Constrained Visualization of 2D Positive Data using Modified Quadratic Shepard Method

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ABSTRACT

This paper is about the visualization of positive data subject to positivity constraint. It presents an algorithm that produces a non-negative graph through scattered positive data sets using Modified Quadratic Shepard method. The objective of positivity has been achieved by scaling of basis functions as far as it is necessary. This method is improved in that it produces the positive graph without much deviation of shapes from the ones due to Modified Quadratic Shepard scheme. The method is developed and implemented as a global scheme.

Keywords
Non-negativity, positivity, quadratic surface, shape preservation, constrained interpolation and scattered data.

1. INTRODUCTION
Visualization of a data set generally involves constraints depending upon the inherent features of that data set. The data to be visualized usually is only a sample and may not be sufficient to visualize the entire reality. Researchers use interpolation to construct the models that match the data samples and approximate the unknown reality around the data samples. The models of data should reflect the inherent features of the data.

The preservation of features, inherent to the data, for example monotonicity, convexity and positivity has always been of great interest. The significance of positivity lies in the fact that sometimes it does not make sense to talk of some quantity to be negative. For example, percentage mass concentrations in a chemical reaction, volume and mass of something are meaningless when negative.

Many researchers have considered the problem of positivity. For related literature and background we refer to the papers of Brodlie and Butt [Bro93],

Sarfraz, Hussain and Butt [Sar00] and Sarfraz, Al-Mulhem and Ashraf [Sar97], Asim and Brodlie [Asi00a] and Asim [Asi00] and the papers referred there in.

Modified Quadratic Shepard (MQS) method is widely used for visualization of scattered data particularly large one. This method does not guarantee to preserve positivity. Work has been done by Asim [Asi00], Asim and Brodlie [Asi00a], Brodlie, Asim and Unsworth [Bro03] to constrain MQS interpolation method.

A scheme suggested by Asim [Asi00] is an efficient, positive and C^1 but does not produce promising results for data sets having large number of basis functions that need scaling. The scaling adversely effects the least square feature of this method. This trend aggravates for basis functions with zero reference values.

This gave the motivation to this research and hence enabled us to present a scheme with the following features:

- This scheme reduces the deviation from original shape while preserving positivity that indirectly reduces the departure from least square fit.
- Minor change in existing software is required.

In this scheme, the basis functions due to original Modified Quadratic Shepard method are kept un-scaled above the reference points but are scaled below the reference points.

2. MODIFIED QUADRATIC SHEPARD (MQS) METHOD

Let $(x_1, y_1, f_1), (x_2, y_2, f_2), …, (x_N, y_N, f_N)$ be the set of given N data points, where the f-values are samples of some function $f(x, y)$ that is non-negative for every $x \in [x_1, x_N]$ and $y \in [y_1, y_N]$. The Modified Quadratic Shepard method is given by:

$$F(x, y) = \frac{\sum_{i=1}^{N} w_i(x, y) Q_i(x, y)}{\sum_{i=1}^{N} w_i(x, y)} \quad (1)$$

where $w_i(x, y) = \dfrac{1}{(x - x_i)^2 + (y - y_i)^2}$ and the basis functions $Q_i(x, y)$ is defined as follow:

$$Q_i(x, y) = f_i + a_{i1}(x - x_i)^2 + a_{i2}(x - x_i)(y - y_i) + a_{i3}(y - y_i)^2 \quad (2)$$
$$+ a_{i4}(x - x_i) + a_{i5}(y - y_i)$$

where the coefficients a_{i1}, a_{i2}, a_{i3}, a_{i4} and a_{i5} are related to data points (x_i, y_i, f_i). By definition $Q_i(x_i, y_i) = f_i$. All other coefficients $a_{ij}, j = 1, 2, ….., 5$ are evaluated so that Q_i is the best distance–weighted least-squares approximation to the other data points as given in Franke and Neilson [Fra80].
The original method due to Shepard D.[She68] uses $Q_i(x, y) = f_i$.

2.1 Loss of Positivity by Modified Quadratic Shepard (MQS) Method

The Modified Quadratic Shepard Method does not guarantee to preserve positivity as shown in Figure 2(a) and Figure 3. Positive scattered data given in Table 1 is used for Figure 1&2. The data for surfaces in this paper has been taken from Asim[Asi00].

2.2 Preserving Positivity using MQS Method.

The Modified Quadratic Shepard method calculates inverse distance weighted average of basis functions' values at each sampling position. The basis functions, Q, are the best distance weighted least square fit to the reference data points. As the weight functions are always positive, the function value, F, does not go negative if all basis functions are individually non-negative.
The problem of positivity using Modified Quadratic Shepard method can be addressed in many ways. One can simply truncate the basis function when it goes negative. This is very simple scheme but is not acceptable because of loss of continuity and smoothness as shown in Figure 2©.
Scaling and shifting of the basis function is another approach. This scheme scales and shifts the negative basis functions such that they are positive, in the

region of their participation, without considering the weighing factor. One such scheme is suggested in Asim [Asi00]. This is a low cost, C^1 solution to the positivity problem. A plot of the scaled basis function using this scheme, for point $x = 4$ in the Table 1, is in Figure 1(b). The plot of the MQS basis function for the same point is shown in Figure 1(a). The graph of the data using this simple scaling is shown in Figure 2(b). For this data the graph shown is smooth. But for data sets where scaling effects most of the basis functions, the results are not promising. A 2D plot to this effect is shown in Figure 4. The surface is considerably different from the original MQS surface shown in Figure 3. In fact, for all control points with $f_i = 0$, the scaling suggested causes $Q_i(x, y) = 0$. Therefore, for data sets with large number of zero reference values, departure from the original MQS surface increases significantly.

3. AN IMPROVED, POSITIVE MODIFIED QUADRATIC SHEPARD METHOD.

MQS method guarantees to preserve positivity if each basis function participating in construction of plot is positive. So, we make each basis function, Q_i, positive in the region of its participation. To reduce the effect of scaling, we suggest the alternate strategy given below:

- We constrain only those basis functions that are negative in their region of participation.
- We scale only the part of basis function that is below the reference point. The part of basis function above the reference point remains unchanged.

Let us define quadratic basis function, $Q_i(x, y)$, in terms of its stationary points as follows:

$$Q_i(x, y) = z_s + \frac{1}{2} \delta_s^T A_i \delta_s \quad (3)$$

where $\delta_i = \begin{bmatrix} x - x_i \\ y - y_i \end{bmatrix}$, z_s is stationary point of $Q_i(x, y)$

and

$$A_i = \begin{bmatrix} \dfrac{\partial^2 Q_i}{\partial^2 x} & \dfrac{\partial^2 Q_i}{\partial x \partial y} \\ \dfrac{\partial^2 Q_i}{\partial x \partial y} & \dfrac{\partial^2 Q_i}{\partial^2 y} \end{bmatrix}$$

We make each negative basis function positive by shifting the value of z_s to z_k and hence scaling the Hessian matrix A_i by a positive scaling factor, α_i. The essential idea is to change the eigenvalues λ_1 and λ_2 of Matrix A_i without changing

its eigenvectors so that the contours that make a basis function do not lose their shape during the constraining process. Calculation of a positive scaling factor, α_i, has been discussed in Asim [Asi00].

We define following new basis function, $\hat{Q}_i\ (x,\ y)$, that is positive in the region of its participation

$$\hat{Q}_i\ (x,\ y) = z_k + \frac{1}{2}\ \alpha_i \delta_s^T\ A_i\ \delta_s . \qquad (4)$$

The positivity preserving algorithm given in Asim[Asi00] uses this modified basis function to construct the graph. There are situations where majority of the basis functions with reference values zero or near zero need scaling. In such cases, deviation from least square fit is very large and the graph sometime seems to degenerate to the one due to original Shepard method.

To construct the graph, we replace the part of Q_i, below the reference point, by $\hat{Q}_i$ as shown in Figure 1©.
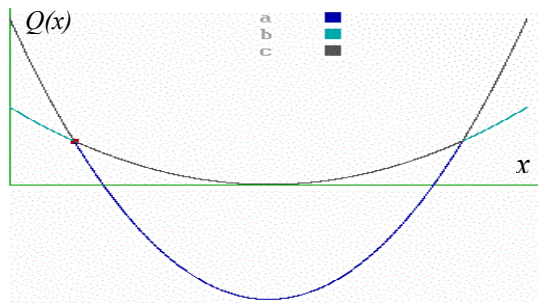

Figure 1 (a) MQS Basis function. (b) Scaled Basis function (c) Basis function proposed in this paper.
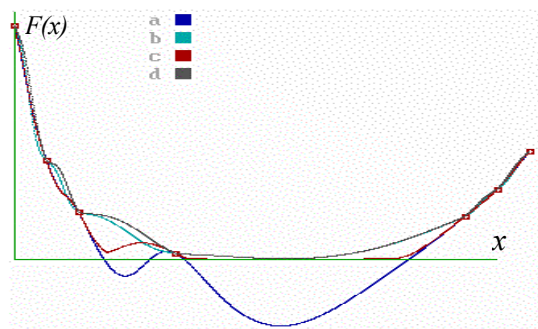

Figure 2. Graph of Data in Table 1 using (a) Original MQS (b) Simple truncation (c) Scaled Basis function (d) Current

x	0	2	4	10	28	30	32
F	20.8	8.8	4.2	.5	3.9	6.2	9.6

Table 1. Oxygen levels in flue gases

The algorithm will scale only a part of the basis functions, which go negative, in the region of participation. Consequently the dependency of the graph on scaling will reduce and the resultant graph is a comparatively closer approximation of the MQS graph. The 1D graph using this scheme is shown in Figure 2(d) and the 2D one is shown in Figure 5.
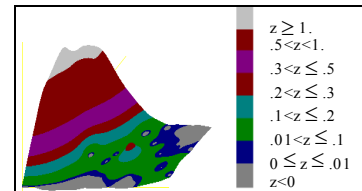

Figure 3. Loss of positivity by surface due to Modified Quadratic Shepard method.
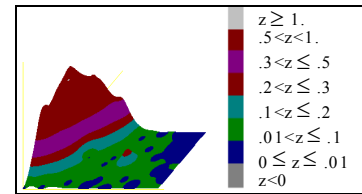

Figure 4. Positive Modified Quadratic Shepard using the algorithm in Asim[Asi00].
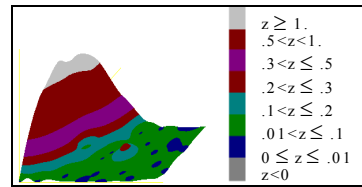

Figure 5. Improved Positive Modified Quadratic Shepard surface.

4. RESULTS AND DISCUSSION

In this section we discuss the results included in this paper and compare the performance of this method with the earlier work by Asim [Asi00]. Data with too many zeroes for surfaces is taken from Asim[Asi00].

The peaks in the surface of Figure 4, adversely affect the visual appearance of the surface. However, poor visual appearance can be disputed being subjective. We think it is due to unnecessary scaling of Hessian matrix that scales the whole basis function. Infact, scaling of the basis function is unavoidable in and close neighborhood of the region where the basis function goes negative and it is avoidable in rest of the region. Otherwise the basis function departs too much from its original shape and hence from its characteristics due to least square fit. We have developed this scheme to reduce the adverse effect of this scaling so that the peaks in Figure 4 disappear.

We have achieved this as shown in Figure 5. However, in this scheme, continuity reduces to G^1.

Since this scheme finds its origin in the constrained MQS suggested in Asim[Asi00], it is also extendible to n-dimensions. Likewise, the scheme can be easily applied to constrain a graph by arbitrary upper and lower bounds.

The cost of the new algorithm is relatively high and depends on the number of basis functions that require scaling. For ideal case, where no basis function requires scaling, extra cost is negligible. All the surfaces given in this paper are drawn using 1190 x 590 sampling positions. Average time taken for the surface Figure 3 using MQS method is 16.68 second. For similar implementation, time taken by new method, to plot Figure 5, is 17.63 seconds. The machine used is PII 350. As such there is an increase of about 6% in execution time.

5. CONCLUSIONS AND FUTURE WORK

We have presented a constrained Modified Quadratic Shepard scheme, which is different from the one presented in Asim [Asi00]. We observed that:

1. We have departed from the least square fit.

2. Continuity of the graph is G^1 as compared to C^1 in Modified Quadratic Shepard method. The graph does not preserve gradient.

Regarding future work, following possibilities are worth mentioning:

a) We are looking forward to incorporate the possible improvements so as to make it a C^1 and gradient preserving at the least for non-zero reference values through dynamic scaling.

b) We are also looking forward to incorporate the possible improvements so as to make it a C^1 and gradient preserving at the least for non-zero reference points. We achieve this by deforming:

All negative concave basis functions into elliptical hats with zero gradients at and beyond the boundary where original basis function is non-positive.

All saddle basis functions into the saddles with partly flat lower wings. Such that their gradients are zero on and beyond the boundary where original basis function is non-positive.

All negative convex basis functions into elliptical bowls. This scheme will give flat-based elliptical bowls for zero value reference points with zero gradients at and within boundary where original basis function is non-positive.

c) We are looking forward to address the problem of negativity that may arise while dealing with sparse data in the MQS method.

d) We are exploring the possibility of achieving positivity by partial scaling of Hessian matrix.

6. ACKNOWLEDGEMENT

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