac{x}{2})$ by multiquadric function $\sqrt{\|x\|^2+r^2}$ (1971, Hardy [38]) on 129 center points extracted from a discretization of 40001 points in interval $[-2\pi,2\pi]$.

In this example, we choose site set by Geometric Greedy Algorithm, ArcLength Equipartition Algorithm and weighted-Leja-Bos sequence respectively. In practice, let shape parameter $r=1$, and use equidistant nodes for the best case of geometric greedy algorithm. The weight function $w(x_i)$ is defined by the sum of forward and backward difference quotient at x_i, and in practice, we take a multiple to increase its effect. When the multiplier is 5, the distribution of the weighted-Leja-Bos sequence of 129 points is shown in Fig. 4.

Numerically, the magnitude of the error using weighted-Leja-Bos sequence is 10^{-8} while the magnitudes according to the other two algorithms are both 10^{-7} about one order of magnitude higher. See Fig. 5-7.

To display the high effectiveness, take the same function $\sin(\frac{x}{2})$ as above on the same interval, in order to attain the same magnitude of the error as that of the error caused by using 129 equidistant nodes, we need a weighted-Leja-Bos sequence only of 54 points. See Fig.8.

V. Conclusion and Future Work.

In this paper, we focus on the effect of center locations on RBF interpolation. This is an important problem as one want to get higher accuracy with fewer data points. According to the theoretical results of RBF methods, the error estimate relies on both center locations and the unknown function. So, to found the optimal data sets, a data-dependent method is required. We have done

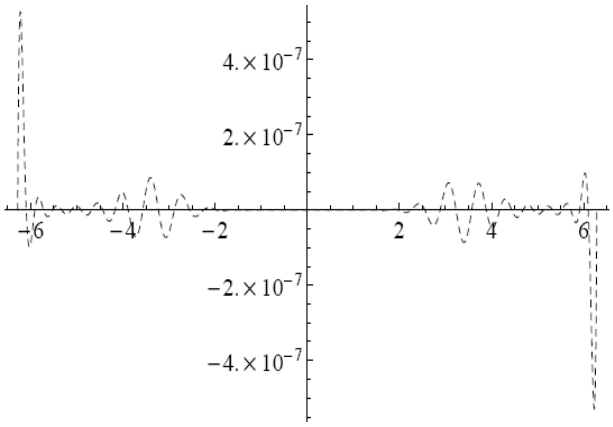

Figure 8. Error function corresponding to weighted-Leja-Bos sequence of 54 points

preliminary research on this topic. Although the weighted-Leja-Bos method performs well, a rule for the best weight function is still unfound. These will be our future work.

Acknowledgment

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