Journal of Scientific Research
Vol. XXXIX No. 2, December, 2009
ISSN 0555-7674

POSITIVE MODIFIED QUADRATIC SHEPARD LEAST-SQUARE-FIT CURVES

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Abstract: In this paper, we constrain the Modified Quadratic Shepard interpolant to preserve positivity in one-dimensional interpolation such that the constrained interpolant also retains the least-squares fit to data. We preserved positivity by obtaining control over the extremum point of the basis functions of the Modified Quadratic Shepard interpolant. The constraining process destroyed the least-squares fitting character of the Modified Quadratic Shepard method. We insert an extra knot to convert each basis function into a spline and use the resultant freedom to make the provision for least-squares fit. Since each basis function is a positive spline which interpolates its respective data point being the least-square fit to other, the consequent Modified Quadratic Shepard interpolant is positive as well as a least-squares fit.

KEYWORDS: Constrained curve, positivity, least-square fit, interpolant, Shepard curve.

1. Introduction

Generally in computer graphics and particularly in CAD (Computer Aided Design) and / or CAGD (Computer Aided Geometric Design) environments a user is usually in need of visualizing scientific data, through a curve representation, that possesses certain shape characteristics inherent in data. As such the preservation of shapes, inherent in the data, by the interpolants has always been an important matter. Positivity is one such shape. The significance of Positivity lies in the fact that sometimes it does not make any sense to talk of some of the quantities to be negative, for example a negative amount of a particular bacteria in a specimen tissue from a human body or the probability of a rainfall or a snowfall in a given area has no meaning if negative.

In this paper we focus on one-dimensional interpolation, constructing a curve through a set of positive data. The work contained in this paper also includes work in Asim [2]. The earlier work related to shape preservation can be found in Hussain M.Z., Ayuab N. & Irshad M. [7] and the papers mentioned therein. The Hussain M.Z. and Sarfraz M. [6], starts with a positive rational cubic curve through 1D positive data and it also extends it to an economical positive rational bicubic for a 2D data arranged over a rectangular grid. A C^1 curve interpolation scheme is discussed in Hussain M.Z., Hussain M and Shamaila [8]. Their scheme is also flexible due to the provision of a free parameter.

However, piecewise cubic approach does not extend so easily to higher dimensions when the data is scattered and is G^1 continuous only. Consequently we developed a method Asim and Brodlie 2000 [1] which is C^1 and cheaper than the original modified Shepard interpolant but loses least-square fit to data. This idea has already been extended to 2D and surface through scattered data is constructed Asim and Nadeem [3]. However this paper too has a drawback

1-For Proof and Correspondence: **Muhamad Rafiq Asim**

of loss of least-squares fit. The loss of least-squares fit property affects the visual appearance some what adversely (see Figure 1). Also the least-squares fit property is the key characteristic of the modified quadratic Shepard interpolant. So the development of constrained modified Shepard interpolant which retains both C^1 continuity and least-square fit properties, and is also extendible to higher dimensions easily is justified. The slope preserving 1D positive method Asim and Sajid L. R. 2007 [4] is an other version of the series of quadratic Shepard interpolants starting with Asim and Brodlie [1].

The Shepard family of interpolants is a famous approach Shepard [11]. The Shepard interpolants are a distance-weighted average of basis functions defined for each data point. Each basis function interpolated its respective data point and is the best weighted least-square fit to others. The modified quadratic Shepard interpolant, with basis functions that are quadratic, is the most popular version in this family (Nielson 1993). The Shepard methods have C^1 continuity Lancaster and Salkauskas [9] and are applicable to a space of any dimension for data of any distribution. However, to their disadvantage they do not preserve any of the local shapes implied by the data Nielson [5]. Recent work on Shepard methods have focused on reducing the computational cost by limiting the least-squares fitting process to a local subset of the data.

Shepard method is widely used for 2D and 3D data, but is equally applicable to a curve interpolation technique. In this paper we show how it can be constrained so as to generate positive 1D interpolants from positive data without losing its least-square fit property.

In section 1 we develop a constrained interpolant that retains the least-squares fit characteristic. Each quadratic basis function is replaced by a spline which is not only a least-squares fit to positive data but also positive over the interpolation interval. This provides us with the Shepard interpolant which itself is not only a least-squares fit to positive data but also positive. The boundedness of the interpolant developed by us in this paper is discussed in section 2. Section 3 elaborates conclusion and future research.

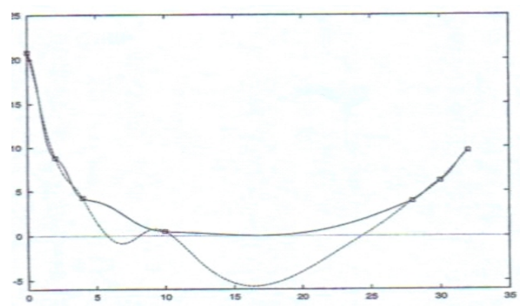

Figure 1: Preservation of positivity by constrained quadratic Shepard method lacking least square fit.

2. Constrained Least-Squares Fit for Curve Drawing

Let $(x_1, f_1), (x_2, f_2), \ldots, (x_N, f_N)$ be given data points, where the f-values are samples of some functions f(x) which is non-negative for every $x \in [x_1, x_N]$ and $x_1 < x_2 < . \quad . \quad . < x_N$.

The modified quadratic Shepard curve $F(x)$ is defined as

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

where the weight function and the basis function $Q_i(x) = f_i + b_i(x - x_i) + a_i(x - x_i)^2$ is related to data point (x_i, f_i). By definition $Q_i(x_i) = f_i$ and the coefficients a_i an b_i are chosen so that Q_i is a best distance-weighted least-squares approximation to the other data points.

In Asim and Brodlie [1], the quadratic basis functions Q_i, were fully defined by three conditions, namely

- Interpolation at $x = x_i$,
- value fixed at $x = x_s$ equal to zero for convex and y_c for concave.
- derivative at $x = x_s$, equal to zero.

So the least-squares approximation was lost. In order to retain the condition of best least-squares approximation to other data points, we need to relax the stipulation that the basis function be a quadratic. Somewhat similar to the idea of Schumaker [10] we use instead a quadratic spline, with a single knot, to give us the extra flexibility in a convex case. For a concave case too, we construct a quadratic spline using freedom in the choice of the y-coordinate of the maximum point to give the flexibility. The two cases are discussed separately.

Convex Case

Suppose first that $x_i < x_s$, so the interpolation point lies to the left of the minimum of the original basis function. We shall define a quadratic spline, $Q_i(x)$, with quadratic pieces S_1 and S_2 joined at a knot (x_{knot}, f_{knot}) where x_{knot} is the mid-point of $[x_i, x_s]$. The value f_{knot} of the spline at x_{knot} gives the extra degree of freedom required. However, to ensure positivity, it is necessary to include a constraint that the spline is convex.

More precisely, the constrained basis function is a quadratic spline,

$$Q_i(x) = \begin{cases} S_1(x) & \text{if } x1 \le x < x_{knot} \\ S_2(x) & \text{if } x_{knot} \le x \le x_N \end{cases} \qquad (2)$$

Where (omitting subscript i for simplicity of notation)

$$S_1(x) = f_{knot} + b_{knot}(x - x_{knot}) + a_{knot}(x - x_{knot})^2 \qquad (3)$$

and

$$S_2(x) = a_s(x - x_s)^2 \qquad (4)$$

The definition of S_2 ensures that the spline has zero value and derivative at $x = x_s$. For interpolation at $x = x_i$ we require:

$$S_1(x_i) = f_i \qquad (5)$$

while for C^1 continuity of the spline we require

$$S_1(x_{knot}) = S_2(x_{knot}), \qquad (6)$$

$$S'_1(x_{knot}) = S'_2(x_{knot}). \qquad (7)$$

Finally to ensure convexity, and hence positivity, we require $a_s > 0$ and $a_{knot} > 0$. The equation (6) and (7) respectively give us

$f_{knot} = a_s(x_{knot} - x_s)^2$ and

$b_{knot} = 2a_s(x_{knot} - x_s)$.

Hence from (3),

$$S_1(x) = a_s(x_{knot} - x_s)^2 + 2a_s(x_{knot} - x_s)(x - x_{knot}) + a_{knot}(x - x_{knot})^2. \qquad (8)$$

Then, from the interpolation condition (5), we have:

$$f_i = a_s(x_{knot} - x_s)^2 + 2a_s(x_{knot} - x_s)(x_i - x_{knot}) + a_{knot}(x_i - x_{knot})^2$$

$$f_i = a_s h^2 + 2a_s h^2 + a_{knot} h^2$$

$$f_i = (3a_s + a_{knot})h^2$$

where $h = x_{knot} - x_i$.

Hence

$$a_{knot} = \frac{f_i}{h^2} - 3a_s. \qquad (9)$$

Thus, the quadratics $S_1(x)$ and $S_2(x)$ of the spline can be rewritten in terms of a_s as:

$$S_1(x) = a_{knot}(x - x_{knot})^2 - 2a_s h(x - x_{knot}) + a_s h^2 \qquad (10)$$

With a_{knot} as defined in (9) and

$$S_2(x) = a_s(x - x_s)^2. \qquad (11)$$

We now have to chose the optimum value of a_s such that $Q_i(x)$ is the best weighted least-squares fit to the other data points, with the restriction that $Q_i(x)$ be convex. Thus we need to minimize:

$$\sum_{x_k \ne x_i} \omega_i(x_k)[Q_i(x_k) - f_k]^2 \qquad (12)$$

subject to the conditions $a_s > 0$ and $a_{knot} > 0$ where the weight function $\omega_i(x) = \frac{1}{(x - x_i)^2}$, From (10) and (11) we need to minimize:

$$P(a_s) = \sum_{x_k < x_{knot}, x_k \ne x_i} \omega_i(x_k)[S_1(x_k) - f_k]^2 + \sum_{x_k > x_{knot}} \omega_i(x_k)[S_2(x_k) - f_k]^2 \qquad (13)$$

or

$$P(a_s) = \sum_{x_k < x_{knot}, x_k \neq x_i} \omega_i(x_k)[a_{knot}$$

$$(x_k - x_{knot})^2 - 2a_s h(x_k - x_{knot}) + a_s h^2 - f_k]^2$$

$$+ \sum_{x_k > x_{,knot}} \omega_i(x_k)[a_s(x_k - x_s)^2 - f_k]^2.$$

Rewriting in terms of a_s

$$P(a_s) = \sum_{x_k \neq x_i} \omega_i(x_k)[\alpha_k a_s - \beta_k]^2 \tag{14}$$

where for $x_k < x_{knot}$

$$\alpha_k = -3(x_k - x_{knot}) - 2h(x_k - x_{knot}) + h^2, \tag{15}$$

$$\beta_k = f_k - \frac{1}{h^2} f_i (x_k - x_{knot})^2 \tag{16}$$

and $x_k > x_{knot}$

$$\alpha_k = (x_k - x_s)^2, \tag{17}$$

$$\beta_k = f_k. \tag{18}$$

Differentiating (14) with respect to a_s:

$$P'(a_s) = 2\sum_{x_k \neq x_i} \omega_i(x_k)[\alpha_k a_s - \beta_k]\alpha_k \tag{19}$$

or

$$P'(a_s) = 2a_s \sum_{x_k \neq x_i} \omega_i(x_k)\alpha_k^2 - 2\sum_{x_k \neq x_i} \omega_i(x_k)\alpha_k \beta_k. \tag{20}$$

Hence minimum is achieved for

$$a_s = \frac{\sum_{x_k \neq x_i} \omega_i(x_k)\alpha_k \beta_k}{\sum_{x_k \neq x_i} \omega_i(x_k)\alpha_k^2}. \tag{21}$$

with α_k, β_k given by (15), (16), (17) and (18).

If $a_s < 0$, then we set $a_s = 0$ in which case $a_{knot} > 0$ from (9).

If $a_s > 0$, then again from (9), $a_{knot} = \frac{1}{h^2} f_i - 3a_s$ which is positive provided $a_s \geq \frac{f_i}{3h^2}$ *so we constrain* $a_s = \frac{f_i}{3h^2}$ *as a maximum value. In conclusion, we calculate as according to (21),* $[0, \frac{f_i}{3h^2}]$ *but restrict its value to the interval.* Because we want to retain convexity of the basis function while constraining it to be positive.

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

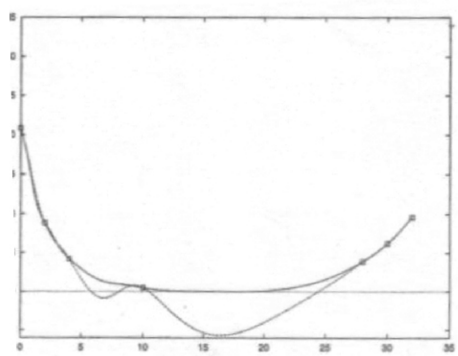

Table1: Oxygen levels in flue gas.

Figure 2: Preservation of positivity by quadratic Shepard method due to constrained least-square fit for data in Table 1.

if $x_i > x_s$, that is when minimum is on the left side of the data point, we proceed in the same way as we did in case $x_i < x_s$ except that:

- quadratics S_1 and S_2 swap their domains of definition.
- $x_{knot} \in [x_s, x_i]$.

The graph (corresponding to the data in Table 1) thus obtained is in Figure 2 whose visual appearance is much better than the one in Figure 1. The noisy behavior of the data has been tackled successfully but at a cost higher than that of the original modified quadratic Shepard method. The discussion so far has dealt with the convex case. Now let us consider the concave case.

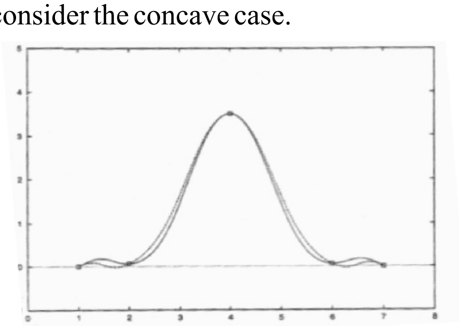

Figure 3: Preservation of positivity by quadratic Shepard method due to constrained least-square fit for data in Table 2.

Concave Case

In the case where $Q_i(x)$ is concave Asim and Brodlie [1], the focus changes from raising the minimum value to zero, to raising the value at one or both end-points to zero. The addition of a least-squares fitting condition again requires extra flexibility, which we get by using a quadratic spline with one knot. In fact this case is slightly simpler because we can place the knot at x_s (we could not do this in convex case because the value at x_s was fixed, and therefore placing a knot there did not provide the extra flexibility required).

x	1	2	4	6	7
y	0	0.06	3.5	0.06	0

Table 2: Data that provides concave basis function.

Suppose $x_i < x_s$, and suppose the original basis function is negative at x_N. We create a constrained basis function which is a quadratic spline, with S_1 interpolating (x_i, f_i) and S_2 interpolating $(x_N, 0)$. This gives us:

$$Q_i(x) = \begin{cases} S_1(x) & if \quad x_1 \le x < x_s \\ S_2(x) & if \quad x_s \le x \le x_N \end{cases} \tag{22}$$

such that

$$S_1(x) = y_s + \frac{f_i - y_s}{(x_i - x_s)^2}(x - x_s)^2 \tag{23}$$

$$S_2(x) = y_s - \frac{y_s}{(x_N - x_s)^2}(x - x_s)^2 \tag{24}$$

with freedom to vary y_s to provide best least-square fit. We need to minimize:

$$\sum_{x_k \ne x_i} \omega_i(x_k)[Q_i(x_k) - f_k]^2 \tag{25}$$

subject to $Q_i(x_1) \geq 0$. That is we need to minimize

$$P(y_s) = \sum_{x_k < x_s, x_k \ne x_i} \omega_i(x_k)[S_1(x_k) - f_k]^2 + \sum_{x_k > x_s} \omega_i(x_k)[S_2(x_k) - f_k]^2 \tag{26}$$

or

$$P(y_s) = \sum_{x_k \ne x_i} \omega_i(x_k)[\alpha_k y_s - \beta_k]^2 \tag{27}$$

where for $x_k < x_s$

$$\alpha_k = 1 - \frac{(x_k - x_s)^2}{(x_i - x_s)^2},$$

$$\beta_k = f_k - f_i \frac{(x_k - x_s)^2}{(x_i - x_s)^2}$$

and for $x_k > x_s$

$$\alpha_k = 1 - \frac{(x_k - x_s)^2}{(x_N - x_s)^2},$$

$$\beta_k = f_k.$$

Then as in (21), the minimum is achieved when:

$$y_s = \frac{\sum_{x_k \ne x_i} \omega_i(x_k)\alpha_k \beta_k}{\sum_{x_k \ne x_i} \omega_i(x_k)\alpha_k^2}. \tag{28}$$

This value of y_s when put in to (23) and (24) gives a quadratic spline which interpolates $(x_N, 0)$ and (x_i, f_i), and is a best least-squares fit to the other data points. To guarantee that S_1 and S_2 are both concave we restrict $y_s > f_i$. In addition we need $Q_i(x_i) > 0$ which requires: $S_1(x_1) > 0$.

That is

$$y_s + \frac{f_i - y_s}{(x_i - x_s)^2}(x_1 - x_s)^2 > 0,$$

or

$$y_s\left(1 - \frac{(x_1 - x_s)^2}{(x_i - x_s)^2} + \frac{f_i(x_1 - x_s)^2}{(x_i - x_s)^2}\right) > 0$$

which after re-arrangement gives

$$y_s < \frac{f_i(x_1 - x_s)^2}{(x_1 - x_s)^2 - (x_i - x_s)^2} >= \theta \quad f_i.$$

Since $(x_1 - x_s)^2 > (x_i - x_s)^2$, $\theta > 1$. In other

Words finally we need to restrict y_s by $y_s \in [f_i, \theta\ f_i]$.
Similar discussion follows for the case $x_i > x_s$, where the original basis function is negative at x_1.
Finally, consider the case $(x_i, f_i) = (x_s, y_s)$, that is both the data point and the maximum coincide with each other. Since y_s in this case cannot be changed, the only freedom available is that of a change in curvature. We avail this freedom to fit a spline

$$Q_i(x) = \begin{cases} S_1(x) & if\ x_1 \le x < x_s \\ S_2(x) & if\ x_s \le x \le x_N \end{cases} \quad (29)$$

such that $S_1(x) = f_i + a_1(x - x_s)^2$, (30)

With $a_1 \ge -\dfrac{f_i}{(x_1 - x_s)^2}$ and

$$S_2(x) = f_i + a_N(x - x_s)^2, \quad (31)$$

With $a_N \ge -\dfrac{f_i}{(x_N - x_s)^2}$. It may be mentioned here that if x_1 and x_N are equidistant from x_s, then only one quadratic covers both sides. For x_s in a close neighbourhood of x_i, we take $x_s = x_i$ and proceed as above. The graph thus obtained is shown in Figure 3. We may observe that the visual appearance of the curve due to the original constrained Shepard interpolant has been maintained by the one drawn by the constrained least-square fit Shepard interpolant in Figure 3. We may mention that we carried out a lot of experimentation and figures given here are only a specimen of the results obtained.

3 Extension of Constrained Least-square Fit to a Linear Constraint

The idea of positive least-square fit based interpolation is extendible to the more general constraint so as to keep the interpolant greater than some linear function of the independent variable. For this we need to reframe the above problem as follows.

Consider data points $(x_1, f_1), (x_2, f_2), \ldots, (x_N, f_N)$, and the linear function given by $y = mx + c$ with
$x_1 < x_2 < \cdots x_N$ and $f_i \ge mx_i + c\ \forall\ i$.
to seek a basis quadratic $Q_i(x)$ such that
$Q_i(x_i) = f_i$ and $Q_i(x) \ge mx + c\ \forall\ x \in [x_1, x_N]$.
We construct a basis quadratic $L_i(x)$ such that

$$L_i(x) = Q_i(x) - mx - c$$

or

$$L_i(x) = a_i(x - x_i)^2 + (b_i - m)(x - x_i) - mx_i - c + f_i$$

or

$$L_i(x) = a_i(x - x_i)^2 + (b_i - m)(x - x_i) + g_i$$

For

$g_i = f_i - mx_i - c$, with

$L_i(x_i) = f_i - mx_i - c$ and $L_i(x) \ge 0\ \forall\ x \in [x_1, x_N]$.
It transforms the problem to that of preservation of positivity while retaining the least-squares fit. As such the technique laid down for the constrained Modified Quadratic Shepard method to be a least-square fit in section 4 is now applicable to L_i. This discussion has just covered the curve bounded below, and the similar argument works for the one bounded above.

We are confident that the same applies to the boundedness by a higher degree curve such as quadratic as well.

4 Conclusion

This paper shows how the modified quadratic Shepards method can be extended in order to provide a constrained least-square fit to a 1D data. As mentioned in section 3 constraint can be any linear or non-linear function. But we have restricted the practical implementation to the extensively used special case of positive interpolant through positive data. The flexibility required for the least-squares fit is provided by inserting a knot. The essential idea is to ensure that each individual quadratic basis function is obtained by the constrained least-squares fit to the data. This in turn gives rise to a constrained interpolant which is the least-square fit to the data as a whole.

The further work in the area is to obtain the least-squares fit based constrained modified quadratic Shepards interpolant in higher dimensions. Also there is an interest in looking at the similar work in the areas of monotonicity and convexity.

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