Shape Control in Multivariate Barycentric Rational Interpolation

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Abstract. The most stable formula for a rational interpolant for use on a finite interval is the barycentric form [1, 2]. A simple choice of the barycentric weights ensures the absence of (unwanted) poles on the real line [3]. In [4] we indicate that a more refined choice of the weights in barycentric rational interpolation can guarantee comonotonicity and coconvexity of the rational interpolant in addition to a polefree region of interest.

In this presentation we generalize the above to the multivariate case. We use a product-like form of univariate barycentric rational interpolants and indicate how the location of the poles and the shape of the function can be controlled. This functionality is of importance in the construction of mathematical models that need to express a certain trend, such as in probability distributions, economics, population dynamics, tumor growth models etc.

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BARYCENTRIC RATIONAL INTERPOLATION

Given $n + 1$ mutually distinct points $x_0, \dots, x_n$ and function values $f_0, \dots, f_n$, the rational functions

$$r_n(x) = \frac{\sum_{i=0}^n f_i \frac{w_i}{(x - x_i)}}{\sum_{i=0}^n \frac{w_i}{(x - x_i)}}, \quad w_i \neq 0 \quad (1)$$

interpolate the values f_i at the points x_i for any nonzero weights w_i , in other words $r_n(x_i) = f_i$. Hence, with respect to interpolation of the given data, the function $r_n(x)$ when represented as in (1), is immune to rounding errors in the computation of the coefficients. If we denote

$$\begin{aligned} \ell(x) &= (x - x_0) \cdots (x - x_n) \\ \ell_i(x) &= \ell(x) / (x - x_i), \end{aligned}$$

then $r_n(x)$ can be written as $r_n(x) = p_n(x)/q_n(x)$ with

$$\begin{aligned} p_n(x) &= \sum_{i=0}^n f_i w_i \ell_i(x) \\ q_n(x) &= \sum_{i=0}^n w_i \ell_i(x). \end{aligned}$$

Hence it is easy to see that the degree in numerator and denominator of $r_n(x)$ is at most n . A necessary condition for the barycentric weights to satisfy when $r_n(x)$ is polefree in $[x_0, x_n]$ is [1]

$$w_i w_{i+1} < 0, \quad i = 0, \dots, n-1.$$

Making use of Descartes' rule of signs or a Lorentz representation of $q_n(x)$ [5] we can make $r_n(x)$ polefree on the positive real line or in an interval $[a, b]$ respectively. By balancing the weights w_i as in [3] we can make $r_n(x)$ polefree on the entire real line.

A rational function of the form (1) clearly does not deliver the minimal degree solution of the rational interpolation problem. There are $n + 1$ additional degrees of freedom in the barycentric weights $w_0, \dots, w_n$. One way to make good use of these is by imposing some shape conditions on $r_n(x)$ [4]. Another way is to add conditions to obtain the minimal degree solution [6, 1, 7].

In the next sections we show how the above can be generalized to the multivariate case. We restrict our description to the bivariate case, without any loss of generality.

MULTIVARIATE BARYCENTRIC INTERPOLATION

Let the points $(x_i, y_i), i = 0, \dots, n$ be given in $\mathbb{R}^2$ and the function values f_i at these points. The points are assumed to be mutually distinct, so for $j \neq i$ we have $x_j \neq x_i$ or $y_j \neq y_i$. But the coordinates x_i need not be mutually distinct and neither do the coordinates y_i . However, in order to avoid a maze of notations, we assume for simplicity either that the x_i are distinct and likewise for the y_i (as in Figure 1), or that we are interpolating a full grid of $n + 1 = (m + 1)^2$ datapoints (as in Figure 2). In the more general intermediate situation, where some of the x_i or y_i coincide, one retains in the formulas below only the distinct coordinates and this in each variable.

FIGURE 1. Scattered data with $n = 8$.

FIGURE 2. Grid data with $m = 2$.

The functions

$$\begin{aligned}\ell_j(x) &= \prod_{i=0, i \neq j}^n (x - x_i) \\ \ell_k(y) &= \prod_{i=0, i \neq k}^n (y - y_i) \\ \ell_{jk}(x, y) &= \ell_j(x) \ell_k(y)\end{aligned}$$

satisfy

$$\ell_{jk}(x_i, y_h) = 0, \quad i \neq j \text{ or } h \neq k.$$

The multivariate polynomial

$$\sum_{i=0}^n f_i \frac{\ell_{ii}(x, y)}{\ell_{ii}(x_i, y_i)} \quad (2)$$

interpolates the data f_i at the points (x_i, y_i) . The functions $\ell_{ii}(x, y)/\ell_{ii}(x_i, y_i)$ in (2) are not the lowest degree polynomials that interpolate zeroes and ones at the $n + 1$ datapoints [8, 9], but they serve our purpose. More generally, for a grid of $(m + 1)^2$ function values f_{jk} at points (x_j, y_k) , the polynomial

$$\sum_{j,k=0}^m f_{jk} \frac{\ell_{jk}(x, y)}{\ell_{jk}(x_j, y_k)}$$

interpolates the data f_{jk} . However, as explained, we need not have a grid of function values at our disposal.

The values $1/\ell_{ii}(x_i, y_i)$ in (2) can be considered as weights in a barycentric formula. It is then easy to see that the multivariate rational function

$$r_n(x, y) = \frac{\sum_{i=0}^n f_i v_i w_i \ell_{ii}(x, y)}{\left(\sum_{i=0}^n v_i \ell_i(x) \right) \left(\sum_{i=0}^n w_i \ell_i(y) \right)} \quad (3)$$

interpolates the data f_i at the points (x_i, y_i) for whatever nonzero values for the weights v_i and w_i . Again (3) does not constitute the minimal degree multivariate rational interpolant. Additional conditions can be imposed on the barycentric weights v_i and w_i . Also, more generally, the rational function

$$\frac{\sum_{j,k=0}^m f_{jk} v_j w_k \ell_{jk}(x, y)}{\left(\sum_{i=0}^n v_i \ell_i(x) \right) \left(\sum_{i=0}^n w_i \ell_i(y) \right)}$$

interpolates a grid of $(m+1)^2$ values f_{jk} at points (x_j, y_k) .

It is easy to choose the weights v_i and w_i such that the rational function $r_n(x, y)$ does not have poles in a specified interval or in $\mathbb{R}^2$. The following lemma takes care of that.

Let the orderings $\kappa(i)$ and $\lambda(i)$ of the indices $0, \dots, n$ be such that $x_{\kappa(0)} < x_{\kappa(1)} < \dots < x_{\kappa(n)}$ and $y_{\lambda(0)} < y_{\lambda(1)} < \dots < y_{\lambda(n)}$. In the case of a grid of datapoints n needs to be replaced by m .

Lemma 1. Let $v_{\kappa(i)} = (-1)^{\kappa(i)} v_i$ and $w_{\lambda(i)} = (-1)^{\lambda(i)} w_i$ with $v_i > 0$ and $w_i > 0$. If for $a < x_{\kappa(0)}, b > x_{\kappa(n)}, c < y_{\lambda(0)}, d > y_{\lambda(n)}$ we have

$$\begin{aligned} \frac{v_{i-1}}{b - x_{\kappa(i-1)}} &< \frac{v_i}{b - x_{\kappa(i)}} & i = 1, \dots, n \\ \frac{v_i}{x_{\kappa(i)} - a} &> \frac{v_{i+1}}{x_{\kappa(i+1)} - a}, & i = 0, \dots, n-1 \\ \frac{w_{i-1}}{d - y_{\lambda(i-1)}} &< \frac{w_i}{d - y_{\lambda(i)}} & i = 1, \dots, n \\ \frac{w_i}{y_{\lambda(i)} - c} &> \frac{w_{i+1}}{y_{\lambda(i+1)} - c}, & i = 0, \dots, n-1 \end{aligned} \quad (4)$$

then $r_n(x, y)$ given by (3) does not have poles in $(a, b) \times (c, d)$. With $a = x_{\kappa(0)}, b = x_{\kappa(n)}, c = y_{\lambda(0)}, d = y_{\lambda(n)}$ the conditions (4) need only be satisfied for $i = 1, \dots, n-1$.

Proof. It is clear that the denominator of $r_n(x, y)$ can only have zeroes of the form $x = \alpha$ or $y = \beta$. We show that such zeroes are excluded in the region of interest by proving that the factor in x and that in y in the denominator of (3) are zero-free in (a, b) and (c, d) respectively. To do so we use an idea similar to the one in [3]. Because the x_i and the y_i are assumed mutually distinct to simplify the notation (otherwise it is just a matter of keeping track which and how many distinct coordinates x_i and y_i we have), we can denote

$$\begin{aligned} \ell(x, y) &= \prod_{i=0}^n (x - x_i)(y - y_i) \\ q_n(x, y) &= \ell(x, y) \left(\sum_{i=0}^n \frac{v_i}{x - x_i} \right) \left(\sum_{i=0}^n \frac{w_i}{y - y_i} \right). \end{aligned}$$

Numerator and denominator of (3) can be rewritten as

$$r_n(x, y) = \frac{\ell(x, y) \sum_{i=0}^n \frac{f_i v_i w_i}{(x - x_i)(y - y_i)}}{\ell(x, y) \left(\sum_{i=0}^n \frac{v_i}{x - x_i} \right) \left(\sum_{i=0}^n \frac{w_i}{y - y_i} \right)}.$$

With the interpolation points (x_i, y_i) we associate open intervals $I_i = (x_{\kappa(i-1)}, x_{\kappa(i)})$ and $H_i = (y_{\lambda(i-1)}, y_{\lambda(i)})$ where we put $x_{\kappa(-1)} = y_{\lambda(-1)} = -\infty$ and $x_{\kappa(n+1)} = y_{\lambda(n+1)} = +\infty$. Then for $(x, y) \in I_j \times H_k$ we can write

$$q_n(x, y) = \ell(x, y) (r(x) + s(x)) (u(y) + v(y))$$

where

$$\begin{aligned} r_i(x) &= \begin{cases} 0, & x < x_{\kappa(i)} \\ v_{\kappa(i)} / (x - x_{\kappa(i)}), & x > x_{\kappa(i)} \end{cases} \\ s_i(x) &= \begin{cases} v_{\kappa(i)} / (x - x_{\kappa(i)}), & x < x_{\kappa(i)} \\ 0, & x > x_{\kappa(i)} \end{cases} \\ r(x) &= \sum_{i=0}^{j-1} r_i(x), \quad s(x) = \sum_{i=j}^n s_i(x). \end{aligned}$$

and

$$\begin{aligned} u_i(y) &= \begin{cases} 0, & y < y_{\lambda(i)} \\ w_{\lambda(i)} / (y - y_{\lambda(i)}), & y > y_{\lambda(i)} \end{cases} \\ v_i(y) &= \begin{cases} w_{\lambda(i)} / (y - y_{\lambda(i)}), & y < y_{\lambda(i)} \\ 0, & y > y_{\lambda(i)} \end{cases} \\ u(y) &= \sum_{i=0}^{k-1} u_i(y), \quad v(y) = \sum_{i=k}^n v_i(y). \end{aligned}$$

If the weights v_i and w_i are such that for $x \in I_j, j = 1, \dots, n$ and $y \in H_k, k = 1, \dots, n$ we have

$$\begin{aligned} |r_i(x)| &> |r_{i-1}(x)|, & i = 1, \dots, j-1 \\ |s_i(x)| &> |s_{i+1}(x)|, & i = j, \dots, n-1, \\ |u_i(y)| &> |u_{i-1}(y)|, & i = 1, \dots, k-1 \\ |v_i(y)| &> |v_{i+1}(y)|, & i = k, \dots, n-1, \end{aligned} \tag{5}$$

then the signs of both $r(x)$ and $s(x)$ are that of $(-1)^{\kappa(j-1)}$ and the signs of both $u(y)$ and $v(y)$ are that of $(-1)^{\lambda(k-1)}$. This can be seen by summing $r(x)$ and $u(y)$ from 0 to $j-1$ and $k-1$ respectively and summing $s(x)$ and $v(y)$ from n to j and k respectively. So $r(x) + s(x)$ only changes sign at each $x_{\kappa(i)}$, as does $\ell(x, y)$, and consequently $q_n(x, y)$ does not change sign. The same is true for $u(y) + v(y)$. Hence both factors in $q_n(x, y)$ are zero-free in $(a, b) \times (c, d)$. Making use of the fact that the $r_i(x), u_i(y)$ and $s_i(x), v_i(y)$ are hyperbola and that their vertical asymptotes are ordered since $x_{\kappa(0)} < x_{\kappa(1)} < \dots < x_{\kappa(n)}$ and $y_{\lambda(0)} < y_{\lambda(1)} < \dots < y_{\lambda(n)}$, the conditions (5) are satisfied if with $v_i = (-1)^{\kappa(i)} v_i$ and $w_i = (-1)^{\lambda(i)} w_i$ the conditions (4) are satisfied. $\square$

It is obvious that the same property holds for the rational interpolant on a grid of values because its denominator has the same form.

The choice to take both v_i and w_i nonzero also guarantees that $r_n(x, y)$ is always defined and finite in $(a, b) \times (c, d)$. The denominator does not have zeroes in $(a, b) \times (c, d)$ and hence numerator and denominator of $r_n(x, y)$ cannot have common zeroes in $(a, b) \times (c, d)$. Consequently the occurrence of so-called unattainable interpolation points [10] is impossible.

Let us illustrate the above with some graphs of functions $r_n(x, y)$ where the different weights v_i and w_i satisfy (4). It is clear from these graphical illustrations that there is still an ample choice of interpolants, each displaying a different shape. In the following section we indicate the possibilities for further control of the shape.

Given here are values $f_{k\ell}$ at points (x_k, y_ℓ) on a 3×3 grid with $x_0 = -3, x_1 = 1, x_2 = 3, y_0 = -3, y_1 = -0.5, y_2 = 3$. The function values $f_{k\ell}$ (in matrix notation where the row index is $k+1$ and the column index $\ell+1$) are

$$\begin{pmatrix} 0 & -0.3 & 0 \\ 0.2 & 2.5 & -0.2 \\ 0 & 0 & 0.3 \end{pmatrix}.$$

For v_i and w_i given by $v_0 = 0.4950, v_1 = -1.000, v_2 = 0.4288, w_0 = 0.4287, w_1 = -1.000, w_2 = 0.4603$ the rational interpolant is shown in Figure 3. Another look and feel is obtained by choosing $v_0 = 1.000, v_1 = -0.3402, v_2 = 0.4555$ and $w_0 = 1.000, w_1 = -5.9536, w_2 = 14.0084$ as in Figure 4.

FIGURE 3. $r_8(x, y)$.

FIGURE 4. $r_8(x, y)$.

DERIVATIVES OF THE BARYCENTRIC INTERPOLANT

The representation (3) takes the form of the univariate barycentric formula (1) by introducing either

$$F_i = r_n(x_i, y) = \frac{f_i w_i \ell_i(y)}{\sum_{i=0}^n w_i \ell_i(y)}$$

or

$$G_i = r_n(x, y_i) = \frac{f_i v_i \ell_i(x)}{\sum_{i=0}^n v_i \ell_i(x)}.$$

The same can be done on a grid of $(m+1)^2$ data. Then regarded as a function in x , (3) takes the form

$$\frac{\sum_{i=0}^n F_i v_i \ell_i(x)}{\sum_{i=0}^n v_i \ell_i(x)}$$

and as a function in y ,

$$\frac{\sum_{i=0}^n G_i w_i \ell_i(y)}{\sum_{i=0}^n w_i \ell_i(y)}.$$

Consequently we can use the formulas for the derivatives given in [1] to obtain the partial derivatives

$$\frac{\partial r_n(x, y)}{\partial x} = \begin{cases} \frac{\sum_{i=0}^n \frac{r_n(x, y) - r_n(x_i, y)}{x - x_i} \frac{v_i}{x - x_i}}{\sum_{i=0}^n \frac{v_i}{x - x_i}}, & x \neq x_j, \quad j = 0, \dots, n \\ - \frac{\left(\sum_{i=0, i \neq j}^n v_i \frac{r_n(x_j, y) - r_n(x_i, y)}{x - x_i} \right)}{v_j}, & x = x_j, \end{cases}$$

$$\frac{\partial r_n(x,y)}{\partial y} = \begin{cases} \frac{\sum_{i=0}^n \frac{r_n(x,y) - r_n(x,y_i)}{y - y_i} \frac{w_i}{y - y_i}}{\sum_{i=0}^n \frac{w_i}{y - y_i}}, & y \neq y_j, \quad j = 0, \dots, n \\ - \left(\frac{\sum_{i=0, i \neq j}^n w_i \frac{r_n(x,y_j) - r_n(x,y_i)}{y - y_i}}{w_j} \right), & y = y_j, \end{cases}$$

These partial derivatives can be combined into directional derivatives or used for the computation of higher derivatives. Then following the ideas of [4] conditions can be imposed to control the shape of the polefree barycentric rational interpolant. We conclude with the following example.

We take the same data as above. It is easy to see from Figure 4 that for $y = 3$ the rational interpolant is not convex. Imagine we want it to be convex along that stretch. Then using the technique from [4] for the partial derivative $\partial r_8(x, 3)/\partial x$ we find that the weights v_i need to be changed to (for instance) $v_0 = 1, v_1 = -1.8, v_2 = 1$. We emphasize that the change is computed such that it preserves the guarantee of a polefree interpolant. The result of the change is shown in Figure 5 and in Figure 6 one finds the projection $r_8(x, 3)$ before and after the change of weights.

FIGURE 5. Convex $r_8(x, y)$.

FIGURE 6. Before and after.

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