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## A DATA-BOUNDED QUADRATIC INTERPOLANT ON TRIANGLES AND TETRAHEDRA.

## M. $\mathrm{BERZ\,INS}^*$

**Abstract.** Many real world problems are successfully modelled by partial differential equations. Many numerical solvers for these problems use triangular and tetrahedral meshes to accurately model complex geometries. Such problems often involve shocks and discontinuities and it is important to devise interpolation methods that can accurately approximate solutions containing such features. These interpolants are required for the post-processing of the solution e.g. for visualization and to recover solution values at arbitrary points over the numerical domain. This paper describes a triangle-based quadratic interpolant that is "data bounded" and so will not create any values outside of the range of the existing data points. The method is compared with the standard quadratic interpolant and extended to the case of quadratic tetrahedral elements.

Key words. Interpolation, Triangles, Tetrahedra, Quadratic Elements.

AMS subject classifications. 65M20, 65M15

1. Introduction. In scientific computing, the visualization of the solution to real-world problems is an essential aid to the understanding of the physical problem being modelled. Interpolation schemes that will respect the physical properties of the underlying data are thus needed, one example being to preserve positivity. Many data sets that require such interpolants result from the numerical solution of partial differential equations (PDEs). Many of the methods used to solve such p.d.e. problems compute solutions on rectangular or hexahedral meshes. A good survey of a number of interpolants for such meshes which are appropriate for scientific visualization in that they provide values that are bounded by the data values "data-bounded" and possibly preserve the shape of data values is given by Brodlie and Mashwama [6]. These interpolants are piecewise linear bilinear and tri-linear and are piecewise cubic and bi-cubic. One such interpolant is a bounded bi-cubic interpolant on a rectangular mesh, [6].

In two and three spatial dimensions a number of general purpose PDE solvers employ triangular and tetrahedral elements in conjunction with triangular and tetrahedral mesh generators to solve problems defined on complex domains. The best example of this being the finite element method [12]. Alternatively, number of authors use a cell-centered or cell-vertex finite volume spatial discretization schemes to solve convection-dominated PDEs, see [5] [7] and [11] for details. An important feature of these problems is that initial smooth conditions may develop into steep gradients or even shocks and discontinuities.

Standard quadratic interpolation techniques [8], [12] can be used to fit six shape functions over each triangle to give an approximation to the surface. Section 2 below and the paper of [10] both show that this method can easily produce interpolated values outside the physical range of the data values. Similar problems arise with the standard quadratic interpolant for tetrahedra, [12].

There have been many methods which have attempted to overcome some of the problems associated with such interpolants. Some of the earliest work is that of Barnhill et al. [2] [3]. This work will be described in outline form and used as a starting point for the new triangular interpolant developed here. Two other important interpolation methods in this area are those of Abgrall [1] and Barth [4]. Both these

<sup>\*</sup> School of Computer Studies, The University of Leeds, Leeds LS2 9JT, U.K.

schemes have the common approach of using adaptive multi-triangle stencils to achieve high order accuracy for problems which may have shocks and discontinuities. The problem is that the number of possible combinations grows rapidly, the stencil used is potentially large, and the points considered may be some distance from the original node. Abgrall's good results provide a more than adequate justification of the scheme however.

A recent paper by Pratt and Berzins, [10], showed that by adopting a relatively simple approach which involved sacrificing accuracy at the mid-points of edges it was possible to achieve positivity for problems with steep gradients. The aim here is to overcome this deficiency and to consider a simpler alternative to Abgrall's scheme. This will be done by decomposing a standard quadratic interpolant into a combination of four one-dimensional quadratics. Replacing each of these one dimensional interpolants by ones which preserve data boundedness, possibly by replacing one quadratic by two piecewise quadratics, enables a new data-bounded interpolant to be devised. This interpolant is bounded by the minimum and maximum data values defining it and so may therefore be utilised to preserve positivity. It can also be used for the visualization of the solution and by the numerical solver to recover values over the numerical domain. A novel feature of the new scheme is that the method is local to each triangle or tetrahedral element. The price that is paid for this is that when the interpolant is modified to preserve data-boundedness the resulting piecewise polynomial is only  $C^0$  continuous rather than  $C^1$  continuous.

The extension of the approach to tetrahedra proves to be straightforward by using a combination of positivity preserving one dimensional and triangular interpolants.

2. The Standard Quadratic Triangular Interpolation Scheme. A 2D quadratic triangular interpolant of an unknown function u(x, y) needs six data points: these points are usually at the vertices of the triangle and the mid-points of the sides, [12]. These can be mapped to area coordinates  $(L_1, L_2, L_3)$ . Six shape functions can be fitted to these points such that each is unity at one point and zero at the others. These shape functions are shown in equation (1).

(1)  

$$\begin{aligned}
\phi_1 &= (2L_1 - 1)L_1, & \phi_2 &= (2L_2 - 1)L_2 \\
\phi_3 &= (2L_3 - 1)L_3, & \phi_4 &= 4L_2L_1 \\
\phi_5 &= 4L_3L_2, & \phi_6 &= 4L_1L_3
\end{aligned}$$

The area co-ordinates of points,  $(L_1, L_2, L_3)$ , 1 to 6 being (1, 0, 0), (0, 1, 0), (0, 0, 1),  $(\frac{1}{2}, \frac{1}{2}, 0)$ ,  $(0, \frac{1}{2}, \frac{1}{2})$  and  $(\frac{1}{2}, 0, \frac{1}{2})$  respectively. The interpolated value  $U_I$  is then defined by

(2) 
$$U_I(L_1, L_2, L_3) = \sum_{i=1}^6 \phi_i(L_1, L_2, L_3) U_i$$

The position of the points  $U_i$  is shown in Figure 1.  $U_i$ , i = 1, 2, 3 being the points at which the corresponding  $L_i = 1$ .

The problem with the standard interpolation formula is that the shape functions associated with the three vertex values are negative over large parts of the triangle. Thus it is possible that new and unphysical extrema may be introduced, [10]. Consider for example the centroid of the triangle marked as  $U_7$  in Figure 1.In the case when standard quadratic interpolation based on the values  $U_i$ , i = 1, 6 is used then



FIG. 1. Example Triangle.

(3) 
$$U_7 = U(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) = \frac{4}{9}(U_4 + U_5 + U_6) - \frac{1}{9}(U_1 + U_2 + U_3)$$

Hence if all the values  $U_i$ , i = 1, 6 are positive but the values  $U_1, U_2$  and  $U_3$  are in some sense large compared to  $U_4, U_5$  and  $U_6$  then  $U_7$  may be negative. More generally, possible extrema of the standard quadratic interpolant polynomial  $U_I$  defined by equation (2) lie at the points at which (after replacing  $L_3$  with  $1 - L_1 - L_2$ )  $\frac{\partial U}{\partial L_1} = 0$ and  $\frac{\partial U}{\partial L_2} = 0$ . Differentiating  $U_I$  and collecting terms together gives a pair of equations for  $L_1, L_2$ , the critical points:

$$4L_1(U_1 + U_3 - 2U_6) + 4L_2(U_3 + U_4 - U_5 - U_6) = (U_1 + 3U_3 - 4U_6),$$
  

$$4L_1(U_3 + U_4 - U_5 - U_6) + 4L_2(U_3 + U_2 - 2U_5) = (U_2 + 3U_3 - 4U_5).$$

The standard multivariable calculus test for determining extrema is that D < 0 where  $D = \left(\frac{\partial^2 U_I}{\partial x^2 y} - \frac{\partial^2 U_I}{\partial x^2} \frac{\partial^2 U_I}{\partial y^2}\right)$ . The case when D > 0 defines saddle points or if D = 0 the test fails and there may be no maximum or minimum or a line of critical points. A lengthy but straightforward derivation shows that D has the same sign as -Det where Det is the determinant of the preceeding pair of equations.

Although this test provides useful help in understanding why the standard interpolant may not be data-bounded it does not directly help to construct a data-bounded interpolant. It is this problem, that of constructing a data-bounded quadratic interpolant that will be addressed in Sections 4 and 5 below. This will be achieved by showing that the original polynomial may be interpreted as a combination of onedimensional quadratics. A geometrical outline of the approach is indicated by Figure 1 which indicates how a point on the line A B C is defined in terms of quadratics using  $U_2, U_4$  and  $U_1$  to define a value at A,  $U_3, U_7$  and  $U_1$  to define a value at B and using  $U_3, U_6$  and  $U_1$  to define a value at C. A further quadratic interpolation using A,B,C then defines points on that line. The problems are thus reduced to that of finding data-bounded quadratic polynomials in one space dimension and of finding a suitable centroid value.

3. Two Data-Bounded Piecewise Quadratic Polynomials . In this section two data-bounded one-dimensional piecewise quadratic polynomials are devised. These polynomials will play an important role in the triangular interpolant in Section 4 and in the tetrahedral interpolant in Section 8. The approach taken to ensure data boundedness will be, when necessary, to decompose the original quadratic polynomial into two piecewise polynomial quadratics.

**3.1.** Polynomial  $P_1$ . Consider the case of the standard one dimensional quadratic interpolant for the function u(x) defined on the interval [0, h] mapped onto [0, 1] with data points at  $0, \frac{1}{2}$  and 1 given by  $U_0, U_{\frac{1}{2}}$  and  $U_1$ . Let this polynomial be defined by

(4) 
$$q_1(U_0, U_{\frac{1}{2}}, U_1, L_1) = U_0 \hat{\phi}_1 + U_{\frac{1}{2}} \hat{\phi}_2 + U_1 \hat{\phi}_3,$$

where

$$\hat{\phi}_1 = (1 - L_1)(1 - 2L_1), \quad \hat{\phi}_2 = 4L_1(1 - L_1), \quad \hat{\phi}_3 = L_1(2L_1 - 1)$$

and  $L_1 + L_2 = 1$ . Differentiating with respect to  $L_1$  gives

(5) 
$$\frac{dq_1}{dL_1} = 0 \text{ at } L_1 = \frac{1}{2} + r \text{ where } r = \frac{U_1 - U_0}{4(2U_{\frac{1}{2}} - U_1 - U_0)}$$

and differentiating again with respect to  $L_1$  gives

(6) 
$$\frac{d^2q_1}{dL_1^2} = 4(-2U_{\frac{1}{2}} + U_1 + U_0),$$

which is also a second order difference approximation to  $h^2 \frac{d^2 u}{dx^2}(\frac{1}{2})$ . This result shows that the polynomial may have extrema at non-nodal points. If the second derivative is zero then as q is linear and hence takes its extrema at the ends of the interval.

In order to get a data bounded interpolant for which any extrema lie at data points, the key observation in modifying the polynomial is that on the interval  $[0, \frac{1}{2}]$ a completely different value of  $U_1$  may be used from the original. Similarly, on the interval  $[\frac{1}{2}, 1]$  a completely different value of  $U_0$  from the original may be used without destroying  $C^0$  but not  $C^1$  continuity of the solution. Thus the original polynomial is replaced by two piecewise quadratic polynomials.

Let these new values of  $U_0$  and  $U_1$  be denoted by  $U_0^*$  and  $U_1^*$  respectively. The new piecewise polynomial is then defined by

(7) 
$$p_1(U_0, U_{\frac{1}{2}}, U_1, L_1) = U_0 \hat{\phi}_1 + U_{\frac{1}{2}} \hat{\phi}_2 + U_1^* \hat{\phi}_3 , \quad 0 \le L_1 \le \frac{1}{2}$$

(8) 
$$= U_0^* \hat{\phi}_1 + U_{\frac{1}{2}} \hat{\phi}_2 + U_1 \hat{\phi}_3 , \quad \frac{1}{2} < L_1 \le 1$$

These new values of  $U_0^*$  and  $U_1^*$  will be defined by moving extrema to the closest nodal point, denoted by  $L_{ext}^{new}$ , by using equation (5). In the case when  $r \leq -\frac{1}{2}$  or  $r \geq \frac{1}{2}$  then  $U_0^* = U_0$  and  $U_1^* = U_1$  and the original polynomial is unchanged

(9) 
$$L_{ext}^{new} = 0, \quad -\frac{1}{2} < r \le -\frac{1}{4}, \quad U_1^* = 4U_{\frac{1}{2}} - 3U_0,$$

(10) 
$$L_{ext}^{new} = \frac{1}{2}, \quad -\frac{1}{4} < r \le 0, \quad U_1^* = U_0$$

(11) 
$$L_{ext}^{new} = \frac{1}{2}, \qquad 0 < r \le \frac{1}{4}, \qquad U_0^* = U_1,$$

(12) 
$$L_{ext}^{new} = 1, \quad \frac{1}{4} < r \le \frac{1}{2}, \quad U_0^* = 4U_{\frac{1}{2}} - 3U_1.$$

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In all the above four cases  $U_1 - U_1^*$  and  $U_0 - U_0^*$  may be rewritten in a more convenient form as

$$(13) L_{ext}^{new} = 0, \quad U_1^* - U_1 = 4U_{\frac{1}{2}} - 3U_0 - U_1 = \frac{(1+2r)}{2} 4 (2U_{\frac{1}{2}} - U_0 - U_1),$$

$$(14) L_{ext}^{new} = \frac{1}{2}, \quad U_1^* - U_1 = U_0 - U_1 = -r \quad 4 (2U_{\frac{1}{2}} - U_0 - U_1),$$

$$(15) L_{ext}^{half} = \frac{1}{2}, \quad U_0^* - U_0 = U_1 - U_0 = r \quad 4 (2U_{\frac{1}{2}} - U_0 - U_1),$$

$$(16) L_{ext}^{new} = 1, \quad U_0^* - U_0 = 4U_{\frac{1}{2}} - 3U_1 - U_0 = \frac{(1-2r)}{2} 4 (2U_{\frac{1}{2}} - U_0 - U_1)$$

From the last four equations and equation (6)

(17) 
$$U_1 - U_1^* = \alpha(r) \frac{d^2 q_1}{dL_1^2} \text{ where } -1/2 \le r \le 0,$$

(18) 
$$U_0 - U_0^* = \alpha(r) \frac{d^2 q_1}{dL_1^2}$$
 where  $0 \le r \le 1/2$ 

and where  $0 \le \alpha(r) \le 1/4$  is the piecewise linear function defined as in equations (13) to (16). Thus the algorithm adds a nonlinear multiple of the second derivative in order to get a data-bounded interpolant. The extra term introduced by this approach is given by

(19) 
$$q_1(...,L_1) - p_1(...,L_1) = (U_1^* - U_1)\hat{\phi}_3, \quad 0 \le L_1 \le \frac{1}{2},$$

(20) 
$$= (U_0^* - U_0)\hat{\phi}_1, \quad \frac{1}{2} < L_1 \le 1.$$

As a consequence of this, the error as defined on  $[\frac{1}{2}, 1]$  is no longer defined by the standard form on, [h/2, h], given by

(21) 
$$u(x) - q_1(U_0, U_{\frac{1}{2}}, U_1, L_1) = x(x - h/2)(x - h) \frac{1}{6} \frac{d^3 u}{dx^3}(\xi_1), \quad \xi_1 \in [0, h]$$

where u(x) is defined at the start of this section, but by

(22)  
$$u(x) - p_1(U_0, U_{\frac{1}{2}}, U_1, L_1) = x(x - h/2)(x - h) \frac{1}{6} \frac{d^3 u}{dx^3}(\xi_1) - \frac{2}{h^2} (U_0^* - U_0)(x - h/2)(x - h).$$

Substituting from equations (15) and (16) for  $U_0^* - U_0$  gives

(23) 
$$(x - h/2)(x - h) \left[ 4 \alpha(r) \frac{4(-2U_{\frac{1}{2}} + U_0 + U_1)}{2 h^2} + \frac{x}{6} \frac{d^3 u}{dx^3}(\xi_1) \right].$$

Thus in the same way as limiter schemes in the solution of hyperbolic partial differential equations vary the order of the method to preserve positivity, see [5], the function  $\alpha(r)$  varies the order between second  $|\alpha(r)| = 1/4$  and third order  $\alpha = 0$  to preserve data boundedness. The case  $\alpha(r) = 1/4$  only occurs if  $U_0 = U_{\frac{1}{2}}$  or  $U_1 = U_{\frac{1}{2}}$  and then the use of a linear polynomial is unavoidable.

In contrast when linear interpolation is used, e.g. on the subinterval [h/2, h], to substitute for the polynomial  $q_1$  the approximation polynomial is

(24) 
$$l_1(U_{\frac{1}{2}}, U_1, L_1) = U_{\frac{1}{2}}2(1 - L_1) + U_1(2L_1 - 1)$$

and the modified form of the error may, for comparison purposes, be written as  $u(x) - l_1(.) = u(x) - q_1(.) - (l_1(.) - q_1(.))$ . After some manipulation this may be written as

(25) 
$$(x - h/2)(x - h) \left[ \begin{array}{c} u(x) - l_1(U_{\frac{1}{2}}, U_1, L_1) = \\ \frac{4(-2U_{\frac{1}{2}} + U_0 + U_1)}{2 h^2} + \frac{x}{6} \frac{d^3u}{dx^3}(\xi_1) \right]$$

A comparison between equations (23) and (25) shows that when the term  $\frac{d^2u}{dx^3}(\xi_1)$  vanishes then the ratio of the two errors is  $4\alpha(r)$ : 1. This is not generally the case. In the examples below, for example, the ratios of the errors in the two cases are obtained by comparing the bracketted terms [] in equations (23) and (25). Furthermore, if the original polynomial  $q_1(.)$  violates the positivity of the data values, then in order for the modified polynomial to be data-bounded there must be a significant cancellation in the two terms in [] in equation (23) and (25). This is also shown in the examples below.

**3.1.1. Numerical Examples.** In this section the cases  $U_0 = 100, U_{\frac{1}{2}} = 0.3$  and  $U_1 = 0.1$ . and  $U_0 = 1.0, U_{\frac{1}{2}} = 0.3$  and  $U_1 = 0.1$  are considered as data points for the function u(x) defined by:

(26) 
$$u(x) = U_1 \ e^{a(1-x)^b},$$

where

$$a = log(U_0/U_1), \ c = log(U_{\frac{1}{2}}/U_1) \ \text{and} \ b = (\log(a) - \log(c))/\log(2).$$

In the first case  $U_0 = 100$  and the new and original polynomials are identical in [0, 0.5]. Table 1 shows the values of the interpolants at points in (0.5, 1.0) and Table 2 shows the errors in the interpolants. In particular the original quadratic polynomial has a minimum of about -12 whereas the new polynomial remains positive. In this case the new value of  $U_0^*$  is 0.9,  $U_0^* - U_0 = -99.1 \alpha(r) = 0.246$  and the change to the original polynomial has to be substantial to achieve data-boundedness. Also shown are the results from the linear polynomial  $l_1$  defined by equation (24).

Now consider the case when the value of  $U_0$  is changed to  $U_0 = 1, U_{\frac{1}{2}} = 0.3$  and  $U_1 = 0.1$ . The new and original polynomials are identical in [0, 0.5]. Table 1 shows the differences at points in (0.5, 1.0). In particular the original quadratic polynomial  $q_1$  has a minimum of about 0.0975 whereas the new polynomial  $p_1$  remains within the range of the data. In this case the new value of  $U_0^*$  is 0.9,  $U_0^* - U_0 = -0.1$  and  $\alpha(r) = 0.05$ . Thus the change to the original polynomial is quite small to ensure that the data values stay within the range of the data. It should be noted that the new polynomial is the same for both values of  $U_0$  as the value of r in both cases defines the same value of  $U_0^*$ . Also shown are the results from the linear polynomial  $l_1$  defined by equation (24).

$U_0$	$L_1$	0.5	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95
100.0	u(x)	0.3	0.230	0.184	0.153	0.133	0.119	0.110	0.105	0.102	0.100
100.0	$p_1$	0.3	0.262	0.228	0.198	0.172	0.150	0.132	0.118	0.108	0.102
100.0	$l_1$	0.3	0.280	0.260	0.240	0.220	0.200	0.180	0.160	0.140	0.120
100.0	$q_1$	0.3	-4.197	-7.700	-10.21	-11.72	-12.24	-11.76	-10.29	-7.820	-4.357
1.0	u(x)	0.3	0.267	0.238	0.212	0.189	0.169	0.151	0.136	0.122	0.110
1.0	$p_1$	0.3	0.262	0.228	0.198	0.172	0.150	0.132	0.118	0.108	0.102
1.0	$l_1$	0.3	0.280	0.260	0.240	0.220	0.200	0.180	0.160	0.140	0.120
1.0	$q_1$	0.3	0.257	0.220	0.178	0.160	0.137	0.120	0.107	0.100	0.098
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TABLE 1

Results for the standard, modified quadratic and linear interpolants

$U_0$	$L_1$	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	
100.0	$p_1 - u(x)$	0.032	0.044	0.045	0.039	0.031	0.022	0.013	0.006	0.002	
100.0	$l_l - u(x)$	0.050	0.076	0.087	0.087	0.081	0.070	0.055	0.038	0.020	
100.0	$q_1 - u(x)$	-4.42	-7.880	-10.36	-11.85	-12.35	-11.87	-10.39	-7.920	-4.458	
1.0	$p_1 - u(x)$	-0.005	-0.010	-0.014	-0.017	-0.019	-0.019	-0.018	-0.014	-0.008	
1.0	$l_1 - u(x)$	0.013	0.022	0.028	0.031	0.031	0.029	0.024	0.018	0.010	
1.0	$q_1 - u(x)$	-0.009	-0.018	-0.024	-0.029	-0.031	-0.031	-0.028	-0.022	-0.012	
	TABLE 2										

IABLE 2

Errors in the standard, modified quadratic and linear interpolants

**3.2.** Polynomial  $P_2$ . Consider now the case of the one dimensional quadratic interpolant to the function u(x) on [0, 1] with data points at  $0, \frac{1}{3}$  and 1 given by  $U_0, U_{\frac{1}{3}}$  and  $U_1$  defined by

(27) 
$$q_2(U_0, U_{\frac{1}{3}}, U_1, L_1) = U_0\bar{\phi}_1 + U_{\frac{1}{3}}\bar{\phi}_2 + U_1\bar{\phi}_3$$

where

$$\bar{\phi}_1 = (1 - L_1)(1 - 3L_1), \quad \bar{\phi}_2 = 4.5L_1(1 - L_1), \quad \bar{\phi}_3 = \frac{1}{2}L_1(3L_1 - 1)$$

and  $L_1 + L_2 = 1$  differentiating with respect to  $L_1$  gives

(28) 
$$\frac{dq_2}{dL_1} = 0 \text{ at } L_1 = \frac{1}{2} + s, \text{ where } s = \frac{U_1 - U_0}{3(3U_{\frac{1}{3}} - U_1 - 2U_0)}.$$

Differentiating again with respect to  $L_1$  gives

(29) 
$$\frac{d^2q_2}{dL_1^2} = 3(-3U_{\frac{1}{3}} + U_1 + 2U_0)$$

As above, this polynomial may have extrema at non-nodal points which may be removed by modifying the polynomial on the interval  $[0, \frac{1}{3}]$  by using a completely different value of  $U_1$  from the original or on the interval  $[\frac{1}{3}, 1]$  by using a completely different value of  $U_0$  from the original. This approach preserves  $C^0$  but not  $C^1$  continuity of the solution. The new polynomial is defined by

(30) 
$$p_2(U_0, U_{\frac{1}{3}}, U_1, L_1) = U_0 \bar{\phi}_1 + U_{\frac{1}{3}} \bar{\phi}_2 + U_1^* \bar{\phi}_3, \quad 0 \le L_1 \le \frac{1}{3}$$

(31) 
$$= U_0^* \bar{\phi}_1 + U_{\frac{1}{3}} \bar{\phi}_2 + U_1 \bar{\phi}_3, \quad \frac{1}{3} < L_1 \le 1$$

Define the values of  $U_0^*$  and  $U_1^*$  by moving extrema to the closest nodal point, denoted by  $L_{ext}^{new}$ . In the case when  $s \leq -\frac{1}{2}$  or  $s \geq \frac{1}{2}$  then  $U_0^* = U_0$  and  $U_1^* = U_1$  and the

original polynomial is unchanged. Define the values of  $U_0^*$  and  $U_1^1$  by again moving extrema to the closest nodal point:

(32) 
$$L_{ext}^{new} = 0, \quad -\frac{1}{2} < s \le -\frac{1}{3}, \quad U_1^* = 9U_{\frac{1}{3}} - 8U_0,$$

(33) 
$$L_{ext}^{new} = \frac{1}{3}, \quad -\frac{1}{3} < s \le -\frac{1}{6}, \quad U_1^* = 4U_0 - 3U_{\frac{1}{3}},$$

(34) 
$$L_{ext}^{new} = \frac{1}{3}, \quad -\frac{1}{6} < s \le \frac{1}{6}, \quad U_0^* = (U_1 + 3U_{\frac{1}{3}})/4,$$

(35) 
$$L_{ext}^{new} = 1, \quad \frac{1}{6} < s \le \frac{1}{2}, \quad U_0^* = (9U_{\frac{1}{3}} - 5U_1)/4.$$

The extra error introduced by this approach is given by

(36) 
$$q_2(...,L_1) - p_2(...,L_1) = (U_1 - U_1^*)\hat{\phi}_3, \quad 0 \le L_1 \le \frac{1}{3},$$

(37) 
$$= (U_0 - U_0^*)\hat{\phi}_1, \quad \frac{1}{3} < L_1 \le 1,$$

where

$$\begin{split} L_{ext}^{new} &= 0, \ U_1^* - U_1 = 9U_{\frac{1}{3}} - 8U_0 - U_1 &= (1+2s) \quad 3(3U_{\frac{1}{3}} - U_1 - 2U_0), \\ L_{ext}^{new} &= \frac{1}{3}, \ U_1^* - U_1 = 4U_0 - 3U_{\frac{1}{3}} - U_1 &= -(\frac{1}{3} + 2s) \ 3(3U_{\frac{1}{3}} - U_1 - 2U_0), \\ L_{ext}^{new} &= \frac{1}{3}, \ U_0^* - U_0 = (U_1 + 3U_{\frac{1}{3}})/4 - U_0 &= (\frac{1}{12} + \frac{s}{2}) \ 3(3U_{\frac{1}{3}} - U_1 - 2U_0), \\ L_{ext}^{new} &= 1, \ U_0^* - U_0 = (9U_{\frac{1}{3}} - 5U_1)/4 - U_0 &= (\frac{1}{4} - \frac{s}{2}) \ 3(3U_{\frac{1}{3}} - U_1 - 2U_0). \end{split}$$

From the last four equations and equation (5)  $U_1 - U_1^* = \beta(s) \frac{d^2 q_2}{dL_1^2}$  where  $0 \le \beta(s) \le 1/3$  and similarly for  $U_0 - U_0^*$ . Hence similar arguments as put forward by equations (21) to (25) in Section 3.1 apply.

4. A Data-Bounded Two Dimensional Quadratic Interpolant. In extending the ideas behind the one-dimensional schemes above to two dimensions there are a number of possible ways to proceed. A direct two dimensional analogy with the previous section would be to notice that the value of  $U_1$  could be changed to  $U_1^*$  for values of  $L_1 < \frac{1}{2}$  and similarly for  $U_2$  and  $U_3$ . Although this approach can be made to work for a single triangle there is a problem in enforcing continuity of the solution along exterior edges in a mesh of triangles. For a positive interpolant in a mesh of triangles it is thus important for the scheme to treat edges independently.

The starting point for the two-dimensional quadratic scheme is the observation that the ordinary quadratic interpolant may be written as a combination of four onedimensional quadratic interpolants; two along exterior edges, one through the centroid and the final one across the other three. There are three such interpolants which will be denoted by  $U_{I,j}$ , j = 1, 2, 3; the subscript I being used to avoid confusion with data points. For example, referring to Figure 1, let

$$U_A = q_1(U_2, U_4, U_1, L_1),$$

$$U_B = q_2(U_5, U_7, U_1, L_1),$$

$$U_C = q_1(U_3, U_6, U_1, L_1),$$

$$U_{I,1} = q_1(U_A, U_B, U_C, \frac{L_3}{L_2 + L_3}).$$
(38)

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where  $L_3/(L_2 + L_3)$  represents the position along the line ABC in that  $L_3 = 0$  at A and  $L_2 = 0$  at C. As each polynomial is exact for a quadratic this interpolant will reproduce a quadratic function. This approach has some similarities with that of Barnhill et al. [2] [3] except that they use three combinations of two quadratics along edges only with linear interpolation between them and subtracted a multiple of linear interpolation using the values  $U_1, U_2$  and  $U_3$ . The main differences here are the use of the centroid value  $U_7$  and the use throughout of quadratic polynomials. The two other ways of writing the interpolant are:

$$U_D = q_1(U_2, U_5, U_3, L_3),$$

$$U_E = q_2(U_4, U_7, U_3, L_3),$$

$$U_F = q_1(U_1, U_6, U_3, L_3),$$

$$U_{I,2} = q_1(U_D, U_E, U_F, \frac{L_1}{L_2 + L_1})$$
(39)

(40)  

$$U_{G} = q_{1}(U_{1}, U_{4}, U_{2}, L_{2}),$$

$$U_{H} = q_{2}(U_{6}, U_{7}, U_{2}, L_{2}),$$

$$U_{K} = q_{1}(U_{3}, U_{5}, U_{2}, L_{2}),$$

$$U_{I,3} = q_{1}(U_{G}, U_{H}, U_{K}, \frac{L_{3}}{L_{1} + L_{3}}).$$

In the case of the standard quadratic interpolant the centroid value,  $U_7$  is computed using equation (3). This value will, as has already been shown in Section 2, not preserve data boundedness.

Using the notation of Section 2 it is now straightforward to describe the bounded positive quadratic interpolant. Let  $\hat{U}_A$  be the value corresponding to  $U_A$  above but replacing the polynomial  $q_1$  with  $p_1$  and let the values  $\hat{U}_B, \hat{U}_C, \hat{U}_D, \hat{U}_E, \hat{U}_F, \hat{U}_G, \hat{U}_H, \hat{U}_K$ be similarly defined using the data-bounded polynomials  $p_1$  and  $p_2$ , and using a centroid value  $U_7$  that is itself bounded by the data values  $U_j, j = 1, ..., 6$ . The method used to compute this centroid value will be given in the next section.

Define the polynomials  $\hat{U}_{I,j}$ , j = 1, 3 by

(41) 
$$\hat{U}_{I,1} = p_1(\hat{U}_A, \hat{U}_B, \hat{U}_C, \frac{L_3}{L_2 + L_3}),$$

(42) 
$$\hat{U}_{I,2} = p_1(\hat{U}_D, \hat{U}_E, \hat{U}_F, \frac{L_1}{L_2 + L_1}),$$

(43) 
$$\hat{U}_{I,3} = p_1(\hat{U}_G, \hat{U}_H, \hat{U}_K, \frac{L_3}{L_1 + L_3}).$$

each of these polynomials being data-bounded and piecewise quadratic. The effect of using the different combinations of bounded quadratics means that the polynomials are no longer identical and may be directionally biased. For these reasons the bounded positive interpolant used is  $\hat{U}_I$  where

(44) 
$$\hat{U}_I(L_1, L_2, L_3) = \frac{1}{3} (\hat{U}_{I,1} + \hat{U}_{I,2} + \hat{U}_{I,3}).$$

5. Choosing the Centroid Value,  $U_7$ . In the case of the cell-centred finite volume schemes [5], [7] values at the centroids of triangles are the primary ones generated by the method. In this case interpolation techniques are used to compute the values at the mid-points of edges, [5], and at the nodes [10]. In the case of triangular quadratic finite element based schemes, [12], however the centroid values are not available and must be computed.

The primary requirement is that the centroid value is itself data bounded and that any error introduced is comparable to other errors already present. In the case when the standard quadratic value  $U_7$  defined by equation (3) is data bounded then this value is used unchanged.

Let  $U_{max}$  and  $U_{min}$  be the maximum and minimum of the values  $U_1, ..., U_6$ . In the case when  $U_7$  lies outside of the range of these values then  $U_7$  is set to either  $U_{max}$  or  $U_{min}$  using the following procedure. For convenience, consider the case when  $U_7 > U_{max}$ , the other case follows without difficulty. Let the (data bounded) linear interpolant value at the centroid be denoted by  $U_7^L$  and defined by

(45) 
$$U_7^L = \frac{1}{3}(U_1 + U_2 + U_3)$$

then from equation(3)

(46) 
$$U_7 = U_7^L - \frac{2}{9} \left[ (U_1 - 2U_4 + U_2) + (U_2 - 2U_5 + U_3) + (U_3 - 2U_6 + U_1) \right]$$

Let  $h_1, h_2$  and  $h_3$  be the lengths of the three edges connecting  $U_1$  and  $U_2$ ,  $U_2$  and  $U_2$ and  $U_3$  and  $U_1$  respectively, then

(47) 
$$U_1 - 2U_4 + U_2 = h_1^2 \frac{\partial^2 U_I}{\partial z_1^2}$$

where  $z_i$  is the local co-ordinate along the *i*th edge with length  $h_i$ . A similar interpretation of the other terms in equation (46) gives:

(48) 
$$U_7 - U_7^L = \frac{2}{9} \left[ h_1^2 \frac{\partial^2 U_I}{\partial z_1^2} + h_2^2 \frac{\partial^2 U_I}{\partial z_2^2} + h_3^2 \frac{\partial^2 U_I}{\partial z_3^2} \right]$$

As the linear value  $U_7^L$  is data-bounded and the quadratic one is not it follows that we can find a constant  $0 \le \gamma \le 1$  such that

(49) 
$$\gamma = \frac{U_{max} - U_7^L}{U_7 - U_7^L}$$

and hence in replacing  $U_7$  by  $U_{max}$  an extra source of error is introduced, which will be denoted by  $e_7$ , where  $e_7 = U_7 - U_{max}$ , and note that

(50) 
$$e_{7} = (1 - \gamma) \frac{2}{9} \left[ h_{1}^{2} \frac{\partial^{2} U_{I}}{\partial z_{1}^{2}} + h_{2}^{2} \frac{\partial^{2} U_{I}}{\partial z_{2}^{2}} + h_{3}^{2} \frac{\partial^{2} U_{I}}{\partial z_{3}^{2}} \right].$$

6. Error and Continuity Analysis. The interpolation error of the standard quadratic triangular interpolant is given by Johnson [9], for example. In order to estimate the value of the extra error incurred by using the one-dimensional databounded polynomials consider the case of the interpolant defined by equation (38). The values  $\hat{U}_A, \hat{U}_B, \hat{U}_C$  each have an error of the type considered in Sections 3.1 and 3.2. Let these errors be denoted by  $e\hat{U}_A, e\hat{U}_B$  and  $e\hat{U}_C$  respectively. In addition there is a possible extra error due to the use of the approximate centroid value. From equation (27) this can be written as  $e_7\bar{\phi}_2(L_1)$ . Hence the additional error due to preserving data-boundedness in  $\hat{U}_{I,1}$  which is denoted by  $e\hat{U}_{I,1}$  is given by

$$e\hat{U}_{I,1} = q_1(U_A, U_B, U_C, \frac{L_3}{L_2 + L_3}) - p_1(U_A + e\hat{U}_A, U_B + e\hat{U}_B + e_7\bar{\phi}_2(L_1), U_C + e\hat{U}_C, \frac{L_3}{L_2 + L_3}).$$

Adding and subtracting the term  $q_1(U_A + e\hat{U}_A, U_B + e\hat{U}_B + e_7\bar{\phi}_2(L_1), U_C + e\hat{U}_C, \frac{L_3}{L_2 + L_3})$ and simplifying using the results in Section 3.1 gives

$$e\hat{U}_{I,1} = -q_1(e\hat{U}_A, e\hat{U}_B + e_7\bar{\phi}_2(L_1), e\hat{U}_C, \frac{L_3}{L_2 + L_3}) + (52) \ \bar{\phi}_1(\frac{L_3}{L_2 + L_3}) \ \alpha(\hat{r}) \left[ (U_A - 2U_B + U_C) + (e\hat{U}_A - 2(e\hat{U}_B + e_7\bar{\phi}_2(L_1)) + e\hat{U}_C) \right]$$

where  $\alpha(\hat{r})$  is calculated by using the modified solution values, i.e.  $\hat{U}_A$  instead of  $U_A$  etc. The errors  $e\hat{U}_{I,2}$  and  $e\hat{U}_{I,3}$  may be similarly estimated. This expression shows how the additional errors introduced by the one dimensional interpolations,  $e\hat{U}_A$ ,  $e\hat{U}_B$  and  $e\hat{U}_C$  combine with the centroid error to introduce an additional error of the same order as the one-dimensional errors, into the interpolant. The first term in equation (60) is the quadratic interpolant of the errors at points A,B, and C while the second term consists of a similar term to that arising from ensuring that the polynomial  $q_1$  is data bounded, e.g. see equation (23), but with errors in the data values.

Regarding the continuity of the interpolant defined in this way: the polynomials defined along the edges of each triangle and through its centroid are clearly continuous. The question remains as to whether or not the dependency of the modified polynomials on r and s might cause discontinuities. Both r and s depend in a fixed well-defined way on the nodal data values and so the new interpolant is a composition of continuous functions of (x, y) and so is continuous.

7. Numerical Examples. In order to illustrate the properties of the interpolant three simple examples defined on a triangle with vertices at (0,0), (0,1) and (1,0) are used. The first problem has a maximum at  $(x_0, y_0)$  the second problem has a minimum at  $(x_0, y_0)$  while the third problem has a ridge of maximum values across the triangle.

Problem 1

(53) 
$$u(x,y) = \frac{1}{0.1 + (x - x_0)^2 + (y - y_0)^2}$$
  $x_0 = 0.25$   $y_0 = 0.1$ .

Problem 2

(54) 
$$u(x,y) = 10[(x-x_0)^2 + (y-y_0)^2] \quad x_0 = \frac{1}{3} \quad y_0 = \frac{1}{3}$$

Problem 3

(55) 
$$u(x,y) = 2 - \frac{1}{2}(x+y_0y)^2 + x_0(x+y_0y) \quad x_0 = -\frac{1}{3} \quad y_0 = -2.0.$$

Figures 1-10 display the results for these three problems and the associated numerical tables in Appendices 1,2 and 3 show the solution values to two significant figures



FIG. 2. Problem 1. Original Values



FIG. 3. Problem 1. New Interpolant



FIG. 4. Problem 1. Errors in New Interpolant



Fig. 5. Problem 2. Data Values and Original Interpolant



FIG. 6. Problem 2. New Positive Interpolant



FIG. 7. Problem 2. Errors in New Interpolant

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FIG. 8. Problem 3. Data Values and Original Interpolant



FIG. 9. Problem 3. New Interpolant



FIG. 10. Problem 3. Errors in New Interpolant

at the mesh points (0.1i, 0.1j) where i = 0, ..., 10, j = 0, ..., 10 and  $i + j \le 10$ . For each of the three problems the original quadratic and new quadratic interpolants are shown. For Problems 2 and 3 the exact solution is identical to the standard quadratic interpolant and so is not shown. In the case of Problem 1 the exact solution is shown.

In the case of Problem 1 the original interpolant has a maximum value of about 9.8 along the line x = 0 whereas the new polynomial does not allow the solution to rise above the largest nodal value of 5.7971, thus giving rise to the large maximum error shown in Figure 4.

For Problem 2 the data and original interpolant are both zero at the centroid  $x = \frac{1}{3}, y = \frac{1}{3}$  but the new interpolant does (correctly given its intent) not allow the solution values to dip below the smallest data value of 0.56.

In the case of Problem 3, the original quadratic interpolant peaks at 2.1 but the new polynomial remains bounded by the maximum nodal value of 2.041 at point 6. Overall, these results show that the new interpolant remains bounded between the maximum and minimum data values.

8. Extension to Tetrahedral Elements. The method described above is readily extended to the case of the standard quadratic interpolant on tetrahedra [12] in which each exterior triangular face has the same data points as the triangular quadratic interpolant in Figure 1. The data points are shown in Figure 11 and are numbered 1 to 10. Suppose that we wish to find the value of the interpolant at a point lying on the Q, R, S triangle defined by the points Q, R and S on which the volume co-ordinate  $L_3$  is constant. Let QR, RS and QS be the midpoints of the lines between Q and R, R and S and between Q and S respectively. Furthermore let  $c_1$ be the centroid of the triangular face defined by points  $1, 2, 3; c_2$  be the centroid of the triangle defined by the points 1, 3, 8 and  $c_3$  be the centroid of the triangle defined by the points 2, 3, 8.



FIG. 11. Example Tetrahedron.

The central idea is to use the monotone positive polynomials  $p_1$  and  $p_2$  defined in Section 2 to compute sufficient values on the triangle defined by Q, R and S so that the triangular interpolant described in Section 3 may be used to find the value of the interpolant. The values at Q, R and S are computed using the  $p_1$  polynomials along the tetrahedral edges while the values at the midpoints QR, RS and QS are computed using the  $p_2$  polynomial and the centroid values  $U_{c_1}$ ,  $U_{c_2}$  and  $U_{c_3}$  respectively on the exterior faces of the tetrahedron. The three centroid values are calculated in the same way as in Section 5. In other words:

$$U_Q = p_1(U_2, U_5, U_3, QL_3),$$
  

$$U_S = p_1(U_8, U_7, U_3, SL_3),$$
  

$$U_R = p_1(U_1, U_6, U_3, RL_3),$$
  

$$U_{QR} = p_2(U_4, U_{c_1}, U_3, QRL_3),$$
  

$$U_{RS} = p_2(U_9, U_{c_2}, U_3, RSL_3),$$
  

$$U_{OS} = p_2(U_{10}, U_{c_2}, U_3, QSL_3)$$

where  $QL_3$  is the  $L_3$  co-ordinate of point Q and similarly for the other five values of  $L_3$ .

The final step is to use the values  $U_Q, U_R, U_S, U_{QR}, U_{RS}, U_{QS}$  in the positive triangular interpolant described in Section 6 to compute the required value. The accuracy and positivity properties follow from the properties of the individual linear and triangular interpolants.

As in the case of triangles where for any point there are three such interpolants of this type there are four such tetrahedral interpolants, the one described being associated with the volume co-ordinate  $L_3$ . Again as in the triangular case, providing that the standard quadratics  $q_1, q_2$  and the standard quadratic triangular interpolant defined by equation (1) are used then all four interpolants will give the same answer. When the positivity preserving polynomials  $p_1$  and  $p_2$  and the positivity preserving triangular interpolant defined by equation (36) are used the four values will no longer be identical, though all will be in the range of the data. One solution is to average the four values. Alternatively the closest value to the original quadratic could be used.

9. Conclusions and Extensions. This new method for quadratic interpolation on triangles and tetrahedra, based on combinations of linear monotone quadratic polynomials, will preserve positivity in the data in that the interpolant created will be bounded by the maximum and minimum function values used to define it.

An obvious extension of the approach is consider the interpolant values on a triangle by global rather than local data values, e.g. [6]. This may be done by locating extrema on each edge, if necessary replacing them by global extremal data values, and using a data bounded quadratic to interpolate in between these new values on that part of the sub-edge where the extremal value lies. In this way, if a non-nodal extremal value outside the data bounds was detected, each quadratic edge polynomial would be decomposed into three piecewise quadratic polynomials.

10. Acknowledgements. The author would like to thank Ken Brodlie for pointing out the work of Barnhill et al. at a critical moment. The referees are also thanked for their thoughtful comments including suggesting the use of the term "databounded".

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Appendix 1 Problem 1. Data Values 1.0 1.2 1.3 1.5 1.6 1.7 1.9 2.1 2.2 2.2 2.4 2.7 2.8 2.8 2.7 3.1 3.5 3.8 3.8 3.5 3.1 4.0 4.7 5.2 5.2 4.7 4.0 3.2 4.9 6.2 7.0 7.0 6.2 4.9 3.8 2.9 5.8 7.5 8.9 8.9 7.5 5.8 4.3 3.2 2.4 6.2 8.2 9.8 9.8 8.2 6.2 4.5 3.3 2.5 1.9 5.8 7.5 8.9 8.9 7.5 5.8 4.3 3.2 2.4 1.9 1.5

## Problem 1. Original Quadratic Interpolant Values,

Data values are shown as []. [1.0] 1.4 1.7 1.8 2.1 2.3 2.2 2.5 2.7 2.7 2.6 3.0 3.2 3.2 3.0 [3.1] 3.4 3.6 3.6 3.4 [3.1] 3.6 3.9 4.1 4.1 3.9 3.6 3.1 4.1 4.4 4.6 4.6 4.4 4.1 3.6 2.9 4.6 5.0 5.2 5.2 5.0 4.6 4.1 3.4 2.6 5.2 5.6 5.7 5.7 5.6 5.2 4.7 4.0 3.1 2.1 [5.8] 6.1 6.3 6.3 6.1 [5.8] 5.3 4.6 3.7 2.7 [1.5]

# Problem 1. New Positive Quadratic Interpolant Values

Data values are shown as []. [1.0] 1.4 1.7 1.8 2.1 2.3 2.2 2.6 2.7 2.7 2.6 3.0 3.2 3.2 3.0 [3.1] 3.5 3.6 3.6 3.4 [3.1] 3.6 3.9 4.1 4.1 3.9 3.5 3.0 4.1 4.44.5 4.6 4.4 4.0 3.5 2.8 5.0 5.0 4.9 4.5 4.0 3.3 4.6 4.9 2.5 5.2 5.4 5.4 5.5 5.4 5.2 4.6 3.9 3.0 2.1 [5.8] 5.8 5.8 5.8 5.8 [5.8] 5.3 4.6 3.7 2.7 [1.5]

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Appendix 2 Problem 2. Data Values and Original Interpolant Values, Data values used are shown as [].

[5.6]										
4.3	3.8									
3.3	2.7	2.4								
2.5	1.9	1.5	1.4							
1.8	1.3	.89	.72	.76						
[1.4]	.82	. 46	.29	.32	[.56]					
1.2	.59	.22	.06	.09	.32	.76				
1.1	.56	.19	.02	.06	.29	.72	1.4			
1.3	.72	.36	.19	.22	. 46	.89	1.5	2.4		
1.7	1.1	.72	.56	.59	.82	1.3	1.9	2.7	3.8	
[2.2]	1.7	1.3	1.1	1.2	[1.4]	1.8	2.5	3.3	4.3	[5.6]

# Problem 2. New Positive Quadratic Interpolant Values

Data v	alues u	sed are	$\operatorname{shown}$	as [ ].						
[5.6]										
4.3	3.8									
3.3	3.0	2.4								
2.5	2.2	1.9	1.4							
1.8	1.6	1.3	1.0	.76						
[1.4]	1.2	.94	.77	.67	[.56]					
1.4	1.0	.75	.63	.67	.67	.76				
1.5	1.1	.77	.60	.61	.77	1.0	1.4			
1.7	1.3	.94	.76	.75	.94	1.3	1.8	2.4		
1.9	1.6	1.3	1.1	1.0	1.2	1.6	2.2	3.0	3.8	
[2.2]	1.9	1.7	1.5	1.4	[1.4]	1.8	2.5	3.3	4.3	[5.6]

# Problem 2. Errors in New Positive Quadratic Interpolant

[0.0]

Appendix 3 Problem 3. Data Values and Original Interpolant Data values used are shown as [].

L.67]										
.98	1.1									
1.3	1.4	1.5								
1.5	1.6	1.7	1.8							
1.7	1.8	1.8	1.9	1.9						
[1.8]	1.9	1.9	2.0	2.0	[2.0]					
1.9	2.0	2.0	2.0	2.1	2.1	2.0				
2.0	2.0	2.1	2.1	2.0	2.0	2.0	2.0			
2.1	2.1	2.0	2.0	2.0	2.0	1.9	1.9	1.8		
2.0	2.0	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	
[2.0]	2.0	1.9	1.9	1.8	[1.7]	1.6	1.5	1.4	1.3	[1.2]

# Problem 3. New Positive Quadratic Interpolant Values

Data v	alues u	sed are	$\operatorname{shown}$	as [ ].						
[.67]										
.98	1.1									
1.3	1.4	1.5								
1.5	1.6	1.7	1.8							
1.7	1.8	1.8	1.9	1.9						
[1.8]	1.9	1.9	2.0	2.0	[2.0]					
1.9	2.0	2.0	2.0	2.0	2.0	2.0				
1.9	2.0	2.0	2.0	2.0	2.0	2.0	1.9			
2.0	2.0	2.0	2.0	2.0	1.9	1.9	1.8	1.7		
2.0	2.0	2.0	1.9	1.9	1.8	1.8	1.7	1.6	1.5	
[2.0]	2.0	1.9	1.9	1.8	[1.7]	1.6	1.5	1.4	1.3	[1.2]

Problem 3. Errors in New Positive Quadratic Interpolant

[0.0]										
0.0	0.0									
0.0	.005	0.0								
0.0	.007	.007	0.0							
0.0	.008	.01	.008	0.0						
[0.0]	.01	.01	.01	.01	[0.0]					
.05	.03	.02	.01	.02	.03	.04				
.08	.06	.04	.02	.01	.02	.03	.06			
.08	.07	.05	.03	.01	.01	.02	.04	.06		
.05	.04	.03	.01	.01	.008	.008	.01	.02	.04	
[0.0]	0.0	0.0	0.0	0.0	[0.0]	0.0	0.0	0.0	0.0	[0.0]

In this case the original quadratic interpolant peaks at 2.1 but the new polynomial remains bounded by the maximum nodal value of 2.041 at point 6.

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