Iterated Approximate Moving Least Squares Approximation

Gregory E. Fasshauer and Jack G. Zhang

Department of Applied Mathematics, Illinois Institute of Technology, Chicago, IL 60616, U.S.A.; E-mail: fasshauer@iit.edu

Abstract. The radial basis function interpolant is known to be the best approximation to a set of scattered data when the error is measured in the native space norm. The approximate moving least squares method, on the other hand, was recently proposed as an efficient approximation method that avoids the solution of the system of linear equations associated with the radial basis function interpolant. In this paper we propose and analyze an algorithm that iterates on the residuals of an approximate moving least squares approximation. We show that this algorithm yields the radial basis interpolant in the limit. Supporting numerical experiments are also included.

Key words: RBP interpolation, MLS approximation, approximate approximation, residual iteration.

1 Introduction

In this paper we will be interested in solving the following approximation problem. For a given set of data $\{(x_i, f(x_i), i = 1, 2, \ldots, N,\ x_i \in \Omega \subseteq \mathbb{R}^s,\ f(x_i) \in \mathbb{R}\}$, we seek a continuous function $\mathcal{P}_f : \mathbb{R}^s \to \mathbb{R}$ that either interpolates the data, i.e.,

$$\mathcal{P}_f(x_i) = f(x_i), \qquad i = 1, 2, \ldots, N, \tag{1}$$

or such that $\mathcal{P}_f$ provides a close approximation to f measured in some appropriate norm.

We will be using *radial basis functions* (RBFs) to solve this problem, and one of the main features of RBFs is the fact that they can be applied without any restriction on the location of the data sites. *Approximate moving least squares* (AMLS) approximation on the other hand is in its current form mainly applicable to uniformly spaced data. This is due to the fact that it is known that the formulation of an approximate

V.M.A. Leitão et al. (eds), Advances in Meshfree Techniques, 221–239.

approximation method for scattered data is significantly more complicated than in the case of uniform data (see, e.g., [8, 9]).

We are interested in the use and comparison of these two multivariate approximation methods. Radial basis function interpolation, on the one hand, is known to yield the best approximation to given (scattered) data with respect to the native space norm of the basic function used. The benefits of this optimality property are somewhat reduced by the need to solve a (generally) large system of linear equations which can also be ill-conditioned. To avoid the solution of such a system of linear equations we recently proposed an alternative meshfree method which we refer to as the approximate moving least squares method (see, e.g., [2–5]). Using the AMLS method the solution is obtained via a simple sum based directly on the given data. Thus, the AMLS method is a quasi-interpolation approach. The drawback associated with the simplicity of the AMLS method is its lesser degree of accuracy.

We will see later that an algorithm which iterates on AMLS residuals converges to the RBF interpolant, and therefore a few iterations can be considered as an efficient and numerically stable alternative to the RBF interpolation approach. While the initial iterate of the algorithm will be an AMLS approximation designed for uniformly spaced data, we will see that the algorithm can generate an equivalently nice solution even when the data sites are irregularly distributed.

The remainder of the paper is organized as follows. In Section 2 we set our notation and present some of the salient facts for the two approximation methods we are interested in. The iterative algorithm is described in Section 3 which also contains an analysis of its convergence. Numerical experiments that demonstrate the performance of the algorithm are presented in Section 4. The paper is concluded with some remarks and an outlook on future work in Section 5.

2 The Two Approximation Methods

2.1 RBF Interpolation

The standard RBF interpolation approach for our data fitting problem is to assume that the interpolant $\mathcal{P}_f$ is a linear combination of radial basis functions Φ_j, i.e.,

$$\mathcal{P}_f(x) = \sum_{j=1}^{N} c_j \Phi_j(x) . \tag{2}$$

where the $\Phi_j : \mathbb{R}^s \to \mathbb{R}$ are defined by shifting a single basic function to the data sites, i.e.,

$$\Phi_j(x) = \varphi\left(\left\|\frac{x - x_j}{h}\right\|\right) \tag{3}$$

for some univariate function $\varphi : [0, \infty) \to \mathbb{R}$. Note that we include a scale factor h in the definition of the basic function. This scale factor is given by the fill distance

$h = \sup_{x\in\Omega} \min_{x_j,\ j=1,\ldots,N} \|x - x_j\|_2$ of the data sites. Note that our definition of the radial basis functions is reminiscent of the *stationary* approximation paradigm, i.e., the basis functions are scaled proportional to the fill distance. On the one hand it is known that most RBFs do not yield a convergent stationary approximation scheme (except when we use such functions as polyharmonic splines). However, it is exactly the stationary setting that is studied in the *approximate approximation* context, and there one can observe convergence subject to a saturation error whose size can be controlled by an initial scaling of the basic function (see, e.g., [5, 9]).

Now, equation (2) can be rewritten as

$$\mathcal{P}_f(x) = \sum_{j=1}^{N} c_j \varphi\left(\left\|\frac{x - x_j}{h}\right\|\right), \tag{4}$$

and with condition (1) this leads to finding the coefficients c_j from the linear system

$$\mathbf{Ac} = \mathbf{f}. \tag{5}$$

Here $\mathbf{A}$ is an $N \times N$ interpolation matrix given by

$$\mathbf{A} = \left\{\varphi\left(\left\|\frac{x_i - x_j}{h}\right\|\right)\right\}_{i,j=1}^{N} \quad \text{or} \quad \mathbf{A} = \left\{\Phi_j\,(x_i)\right\}_{i,j=1}^{N},$$

$\mathbf{c} = [c_1, c_2, \ldots, c_N]^T$, and $\mathbf{f} = [f(x_1), f(x_2), \ldots, f(x_N)]^T$. The interpolation matrix $\mathbf{A}$ is guaranteed to be non-singular if φ is a strictly positive definite radial function on $\mathbb{R}^s$.

Examples of basic functions we could consider for the purpose of interpolation are the strictly positive definite Gaussians $\varphi(r) = e^{-\varepsilon^2 r^2}$ or the inverse multiquadrics $\varphi(r) = \frac{1}{\sqrt{1+\varepsilon^2 r^2}}$. Note that the shape parameter ε will play the role of the initial scaling of the basic function just mentioned in the context of saturated approximate approximation. However, throughout this paper we will use the following set of strictly positive definite functions defined as

$$\varphi(r) := \frac{1}{\sqrt{\pi^s}}\, e^{-r^2} L_n^{s/2}(r^2), \tag{6}$$

with

$$L_n^{s/2}(t) := \frac{e^t t^{-s/2}}{n!} \frac{d^n}{dt^n}\left(e^{-t} t^{n+s/2}\right), \quad n = 0, 1, 2, \ldots,$$

being the generalized Laguerre polynomials. We will refer to φ as a *Laguerre–Gaussian*. Note that we did not include the shape parameter ε here in order to keep the formulas transparent. Later we will consider the functions $\varphi_\varepsilon = \varphi(\varepsilon\cdot)$.

The Laguerre–Gaussian functions are *oscillatory*. They can be explicitly written as

$$\varphi(r) = \sum_{k=0}^{n} \frac{(-1)^k (n + s/2)!}{n!(k + s/2)!} \binom{n}{k} r^{2k} e^{-r^2}.$$

It is known that a (radial) function φ is strictly positive definite and radial on $\mathbb{R}^s$ if its (radial) Fourier transform is non-negative and not identically equal to zero. For the Laguerre–Gaussians one can show

$$\hat{\varphi}(t) = \frac{e^{-\frac{t^2}{4}}}{\sqrt{2^s}} \sum_{k=0}^{n} \frac{t^{2k}}{k! 4^k} \geq 0,$$

and it is obvious that equality holds only when $t = 0$.

Note that the definition of φ depends on the space dimension s, and therefore φ is strictly positive definite and radial only on $\mathbb{R}^s$ for certain values of s. However, in the special case $n = 0$ the basic function φ becomes the regular Gaussian whose definition is independent of the space dimension s and thus it is strictly positive definite on $\mathbb{R}^s$ for all s.

The primary motivation for us to investigate Laguerre–Gaussians lies in the fact that they satisfy certain *continuous moment conditions*. These moment conditions come up when one generates basis functions for approximate moving least squares approximation. Details are given in next section.

2.2 Approximate Moving Least Squares Approximation

Roughly speaking, approximate moving least squares approximation is an approximate version of the standard moving least squares method which does not require the solution of any linear systems. The concept of approximate approximations was first suggested by Maz'ya in the early 1990s. A key ingredient in this approach are the *continuous moment conditions* for the basic function φ. A radial version of this requirement may be described as

$$\int_{\mathbf{R}^s} \|x\|^k \varphi(\|x\|) dx = \delta_{\alpha,0} \qquad \text{for } 0 \leq k \leq d. \tag{7}$$

According to the theory (see, e.g., [9]), a basic function φ that satisfies these conditions provides the following results.

For uniformly spaced $x_j \in \mathbb{R}^s$ and $\varepsilon > 0$, the quasi-interpolant

$$\mathcal{Q}_f(x) := \varepsilon^s \sum_{j=1}^{N} f(x_j) \varphi\left(\varepsilon \left\| \frac{x - x_j}{h} \right\|\right) \tag{8}$$

approximately solves the data fitting problem (1) with a guaranteed convergence

$$\| f - \mathcal{Q}_f \|_\infty = \mathcal{O}(h^{d+1}) + \epsilon(\varphi, \varepsilon).$$

As before, h is the fill distance of the given data points. The quantity $\epsilon(\varphi, \varepsilon)$ is referred to as a *saturation error*, and it depends only on the basic function φ and the initial scale factor ε. By choosing an appropriate scaling parameter ε, this saturation error may be pushed to the order of machine accuracy on any given computer.

One major advantage of the AMLS method is that the continuous moment conditions (7) provide a possibility to explicitly derive such a basic function φ. For example, any normalized integrable φ will satisfy (7) for $d = 0$. In fact, as mentioned earlier, the Laguerre–Gaussian functions satisfy (7) with $d = 2n + 1$ for each corresponding s-dimensional space. Thus, Laguerre–Gaussians are admissible for *both* RBF interpolation and AMLS approximation.

Unlike the standard RBF interpolation or moving least squares method, AMLS approximation is a completely matrix free method and hence significantly improves computational efficiency and successfully avoids the difficulties associated with ill-conditioned system matrices. However, if we are interested in an approximation that exactly interpolates the data given in (8), then the quasi-interpolant $\mathcal{Q}_f$ requires that its generating functions are cardinal functions. In other words, the approximant $\mathcal{Q}_f$ will naturally involve an error at the data sites in addition to the saturation error $\epsilon(\varphi,\ \varepsilon)$. On the other hand, as we pointed out earlier, the interpolant $\mathcal{P}_f$ is the "best" solution to problem (1) in the Hilbert function space defined by the chosen basis functions. Therefore, we are motivated to seek a method that comes close to both ideals, i.e., to find a solution that, on the one hand, does not require solving a linear system but, on the other hand, is closer to the RBF interpolant than the plain AMLS approximant.

Next, we will formulate a residual iteration algorithm that can achieve this goal with an acceptable amount of additional computations.

3 Interpolation via Iterated AMLS Approximation

As shown in the previous section, it is possible that a standard RBF interpolant $\mathcal{P}_f$ and an AMLS quasi-interpolant $\mathcal{Q}_f$ share the same set of basis functions, e.g., basis functions generated by a basic Laguerre–Gaussian function. In this section we will explain how an initial approximant $\mathcal{Q}_f$ can be pushed closer towards the corresponding interpolant $\mathcal{P}_f$ by a residual iteration process. We will also provide some theoretical analysis of the convergence of such an iteration.

3.1 The Iterative Algorithm

We will now combine all constant parameters h, ε, and ε^s into the definition of the basic function φ. That is, we redefine (4) and (8) in the simple form

$$\mathcal{P}_f(x) := \sum_{j=1}^{N} c_j \varphi\left(\|x - x_j\|\right), \tag{9}$$

$$\mathcal{Q}_f(x) := \sum_{j=1}^{N} f(x_j) \varphi\left(\|x - x_j\|\right). \tag{10}$$

Note that now each of $\mathcal{P}_f$ and $\mathcal{Q}_f$ is a linear combination with the *same* basic function φ. For example, we can use the scaled s-dimensional Gaussian,

$$\varphi(r) = \frac{\varepsilon^s}{\sqrt{\pi^s}} e^{-\varepsilon^2 r^2/h^2}.$$

Clearly, the interpolation matrix based on (9) becomes

$$\mathbf{A} = \left\{\varphi\left(\|x_i - x_j\|\right)\right\}_{i,j=1}^{N}, \tag{11}$$

and the linear system is still in the form $\mathbf{Ac} = \mathbf{f}$, where the vectors $\mathbf{c}$ and $\mathbf{f}$ are as defined earlier.

To construct an algorithm that iterates on residuals, we start with an initial AMLS quasi-interpolant

$$\mathcal{Q}_f^{(0)}(x) = \sum_{j=1}^{N} f(x_j) \varphi\left(\|x - x_j\|\right). \tag{12}$$

We then iteratively define

$$\mathcal{Q}_f^{(n)}(x) = \mathcal{Q}_f^{(n-1)}(x) + \sum_{j=1}^{N} \left[f(x_j) - \mathcal{Q}_f^{(n-1)}(x_j)\right] \varphi\left(\|x - x_j\|\right). \tag{13}$$

That is, the current approximant is successively updated by a residual function which is also constructed by AMLS approximation on the same set of data points.

Certainly, so far we have no evidence that the sequence of these approximating functions $\{\mathcal{Q}_f^{(n)}\}$ converges in any form as $n \to \infty$, or what its limit will be if it is convergent. Next, we will show that under some appropriate assumptions $\mathcal{Q}_f$ does converge to the interpolant $\mathcal{P}_f$ as $n \to \infty$.

3.2 A Necessary and Sufficient Condition

Theorem 1. *The sequence of functions* $\{\mathcal{Q}_f^{(n)}\}$ *defined by (12) and (13) converges to the interpolant* $\mathcal{P}_f$ *defined in (9) if and only if the chosen basic function* φ *generates an interpolation matrix* $\mathbf{A}$ *that satisfies* $\|\mathbf{I} - \mathbf{A}\|_2 < 1$ *for a given set of distinct data points* $\{x_j\} \subseteq \Omega \subseteq \mathbb{R}^s$.

Proof. First, we convert our notation to matrix-vector form. Define a column vector of functions

$$\Psi(x) := [\varphi(\|x - x_1\|), \varphi(\|x - x_2\|), \ldots, \varphi(\|x - x_N\|)]^T.$$

Clearly, $\Psi(x)$ is related to the interpolation matrix $\mathbf{A}$, i.e., due to the symmetry,

$$\mathbf{A}^T = [\Psi(x_1) \mid \Psi(x_2) \mid \cdots \mid \Psi(x_N)] \ (= \mathbf{A}). \tag{14}$$

The interpolant $\mathcal{P}_f$ defined in (9) can also be expressed in matrix-vector form using the vector $\Psi(x)$, i.e.,

$$\mathcal{P}_f(x) = \Psi(x)^T \mathbf{c}. \tag{15}$$

Next, we will inductively prove that the functions $\mathcal{Q}_f^{(n)}$ defined in (13) can also be explicitly expressed in matrix-vector notation

$$\mathcal{Q}_f^{(n)}(x) = \Psi(x)^T \left[\sum_{k=0}^{n} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f}, \quad \text{for all } n = 0, 1, 2, \ldots, \tag{16}$$

where $\mathbf{f} = [f(x_1), f(x_2), \ldots, f(x_N)]^T$ as before.

The initial case $n = 0$ is clear. Suppose (16) holds up to an index n. We need to show that

$$\mathcal{Q}_f^{(n+1)}(x) = \Psi(x)^T \left[\sum_{k=0}^{n+1} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f}.$$

Using the induction hypothesis, the definition of $\mathbf{f}$ and the relation (14) between the interpolation matrix $\mathbf{A}$ and the vector function Ψ we have

$$\begin{aligned}
\mathcal{Q}_f^{(n+1)}(x) &= \mathcal{Q}_f^{(n)}(x) + \sum_{j=1}^{N} \left[f(x_j) - \mathcal{Q}_f^{(n)}(x_j)\right] \varphi\left(\|x - x_j\|\right) \\
&= \Psi(x)^T \left[\sum_{k=0}^{n} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f} \\
&\quad + \sum_{j=1}^{N} \left[f(x_j) - \Psi(x_j)^T \left[\sum_{k=0}^{n} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f}\right] \varphi\left(\|x - x_j\|\right) \\
&= \Psi(x)^T \left[\sum_{k=0}^{n} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f} \\
&\quad + \Psi(x)^T \left[\mathbf{f} - \mathbf{A}^T \left[\sum_{k=0}^{n} (\mathbf{I} - \mathbf{A})^k\right] \mathbf{f}\right].
\end{aligned}$$

Now, straightforward algebra yields

$$\begin{aligned}\mathcal{Q}_f^{(n+1)}(x) &= \Psi(x)^T \left[\mathbf{I} + \sum_{k=0}^{n} (\mathbf{I}-\mathbf{A})^{k+1}\right]\mathbf{f} \\ &= \Psi(x)^T \left[\sum_{k=0}^{n+1} (\mathbf{I}-\mathbf{A})^{k}\right]\mathbf{f}.\end{aligned}$$

As (16) shows, it is clear that each updated approximant $\mathcal{Q}_f^{(n)}$ is still a linear combination of the same basis functions but with an updated coefficient vector of the form

$$\left[\sum_{k=0}^{n} (\mathbf{I}-\mathbf{A})^{k}\right]\mathbf{f}.$$

Thus, the fact that $\mathcal{Q}_f^{(n)} \to \mathcal{P}_f$ as $n \to \infty$ is equivalent to

$$\left[\sum_{k=0}^{n} (\mathbf{I}-\mathbf{A})^{k}\right]\mathbf{f} \to \mathbf{c} \quad \text{as } n \to \infty.$$

Since $\mathbf{c}$ is determined by the linear system (5) defined by the interpolation problem, i.e., $\mathbf{c} = \mathbf{A}^{-1}\mathbf{f}$, the convergence is therefore equivalent to

$$\left[\sum_{k=0}^{n} (\mathbf{I}-\mathbf{A})^{k}\right]\mathbf{f} \to \mathbf{A}^{-1}\mathbf{f} \quad \text{as } n \to \infty,$$

or,

$$\sum_{k=0}^{n} (\mathbf{I}-\mathbf{A})^{k} \to \mathbf{A}^{-1} \quad \text{as } n \to \infty.$$

The proof is completed by noting that a Neumann series satisfies

$$\sum_{k=0}^{\infty} (\mathbf{I}-\mathbf{A})^{k} = \mathbf{A}^{-1}$$

if and only if $\|\mathbf{I}-\mathbf{A}\|_2 < 1$. □

If the assumption of Theorem 1 holds, then a discrete ℓ_2 error of this iterated approximation with respect to the given data can be computed.

Corollary 1. *Let*

$$\mathbf{q}^{(n)} = [\mathcal{Q}_f^{(n)}(x_1), \mathcal{Q}_f^{(n)}(x_2), \ldots, \mathcal{Q}_f^{(n)}(x_N)]^T.$$

If $\|\mathbf{I}-\mathbf{A}\|_2 < 1$ *then* $\|\mathbf{f}-\mathbf{q}^{(n)}\|_2 \to 0$ *for* $n \to \infty$.

Proof.

$$\|\mathbf{f}-\mathbf{q}^{(n)}\|_2 = \left\|\mathbf{A}\mathbf{A}^{-1}\mathbf{f} - \left[\mathbf{A}\sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k\right]\mathbf{f}\right\|_2$$
$$\leq \|\mathbf{A}\|_2 \left\|\mathbf{A}^{-1} - \sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k\right\|_2 \|\mathbf{f}\|_2.$$

Since the matrix $\mathbf{A}^{-1}$ is invertible, using the formula for the sum of a finite geometric series, we have

$$\begin{aligned}\|\mathbf{f}-\mathbf{q}^{(n)}\|_2 &\leq \|\mathbf{A}\|_2 \left\|\mathbf{A}^{-1}(\mathbf{I}-\mathbf{A})^{n+1}\right\|_2 \|\mathbf{f}\|_2 \\ &\leq \|\mathbf{A}\|_2 \|\mathbf{A}^{-1}\|_2 \|\mathbf{I}-\mathbf{A}\|_2^{n+1} \|\mathbf{f}\|_2 \\ &= \operatorname{cond}(\mathbf{A}) \|\mathbf{I}-\mathbf{A}\|_2^{n+1} \|\mathbf{f}\|_2 \to 0,\end{aligned}$$

where $\operatorname{cond}(\mathbf{A})$ is the ℓ_2-condition number of $\mathbf{A}$. □

If the assumption of Theorem 1 holds, then we can also estimate the norm of the residual functions.

Corollary 2. *If* $\|\mathbf{I}-\mathbf{A}\|_2 < 1$ *then*

$$\|R^{(n)}\|_2 = \left\|\sum_{j=1}^{N}\left[f(x_j) - \mathcal{Q}_f^{(n-1)}(x_j)\right]\varphi\left(\|\cdot - x_j\|\right)\right\|_2 \to 0$$

for $n \to \infty$.

Proof. From (13) we have

$$\begin{aligned}R^{(n)} &= \sum_{j=1}^{N}\left[f(x_j) - \mathcal{Q}_f^{(n-1)}(x_j)\right]\varphi\left(\|\cdot - x_j\|\right) \\ &= \mathcal{Q}_f^{(n)} - \mathcal{Q}_f^{(n-1)}.\end{aligned}$$

But now, using matrix-vector notation,

$$\left\|\mathcal{Q}_f^{(n)} - \mathcal{Q}_f^{(n-1)}\right\|_2 = \left\|\Psi(\cdot)^T\left[\sum_{k=0}^{n}(\mathbf{I}-\mathbf{A})^k\right]\mathbf{f} - \Psi(\cdot)^T\left[\sum_{k=0}^{n-1}(\mathbf{I}-\mathbf{A})^k\right]\mathbf{f}\right\|_2$$
$$\leq \|\Psi(\cdot)\|_2 \|\mathbf{I}-\mathbf{A}\|_2^n \|\mathbf{f}\|_2 \to 0,$$

and thus the statement follows. □

Clearly, the speed of convergence is governed by the entries in the interpolation matrix **A**, and thus by the choice of φ (see (11)). A basic function that is strictly positive definite and satisfies the continuous moment conditions does not automatically guarantee such a matrix **A**. This may easily be demonstrated by counterexamples.

3.3 A Sufficient Condition

Theorem 2. *Using the same notation as in Theorem 1, if a basic function φ is strictly positive definite and generates an interpolation matrix* **A** *so that*

$$\max_{i=1,2,\ldots,N} \left\{ \sum_{j=1}^{N} | \mathbf{A}_{i,j} | \right\} < 2, \tag{17}$$

then $\mathcal{Q}_f^{(n)}$ converges to $\mathcal{P}_f$ as $n \to \infty$.

Proof. Let λ_k for $k = 1, 2, \ldots, N$ be the eigenvalues of **A**. That is, $1 - \lambda_k$ are the eigenvalues of the matrix $\mathbf{I} - \mathbf{A}$ for $k = 1, 2, \ldots, N$.

Since φ is a strictly positive definite function, the matrix **A** is positive definite, i.e.,

$$\lambda_k > 0 \quad \text{for } k = 1, 2, \ldots, N.$$

Thus,

$$1 - \lambda_k < 1 \quad \text{for } k = 1, 2, \ldots, N. \tag{18}$$

Recall that

$$\mathbf{A}_{i,j} = \varphi\|x_i - x_j\|, \quad \text{for } i, j = 1, 2, \ldots, N.$$

This shows that all diagonal entries in **A** are identical and equal to $\varphi(0)$. Hence, Gerschgorin's Theorem implies that

$$|\lambda_k - \varphi(0)| \leq \max_{i=1,2,\ldots,N} \left\{ \sum_{j=1}^{N} | \mathbf{A}_{i,j} | \right\} - \varphi(0), \quad \text{for } k = 1, 2, \ldots, N.$$

Using the assumption (17) we get

$$| \lambda_k - \varphi(0) | < 2 - \varphi(0),$$

which is equivalent to

$$\varphi(0) - 2 < \lambda_k - \varphi(0) < 2 - \varphi(0).$$

Rearranging these inequalities yields

$$-1 < 1 - \lambda_k < 3 - 2\varphi(0), \quad \text{for } k = 1, 2, \ldots, N. \tag{19}$$

Combining (18) and (19) we have

$$-1 < 1 - \lambda_k < 1, \quad \text{for } k = 1, 2, \ldots, N,$$

or

$$\max_{k=1,2,\ldots,N} \{|1 - \lambda_k|\} < 1.$$

Since the matrix $\mathbf{I} - \mathbf{A}$ is also symmetric, standard results from linear algebra tell us that the 2-norm of the matrix $\mathbf{I} - \mathbf{A}$ is given by

$$\|\mathbf{I} - \mathbf{A}\|_2 = \max_{k=1,2,\ldots,N} \{|1 - \lambda_k|\}.$$

So

$$\|\mathbf{I} - \mathbf{A}\|_2 < 1,$$

and the convergence of $\mathcal{Q}_f^{(n)}$ to $\mathcal{P}_f$ follows from Theorem 1. □

A simple example that illustrates Theorem 2 is obtained if we use Shepard's partition of unity functions. We define the set of basis functions as

$$w_j(x) = \varphi(\|x - x_j\|) \Big/ \sum_{\ell=1}^{N} \varphi(\|x - x_\ell\|)$$

with a strictly positive definite and positive basic function φ. If an interpolant is constructed with these basic functions, i.e.,

$$\mathcal{P}_f(x) = \sum_{j=1}^{N} c_j w_j(x),$$

then one can easily show that the interpolation matrix $\mathbf{W} = \{w_j(x_i)\}_{i,j=1}^{N}$ is invertible. Moreover, summation of the entries in any row of $\mathbf{W}$ always results in a row sum equal to one due to the partition of unity property. Therefore, if the residual iteration algorithm is started with a quasi-interpolant using the w_j as generating functions, then it will converge to $\mathcal{P}_f$.

In order to ensure convergence of the residual iteration algorithm via Theorem 2 in the first place, and to increase its speed of convergence as much as possible, Theorem 2 and its proof tell us that we want to have an interpolation matrix $\mathbf{A}$ whose entries are not too large in magnitude. From the definition of the basic functions φ we know that the entries of the matrix $\mathbf{A}$ carry a multiplicative factor ε^s. This simply

implies that at least the diagonal entries in $\mathbf{A}$ could become arbitrarily large for $\varepsilon > 0$ being large (recall that $\mathbf{A}_{j,j}$ are indeed positive since φ is strictly positive definite). Therefore, ε must be chosen to be small. On the other hand, however, it is known that for many commonly used strictly positive definite functions (e.g., the Gaussian) a small shape parameter ε implies that the smallest eigenvalue of $\mathbf{A}$, $\lambda_{\min}$ (which again is always positive), will likely be very close to zero (see, e.g., Chapter 12 in [10]). Therefore, again according to the proof of Theorem 2, $\|\mathbf{I}-\mathbf{A}\|_2$ will be at least $1-\lambda_{\min}$ which is very close to 1. Thus, for such a choice of ε the convergence of the iteration will be extremely slow. We will use a set of experiments to demonstrate this trade-off phenomenon caused by the scaling parameter ε.

To conclude this section, we would like to come back to the data point distribution issue as mentioned earlier. Once $\mathcal{Q}_f^{(n)}$ is guaranteed to converge to $\mathcal{P}_f$ it is not so crucial how the initial approximant was constructed since $\mathcal{P}_f$ is still the "best" solution to the problem even when data points are scattered. That is to say, although $\mathcal{Q}_f^{(0)}$ is an AMLS quasi-interpolant formulated with a scaling designed for the uniform data problem, the iterated approximant is still good when the data points are scattered. From the experimental results presented in the next section, we will see that this iterative method does work equivalently well for both regular and irregular grid points.

4 Numerical Experiments

In this sections, we use a set of numerical experiments to illustrate some of the advantages and features of the iterated AMLS approximation method described in previous sections. We will study the behavior of the method with respect to the data size N and the shape parameter ε used in the definition of the basic function φ. Throughout the rest of this section the test function f we use for our experiments is a mollified linear combination of exponentials similar to the famous Franke function. More precisely, in the case $s = 1$ we use

$$f(x) = 15e^{-\frac{1}{1-(2x-1)^2}}\left(\frac{3}{4}e^{-\frac{(9x-2)^2}{4}} + \frac{3}{4}e^{-\frac{(9x+1)^2}{49}} + \frac{1}{2}e^{-\frac{(9x-7)^2}{4}} - \frac{1}{5}e^{-(9x-4)^2}\right) \tag{20}$$

on the interval $[0, 1]$, and for $s = 2$ we let

$$\begin{aligned} g(x, y) &= \frac{3}{4}e^{-1/4((9x-2)^2+(9y-2)^2)} + \frac{3}{4}e^{-(1/49)(9x+1)^2-(1/10)(9y+1)^2} \\ &\quad + \frac{1}{2}e^{-1/4((9x-7)^2+(9y-3)^2)} - \frac{1}{5}e^{-(9x-4)^2-(9y-7)^2} \\ f(x, y) &= 15g(x, y)e^{-\frac{1}{1-(2x-1)^2}}e^{-\frac{1}{1-(2y-1)^2}} \end{aligned} \tag{21}$$

which we will sample in the unit cube $[0, 1]^2$. The basic function used to generate the basis functions for all experiments presented here is the scaled s-dimensional

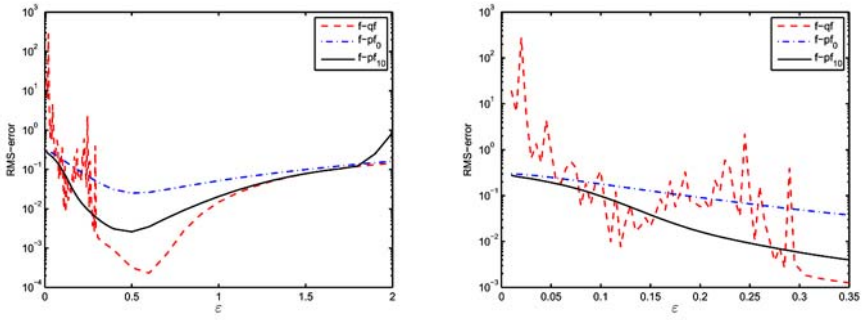

Fig. 1. Comparison of accuracy and stability of the RBF interpolant, AMLS approximant, and iterated AMLS approximant for 1089 Halton data points in 2D.

Gaussian

$$\varphi(r) = \frac{\varepsilon^s}{\sqrt{\pi^s}} e^{-\varepsilon^2 r^2/h^2}, \tag{22}$$

where h is the fill-distance corresponding to a *uniform* distribution of points in the domain. This manner of scaling the basic function proportional to the fill-distance is known as the stationary approximation paradigm. We have performed the same set of experiments also with first-order Laguerre–Gaussians (see (6)). Due to the similarity of these results to those for Gaussians we focus only on Gaussians here.

Although it is known that RBF interpolation theoretically yields the native space best approximation for scattered data fitting problems, the results obtained in practice are sometimes unreliable due to poor numerical stability of the solution of the associated linear system (5). For a given set of data the accuracy of an interpolant may strongly depend on the scale parameter ε that is often part of the definition of the basic function, e.g., the Gaussian function (22).

Generally speaking, when ε is too large, the basic function is very peaked, and thus the resulting interpolant will be very "spiky" so that it can not be considered as a good approximant to the true function. On the other hand, a small ε makes a flat basic function which will generate an ill-conditioned interpolation matrix $\mathbf{A}$ giving rise to computational difficulty (in the extreme case, when $\varepsilon \to 0$, the matrix $\mathbf{A}$ becomes a constant matrix which is singular). The interpolant resulting from such an ill-conditioned calculation is obviously to be trusted less. Figure 1 illustrates both of these observations.

In both plots of Figure 1 we display the root-mean-squared error of the interpolant (`f-qf`, dashed line), the AMLS approximant ($\texttt{f-pf}_0$, dash-dotted line), and the result of ten iterations of the iterated AMLS method ($\texttt{f-pf}_{10}$, solid line) versus the scale parameter ε as used in (22). The data were obtained by sampling the two-dimensional modified Franke function (21) at 1089 non-uniform Halton points (see,

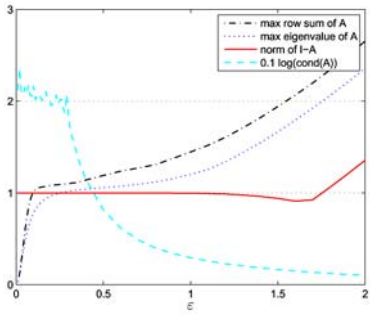

Fig. 2. Maximum row sum, maximum eigenvalue, $\|\mathbf{I} - \mathbf{A}\|$, and cond($\mathbf{A}$), for the matrix $\mathbf{A}$ used in Figure 1.

e.g., [11] for more information on Halton points). The error was computed on a grid of 40×40 equally spaced evaluation points.

In this example ε should be characterized as being "large" if its value is greater than approximately 1.2. For these values the error of the interpolant is not significantly different from that of the AMLS approximation, and a plot of the interpolant would be a very "spiky" surface as mentioned earlier. Within this range for the scale parameter we can distinguish two different behaviors of the iterative algorithm. If ε is so large that convergence of the iterative algorithm is no longer ensured then the iterated approximant blows up. Figure 2 shows that the maximum row sum of the matrix $\mathbf{A}$ is greater than two if $\varepsilon > 1.5$. In fact, the iterated algorithm does not blow up until about $\varepsilon = 1.8$ (when the maximum eigenvalue of $\mathbf{A} > 1$). This also indicates that the maximum row sum criterion is a relatively easy to check and safe criterion to ensure convergence of the iterative algorithm. Clearly, one wants to avoid the use of these "large" ε values.

Moreover, within the "large" ε range we can usually find those values for which the iterative algorithm converges rapidly to the interpolant. For the example shown in Figure 1 this corresponds to about $1.2 < \varepsilon < 1.8$. Since the interpolant is still rather "spiky" for these ε-values neither the interpolant nor the iterated approximant are desirable in this case. However, the (iterated) AMLS apprimant is usually smoother for this range of ε-values and there may be certain circumstances in which this may be more desirable than the interpolant.

A third range of values of the scale parameter corresponds to a "good" interpolant – usually accompanied by slow convergence of the iterative algorithm. For the example shown in Figure 1 this corresponds to about $0.4 < \varepsilon < 1.2$. For most problems of small to modest size (for which we were able to compute the interpolant in Matlab) the smallest achievable RMS-error for the interpolant falls into this range. However, for larger problems the optimal interpolant may be associated

with an ε-value that leads to an ill-conditioned system matrix. This brings us to the last ε-range.

If ε is in the range that causes instability (roughly $\varepsilon < 0.4$ in Figure 1), then the iterated AMLS method can successfully overcome the computational difficulty associated with the solution of the ill-conditioned interpolation system. To illustrate this more clearly we have displayed a "zoomed-in" view for this range of small ε in the right part of Figure 1. Even pure AMLS quasi-interpolation may work better than interpolation for this range of ε. In addition, the error between the test function and the iterated AMLS approximant is significantly improved after only 10 iterations. It is clear that if the number of iterations is much smaller than the number of data points, then the iterated AMLS method requires far less computational work compared to solving for the interpolant. In the experiments reported here we always perform 10 iterations. That is, the computational complexity is of order $\mathcal{O}(10N^2)$ while direct computation of the interpolant usually requires a computational complexity on the order of $\mathcal{O}(N^3)$. Of course, fast summation techniques such as the fast (non-uniform) Fourier transform (see, e.g., [6, 7] or [5]) can be used to improve the efficiency of both approaches.

In order to study the connection between the convergence behavior of the interpolant and that of the iterated AMLS approximant we will now focus on an ε that falls into the "reasonable" range for both the interpolant and the iterative algorithm, say, $0.4 \leq \varepsilon \leq 0.8$ for the examples we present.

It is well-known (see, e.g., [1]) that stationary interpolation with Gaussians is saturated. However, to our knowledge until now no one has provided an explicit estimate for the saturation error. In the quasi-interpolation setting, on the other hand, which is discussed in the literature on approximate approximations (see, e.g., [9]) the saturation error is well understood. This begs the question whether the saturation error of stationary RBF interpolation can be explained by the one of AMLS approximation via the residual iteration process. Since we have shown convergence of iterated approximate MLS approximation to the RBF interpolant we may expect the saturation error of the approximate approximation setting to propagate to the interpolant. This may be intuitively reasonable since the residual function is constructed with the same AMLS functions as the initial AMLS approximant. Further detailed analysis of this phenomenon is required.

The graphs in Figure 3 illustrate how the convergence behavior of the iterated AMLS approximation matches that of the interpolant. The graphs shows RMS-errors versus N, the number of data points, for a 1D approximation problem with data function (20). The graphs in the left column are for uniformly spaced data, and in the right column for Halton points. Each row corresponds to a different (fixed) value of ε.

We see that the behavior is very similar in both the uniform and the non-uniform (Halton) setting. The main difference is the larger error for the basic AMLS approximation ($\texttt{f-pf}_0$, dash-dotted line) in the Halton setting. This is easily explained by the

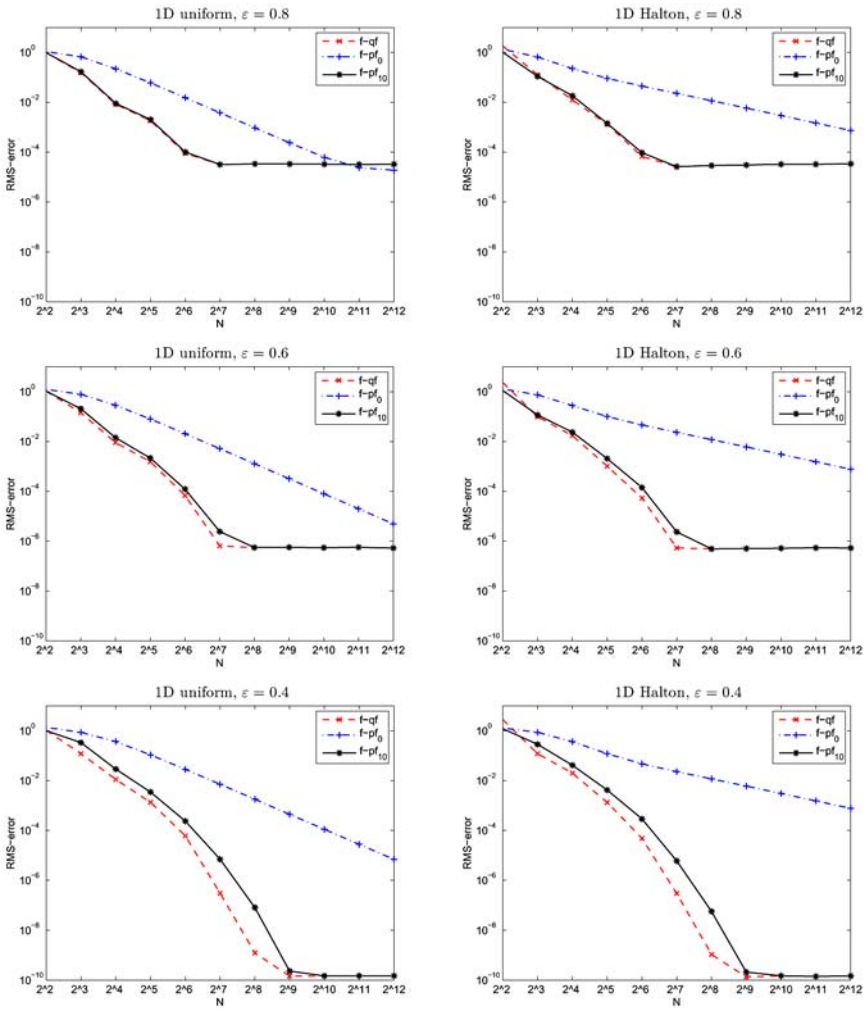

Fig. 3. Saturated convergence of stationary RBF interpolation and iterated AMLS approximation for $\varepsilon = 0.8, 0.6, 0.4$ from top down with uniform (left) and Halton data (right).

fact that we have not adapted the scaling of the basis functions for the non-uniform point distribution (see (22)). The similarity of the errors for the iterated AMLS approximant in the Halton and uniform settings clearly illustrates how the iterative algorithm automatically adapts the AMLS method to the non-uniform setting.

In Figure 4 we collect the error curves for the iterated AMLS approximants from the two columns of Figure 3 in one graph each. We can now clearly see that a larger

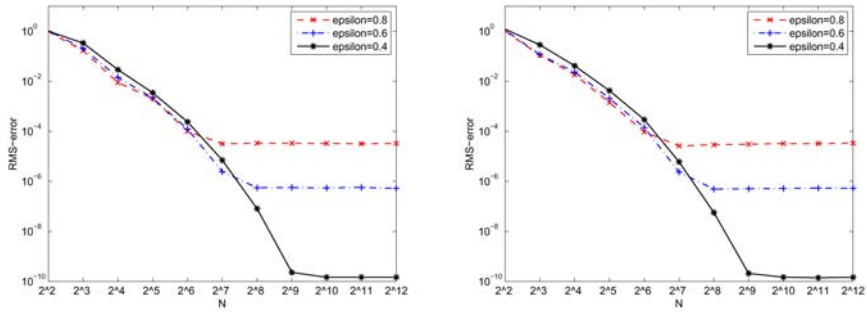

Fig. 4. Saturation errors of iterated AMLS approximation for uniform (left) and Halton (right) data in 1D.

ε makes the saturation error come in earlier, i.e., the drop in the error stops at a larger error value and at a smaller data size N.

5 Conclusions

In this report we have presented a residual iterative algorithm for solving the scattered data fitting problem. As shown by the analysis and numerical results in the previous sections, the method works well for both uniform data and Halton data (an example of irregular data). This is true in terms of accuracy, convergence speed, numerical stability and computational cost.

As illustrated above, the residual iterative algorithm provides a mechanism to transfer the saturation error associated with (stationary) AMLS approximation to RBF interpolation. We plan to investigate this connection more carefully in the future.

As is well known, RBF interpolation is the best approximation in the native space for the data fitting problem. However, in practice, this "best" solution might not be "good enough" – especially if the choice of the shape parameter ε is bad. Moreover, in some cases one may not really desire an interpolant as the "best" solution. This will be true, for example, when the data are obtained from some inaccurate noisy experiments. In this case the residual iterative method will definitely provide a more stable and more reliable solution for the problem.

Clearly, the success of our iterative method is determined by several components such as the scaling parameter ε and the basic function itself. As pointed out above, we want the basic function to be strictly positive definite to ensure uniqueness of the RBF interpolant. Moreover, we want the basic function to satisfy a set of continuous moment conditions defined in (7) required for AMLS approximation. As an example of a class of functions that carry both of these properties we presented the Laguerre–Gaussian functions. In order to obtain more insight and carry out a deeper analysis of

the performance of this iterative method, it is desirable to test the method with some other basic functions besides the Laguerre–Gaussians. Presently we are not aware of any direct connection between strict positive definiteness of a function and the set of continuous moment conditions (7). Of course, it is a simple matter to verify that any integrable normalized strictly positive definite function satisfies condition (7) for (at least) $d = 0$. On the other hand, a function that satisfies condition (7) is not guaranteed to be strictly positive definite. For example, let $\varphi : [0, \infty) \to \mathbb{R}$ be defined as

$$\varphi(r) = \frac{1 + r^2}{1 + r^2 + r^4}.$$

Then its one-dimensional radial version

$$\varphi(\|x\|) = \frac{\sqrt{3}}{2\pi} \frac{1 + \|x\|^2}{1 + \|x\|^2 + \|x\|^4}, \qquad x \in \mathbb{R}$$

satisfies condition (7) for $d = 0$. But it can be verified that the Fourier transform of φ is negative at some points. Therefore φ is not strictly positive definite.

Since finding strictly positive definite functions that satisfy the continuous moment conditions seems to be a non-trivial task, we plan to search for additional function classes that carry both of these properties.

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