

A Weighted Linear Method for Approximation of Irregularly Spaced Data

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Abstract. A new method for the approximation of irregularly spaced data is described that is particularly suitable for very large data sets of highly varying densities. The approximation is defined by a weighted sum of linear functions, each function obtained from a data point and its gradient, and weight functions that adapt to the organization of data. Experimental results are provided comparing the accuracy of the proposed method with that of multiquadrics in the approximation of irregularly spaced data.

§1. Introduction

The problem to be solved is as follows. Given a set of irregularly spaced data

$$\{f_i : i = 1, \dots, N\} \tag{1}$$

correspondingly at

$$\{\mathbf{x}_i = (x_{1i}, x_{2i}, \dots, x_{di}) : i = 1, \dots, N\} \tag{2}$$

in d dimensions, we would like to determine a function $f(\mathbf{x})$ that closely approximates the data.

A large number of approximation/interpolation methods exist in the literature [4, 5, 7, 11]. Methods based on radial basis functions are most widely used when density variations in data do not exist. Radial basis functions are defined by

$$f(\mathbf{x}) = \sum_{i=1}^N R_i(\mathbf{x})F_i \tag{3}$$

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where $R_i(\mathbf{x})$ is a radially symmetric function centered at \mathbf{x}_i . Coefficients $\{F_i : i = 1, \dots, N\}$ are determined by solving the following system of linear equations:

$$\sum_{i=1}^N R_i(\mathbf{x}_j) F_i = f_j \quad j = 1, \dots, N. \quad (4)$$

Franke [4] compared various approximation/interpolation methods using rather small and randomly spaced data and found that multiquadrics (MQ) [8, 9] in general produced the best accuracy. Monotonically increasing basis functions such as MQ and thin-plate splines (TPS), in general, produced a better accuracy in data fitting than monotonically decreasing basis functions such as inverse multiquadrics (IMQ) and Gaussians [4]. When data are noisy or contain errors, however, monotonically decreasing basis functions are preferred because an erroneous data point will affect functional values mostly in the neighborhood of the error. When monotonically increasing basis functions are used, the effect of an erroneous data point spreads over the entire approximation domain.

When data are noisy, approximation methods are preferred over interpolation methods because they can smooth noise in the data through an averaging process. In this paper, a new method for the approximation of irregularly spaced data is introduced that uses monotonically decreasing weight functions to ensure that a data point affects functional values mostly in its neighborhood. Also, local gradients of data are determined and used to control the shape of the approximating function and avoid creation of overshoots and fluctuations in data fitting.

§2. Geometric Interpretation of Radial Basis Functions

Examples of interpolation by radial basis functions in 1-D are depicted in Fig. 1. Fig. 1a shows interpolation by MQ and Fig. 1b shows interpolation by IMQ. The basis functions are shown by the dotted curves. Multiplying the basis functions by their coefficients (the F_i 's in (3)), the solid thin curves are obtained. Adding the thin curves, the interpolation curves shown by the thick curves are obtained.

Monotonically decreasing basis functions produce flat horizontal spots at the data points as can be observed in Fig. 1b, and the spots become more pronounced as the width of the basis functions is reduced. This is usually not a desirable property in interpolation. As the width of the basis functions is reduced, however, the interpolation becomes more local, which is a desired property. Therefore, our goal will be to come up with a formulation that is based on monotonically decreasing basis functions but does not create flat horizontal spots at the data points.

Another way to interpret formula (3) when monotonically decreasing basis functions is used is depicted in Fig. 2a. The coefficients can be

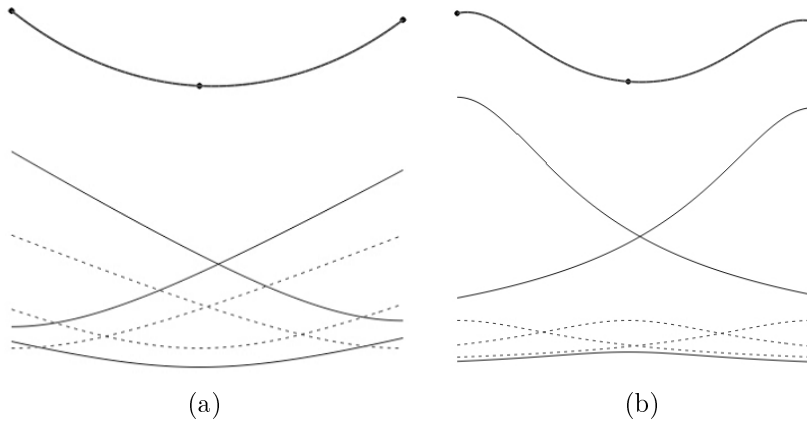


Fig. 1. (a) Interpolation using monotonically increasing basis functions. (b) Interpolation using monotonically decreasing basis functions.

considered horizontal lines. Multiplying the lines point-by-point by the corresponding basis function values (shown by the dotted curves), the thin solid curves are obtained, which when added together produces the interpolation curve shown by the thick solid curve.

Note that at a data point, the horizontal line representing the coefficient there has gradient 0. Also, because the value of the corresponding basis function becomes maximum at the data point, the gradient of the basis function becomes 0 there. This is the reason why flat horizontal spots are obtained at the data points. The gradient of the approximating function at the data points may not be exactly 0 due to influence of nearby basis functions, but they are very small and they become smaller as the width of the basis functions is reduced. We would like to develop a formulation that uses monotonically decreasing weight functions but does not produce flat horizontal spots as is generally obtained in interpolation/approximation methods that use monotonically decreasing basis/weight functions.

One other factor that has to be taken into consideration is the irregular spacing of the data points. When radially symmetric basis/weight functions are used and data are irregularly spaced, large errors may be obtained away from the data points. To avoid this, instead of radially symmetric functions, functions whose shapes adapt to the organization of data will be needed. An example of such weight functions is shown in Fig. 2b. A weighted sum of lines whose slopes are either given or can be estimated from local data is used. By decreasing the widths of the weight functions, the approximation is made more local, forcing it to more closely follow the data.

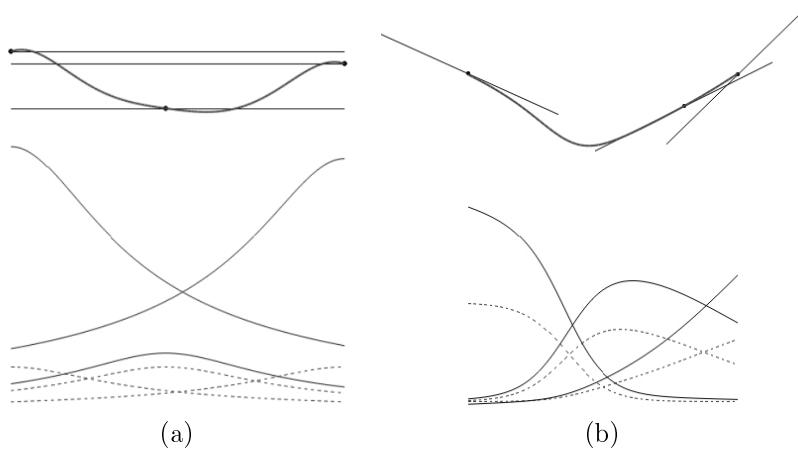


Fig. 2. (a) Interpolation using monotonically decreasing radial basis functions. The dotted curves are the basis functions, the horizontal lines represent the coefficients (appropriately scaled here), the thin solid curves are obtained by multiplying the weight functions and the corresponding lines point-by-point, and the thick solid curve on top shows the interpolating function obtained from the sum of the thin solid curves. (b) Approximation by the proposed method. The dotted curves are the weight functions, the lines represent the local functions obtained from data values as well as their gradients, and the thin solid curves show multiplication of the local functions and the corresponding weight functions. The thick solid curve on top is the resulting approximation obtained from the sum of the thin solid curves.

§3. The Proposed Formulation

The following formula is proposed for the approximation of irregularly spaced data:

$$f(\mathbf{x}) = \sum_{i=1}^N W_i(\mathbf{x})L_i(\mathbf{x}) \quad (5)$$

where

$$W_i(\mathbf{x}) = \frac{R_i(\mathbf{x})}{\sum_{j=1}^N R_j(\mathbf{x})} \quad (6)$$

is the i th weight function, and

$$L_i(\mathbf{x}) = a_{0_i} + a_{1_i}x_1 + a_{2_i}x_2 + \cdots + a_{d_i}x_d \quad (7)$$

is the local function approximating data surrounding the i th data point. In 1-D L_i is a line, in 2-D it is a plane, and in higher dimensions, it is a

hyperplane. The implication of using a weighted sum of linear functions as opposed to a weighted sum of constants is that the approximating function will not produce nearly horizontal spots at the data points but will approximate desired gradients at the data points. The weight functions stretch towards the large gaps (see Fig. 2b for an example) to ensure that the sum of weights everywhere in the approximation domain is 1.

If gradients at \mathbf{x}_i , that is, if $(a_{1i}, a_{2i}, \dots, a_{di})$ are given, a_{0i} is determined such that $L_i(\mathbf{x}_i) = f_i$. If the gradients are not given, they are estimated by fitting $L_i(\mathbf{x})$ to data at and surrounding \mathbf{x}_i . Since this may produce a function that does not evaluate to f_i at \mathbf{x}_i , a_{0i} is recalculated such that $L_i(\mathbf{x}_i) = f_i$.

The weight functions given by formula (6) are rational functions, defined in terms of radial functions. Monotonically decreasing radial functions are used in formula (6) in order to make the approximation sensitive to local data. When the radial functions are Gaussians, we have:

$$R_i(\mathbf{x}) = \exp \left\{ -\frac{\|\mathbf{x} - \mathbf{x}_i\|^2}{2\sigma_i^2} \right\}. \quad (8)$$

The standard deviations of Gaussians control the widths of the weight functions. In order that the widths of the weight functions automatically adjust to the local density of data, σ_i is related to the density of data in the neighborhood of \mathbf{x}_i . In our implementation, σ_i is set to the radius of the radially symmetric region centered at \mathbf{x}_i containing n data points. For example, in 2-D, σ_i will be the radius of the circle centered at \mathbf{x}_i containing n data points. The widths of the weight functions, therefore, automatically adjust to the density of data and since the sum of the weights is required to be 1 everywhere in the approximation domain, the shapes of the weight functions adjust to the organization of data.

Parameter n controls the localness/globalness of the approximation. By decreasing n , the widths of the weight functions decrease, producing an approximation that more closely follows the data, while by increasing n , the process will smooth noisy details in data and capture more of the global features in data. Note that approximation by the proposed method requires the solution of only small systems of equations to obtain the local functions. Therefore, the process is very efficient and can be used to approximate very large data sets.

§4. Experimental Results

A series of experiments were carried out using data in 2-D to determine the behavior and accuracy of the proposed approximation. Four functions: constant, linear, quadratic, and exponential, shown in Fig. 3, were used. The constant and linear functions were used to make sure that the proposed method does not introduce nonexistent fluctuations to

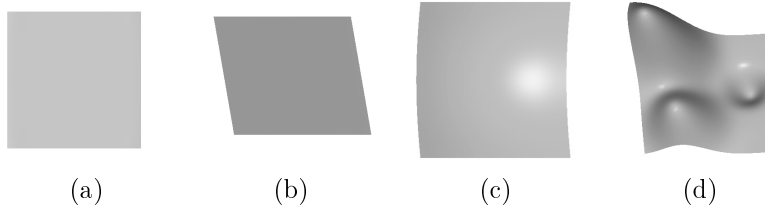


Fig. 3. (a) Constant. (b) Linear. (c) Quadratic. (d) Exponential.

the approximation. The quadratic and exponential functions were used to determine the accuracy of the method in the approximation of moderate to highly varying data. Fig. 3a depicts $f(x_1, x_2) = 1$, Fig. 3b depicts $f(x_1, x_2) = x_1 + x_2$, Fig. 3c shows the segment of the sphere of radius 1 centered at $(0.5, 0.5, 1.0)$ with x_1 and x_2 in the range $[0, 1]$, and Fig. 3d represents the exponential function often used in the literature to determine the accuracy of approximation methods and is attributed to Franke [4]. This function is defined by

$$\begin{aligned}
 f(x_1, x_2) = & 0.75 \exp\{ -[(9x_1 - 2)^2 + (9x_2 - 2)^2]/4 \} + \\
 & 0.75 \exp\{ -[(9x_1 + 1)^2/49 + (9x_2 + 1)/10] \} + \\
 & 0.50 \exp\{ -[(9x_1 - 7)^2 + (9x_2 - 3)^2]/4 \} - \\
 & 0.20 \exp\{ -[(9x_1 - 4)^2 + (9x_2 - 7)^2] \}. \quad (9)
 \end{aligned}$$

Functions in Fig. 3 were sampled at the (x_1, x_2) coordinates shown in Fig. 4 and the obtained data sets were used to estimate the original functions. Fig. 4a shows 100 uniformly spaced points, Fig. 4b shows 100 randomly spaced points (from Franke [3]), Fig. 4c shows 100 points with a moderate density variation, Fig. 4d shows 100 points with a high density variation, and Fig. 4e shows 100 points along curves, representing a very high density variation. There are 4 functions, each sampled 5 different ways; therefore, there are 20 data sets.

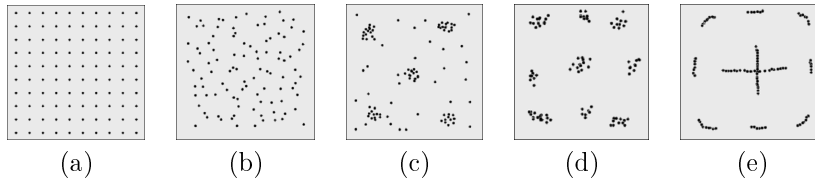


Fig. 4. (a) Uniform. (b) Random. (c) Moderate density variation. (d) High density variation. (e) Very high density variation.

The root-mean-squared errors (RMSEs) between the true functions shown in Fig. 3 and the estimated ones using each of the 20 data sets at

Tab. 1. RMSEs in approximation using a fixed neighborhood size $n = 10$ to calculate all local functions.

	Constant	Linear	Quadratic	Exponential
Uniform	0.0	0.0	0.00181	0.01324
Random	0.0	0.0	0.00203	0.02768
Moderate Density Variation	0.0	0.0	0.00565	0.03966
High Density Variation	0.0	0.0	0.01971	0.10103
Very High Density Variation	0.0	0.0	0.01272	0.11682

Tab. 2. RMSEs in approximation using optimal neighborhood size n to calculate the local functions. The first number in an entry shows the RMSE and the second number shows the optimal neighborhood size n .

	Constant	Linear	Quadratic	Exponential
Uniform	0.0	0.0	0.00156, 5	0.01147, 5
Random	0.0	0.0	0.00203, 10	0.02156, 8
Moderate Density Variation	0.0	0.0	0.00565, 10	0.03966, 10
High Density Variation	0.0	0.0	0.01683, 15	0.08500, 15
Very High Density Variation	0.0	0.0	0.01180, 25	0.105653, 30

100×100 uniformly spaced points in $[0, 1]$ (the approximation domain) were determined and listed in Tab. 1. The number of points, n , used to estimate the local functions was 10. Changing n will change the neighborhood size and that will change the approximation errors. The value of n producing the least error was determined for each data set and reported in Tab. 2. The first number in an entry shows the RMSE and the second number shows the optimal n .

Approximation to the uniform and random data sets by MQ produced the RMSEs shown in Tab. 3. The parameter r in MQ [2] was varied in each case to obtain the least error. The optimal r obtained in each case is shown along with the obtained RMSE. Approximation by MQ was not possible for data sets with moderate, high, and very high density variations.

Although, theoretically, the matrix of coefficients obtained by MQ fitting is known to be positive definite [10], in practice the system of equations to be solved becomes ill-conditioned as variations in the density and in the data values increase. This has been experimentally verified by Carlson and Foley [2] and Goshtasby and O'Neill [6]. The condition number

Tab. 3. Interpolation RMSEs when using MQ with optimal parameter r . The first number in an entry shows the RMSE and the second number shows the optimal r . Approximation by MQ was not possible when data sets with moderate, high, and very high density variations were used.

	Constant	Linear	Quadratic	Exponential
Uniform	0.00030, 0.3	0.00054, 0.3	0.00042, 0.3	0.00126, 0.2
Random	0.00010, 0.3	0.00027, 0.3	0.00018, 0.3	0.00194, 0.2

of the matrix of coefficients increases as parameter r of MQ is increased or as the matrix of coefficients becomes larger. Although clever preconditioned algorithms can be developed to iteratively find the solution to large systems of equations [1], even such preconditioning algorithms become impractical when millions of points are involved. The idea proposed here is to avoid the solution of large systems of equations altogether.

From the above discussions and experimental results, the following conclusions can be reached.

1. For data sets with nearly uniform density, MQ generally produces more accurate results than the proposed method. This can be attributed to the fact that MQ is an interpolation method while the proposed method is an approximation one.
2. If data values in a neighborhood do not vary, the proposed method does a very good job of reproducing the homogeneity in data. When variations in data do not exist, the proposed method does not introduce nonexistent variations to the approximation. The zeros in the “Constant” and “Linear” columns in Tabs. 1 and 2 are anticipated as the convex combinations of a linear function will be that linear function. MQ may create fluctuations in a neighborhood even when no change in data exists as can be observed in the same columns in Tab. 3.
3. In Tabs. 1 and 2, a sharp increase in approximation error is observed from moderate density variations to high and very high density variations for the Exponential case. A closer examination of data organization in Fig. 4 reveals that large gaps exist between data points where large variations in data are present. In data sets with moderate density variations, information about variations in data are provided by the scattered points within the large gaps.
4. The proposed method remains stable under the highest density variations, while data fitting by MQ without preconditioning techniques

becomes impossible even under moderate density variations.

5. Data sets containing 100 points were used in the experiments. These are considered relatively small data sets. In many applications, the number of data points to be used could be in the millions and solution of systems containing millions of equations is impractical. In the proposed method, the systems of equations to be solved are very small and independent of the size of a data set, making the method especially suitable for very large data sets.

§5. Concluding Remarks

In approximation of irregularly spaced data the following properties are desired: 1) The employed method should be able to handle sharp variations in data values. 2) The method should be able to handle large density variations in data. 3) The method should be locally sensitive so that the effect of a noisy or erroneous data point will be mostly in the neighborhood of the point. 4) The method should be able to work with very large data sets.

The proposed method has all these properties. First, the local functions reflect information about local variations in data, so they can reproduce high variation in data. Second, the shape and width of the weight functions automatically adjust to the organization and density of data. Therefore, data sets from uniform density to very high density variation can be used. Third, the approximation can be made more locally sensitive by reducing parameter n of the method. Fourth, the method requires the solution of very small systems of equations to find the local functions; therefore, it can be applied to very large data sets.

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