Regional Conference on Ecological and Environmental Modeling (ECOMOD 2004), Penang Malaysia, 15-16 September 2004. Organized by School of Mathematical Sciences and School of Biological Sciences, Universiti Sains Malaysia.

Visualize Scientific Data using Rational Cubic

[1]Jamaludin Md. Ali, [2] Hadibah Mohd Hassan & [3]Abu Hassan Ahmad.

[1,2] School of Mathematical Sciences & [3] School of Biological Sciences
Universiti Sanis Malaysia , Penang, Malaysia

Abstract Smooth curve representation to visualize scientific data is very significant in Computer Graphics and in particular Data Visualization. It is very important when the data is obtained from some complex functions or from some scientific experiments or phenomena. It becomes crucial to incorporate the inherited features of the data. A very simple example is the visualization of positive data such as the number of mosquito larvae compared to the amount of rainfall in a certain month. Moreover, smoothness is also an important feature for a pleasing visual display of the data. This paper utilized the idea of curve interpolation to display the data, and spline is commonly used and popular. However an alternative approach using piecewise rational cubic is proposed which preserved the desired properties of positivity and smoothness as required by the data.

Keywords: Data visualization, Rational spline, Interpolation, Shape preserving, Monotone, Convex, Positive

1. Introduction

In the area of Computer Graphics and in particular Data Visualization, to visualize data obtained from complex function or the scientific data from scientific experiments or phenomena as smooth curve representation is very important. It becomes crucial to incorporate the inherited features of the data.. A very simple example is the visualization of positive data such as the number of mosquito larvae compared to the amount of rainfall in a certain month. Moreover, smoothness is also an important feature for a pleasing visual display of the data.Therefore, data visualization has been considered by a number of authors. To cite a few are Delbourgo and Gregory (1985), Fritsch and Butland (1984),), Passow and Roulier (1977) and McAllister et. Al. (1977). This paper describes a piecewise rational cubic function which can be used to solve the problem of shape preserving interpolation of convex data.

This paper begins with a definition of the rational function given in section 2 then in section 3, we describe the generation of a C^1 spline, which can preserve the shape of a monotone, convex and positive data. In section 4 an algorithm using mathematical software Mathematica is demonstrated using some real data. A brief conclusinon and further works will be given in the last section.

2. Rational cubic spline with shape control

Data visualization using rational cubic spline consisting of piecewise rational Bezier cubic curves with shape control was thoroughly discussed by Sarfraz (1997, 2000, 2002). In this paper we follow the same approach as Sarfraz but with a rational cubic function defined by Ball (1974) as:

$$s(x) \equiv s_i(x) = \frac{U_i(1-\theta)^2 + v_iV_i\theta(1-\theta)^2 + w_iW_i\theta^2(1-\theta) + Z_i\theta^2}{(1-\theta)^2 + v_i\theta(1-\theta)^2 + w_i\theta^2(1-\theta) + \theta^2}, \quad 0 \le \theta \le 1 \tag{1}$$

where v_i, w_i are the weights and U_i, V_i, W_i, Z_i are the control points (values).

Let $(x_i, f_i), i = 1,2,\dots,n$, be a given set of data points, where $x_1 < x_2 < \dots < x_n$. Let

$$h_i = x_{i+1} - x_i, \qquad \Delta_i = \frac{f_{i+1} - f_i}{h_i}, \qquad i = 1,2,\dots,n-1 \tag{2}$$

where

$$\theta = \frac{x - x_i}{h_i} \quad . \tag{3}$$

To ensure that the rational function (1) is C^1, we impose the following interpolatory properties:

$$s(x_i) = f_i, \qquad s(x_{i+1}) = f_{i+1}$$
$$s^{(1)}(x_i) = d_i, \quad s^{(1)}(x_{i+1}) = d_{i+1} \tag{4}$$

This will provide the following manipulations:

$$U_i = f_i, \qquad Z_i = f_{i+1}$$

$$V_i = f_i + \frac{h_i d_i}{v_i}, \qquad W_i = f_{i+1} - \frac{h_i d_{i+1}}{w_i} \tag{5}$$

where $s^{(1)}$ denotes the first derivative with respect to x, and d_i denotes derivatives value given at the knot x_i. Thus the interpolant $s \in C^1[x_1, x_n]$ is

$$s(x) \equiv s_i(x) = \frac{P_i(\theta)}{Q_i(\theta)} \tag{6}$$

where

$$P_i(\theta) = f_i(1-\theta)^2 + v_i V_i \theta(1-\theta)^2 + w_i W_i \theta^2(1-\theta) + f_{i+1}\theta^2$$

$$Q_i(\theta) = (1-\theta)^2 + v_i\theta(1-\theta)^2 + w_i\theta^2(1-\theta) + \theta^2$$

The parameters v_i's, w_i's and derivatives d_i's are chosen so that the interpolant (6) preserves monotone, convex and positive shape. Variation for values of v_i's and w_i's controls (tighten or loosen) the curve in different pieces of the curve. This behavior is discussed in the following section.

2.1. Shape control analysis

The parameters v_i's and w_i's can be used to modify the shape of the curve according to the user. In Figure 1, the bottom curve of the third piece is a default curve when the weights are equal to two and it has negative values. When the weight increases the curve is tightened and it becomes linear when they are approaching to infinity.

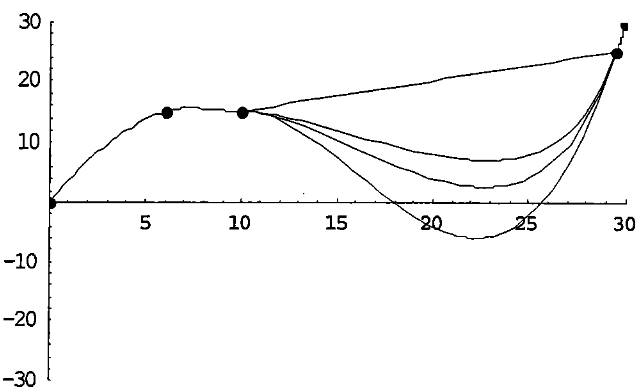

Figure 1: The tightening effect of the curve.

The interval shape control behavior can be observed by rewriting $s_i(x)$ in equation (6) to the following simplified form:

$$s(x) = f_i(1-\theta) + f_{i+1}\theta + \frac{[(1-\theta)(d_i - \Delta_i) + \theta(\Delta_i - d_{i+1}) + \theta(1-\theta)\Delta_i(w_i - v_i)]h_i\theta(1-\theta)}{Q_i(\theta)} \tag{7}$$

When both v_i and $w_i \to \infty$, it converges to the following linear interpolant:

$$s(x) = f_i(1-\theta) + f_{i+1}\theta \ .$$

The shape control analysis is valid only if derivatives values are assumed bounded. A description of appropriate choices for such derivatives values is made in the following section.

2.2. Determination of derivatives

In most applications, the derivative parameters $\{d_i\}$ are not given and hence must be determined either from the given data $(x_i, f_i), i = 1,2,\ldots,n$ or by some other means. In this paper, the pameters $\{d_i\}$ are computed from the given data in such a way that the C^1 smoothness of the interpolant (6) is maintained. These methods are the approximations based on various approaches. For this paper we will discussed two common methods of determining the derivatives; the arithmetic means and geometric means.

2.2.1. Method 1

Arithmetic mean method is the three-point difference approximation based on arithmetic manipulation. This method is given by ,

$$d_i = \begin{cases} 0 & \text{if} \quad \Delta_{i-1} = 0 \text{ or } \Delta_i = 0 \\ \dfrac{(h_i \Delta_{i-1} + h_{i-1}\Delta_i)}{(h_i + h_{i-1})} & \text{otherwise } i = 2,\ldots,n-1 \end{cases} \tag{8}$$

with end conditions

$$d_1 = \begin{cases} 0 & \text{if} \quad \Delta_1 = 0 \quad \text{or} \quad \operatorname{sgn}(d_1^*) \neq \operatorname{sgn}(\Delta_1) \\ d_1^* & \text{otherwise} \end{cases} \tag{9}$$

$$d_n = \begin{cases} 0 & \text{if} \quad \Delta_{n-1} = 0 \quad \text{or} \quad \operatorname{sgn}(d_n^*) \neq \operatorname{sgn}(\Delta_{n-1}) \\ d_n^* & \text{otherwise} \end{cases}$$

(10)

where

$$d_1^* = \Delta_1 + (\Delta_1 - \Delta_2)\frac{h_1}{h_1 + h_2}$$

$$d_n^* = \Delta_{n-1} + (\Delta_{n-1} - \Delta_{n-2})\frac{h_{n-1}}{h_{n-2} + h_{n-1}}$$

These arithmetic mean approximations are suitable for the convex interpolation problem, since they satisfy the inequality

$$d_1 < \Delta_1 < \ldots\Delta_{i-1} < d_i < \Delta_i \ldots < \Delta_{n-1} < d_n \,. \tag{11}$$

These method will be considered as the default choice as it is computationally more economical.

2.2.2. Method 2

These are the non-linear approximations based on geometric means;

$$d_i = \begin{cases} 0 & \text{if} \quad \Delta_{i-1} = 0 \text{ or } \Delta_i = 0 \\ \Delta_{i-1}^{\frac{h_i}{h_{i-1}+h_i}} \Delta_i^{\frac{h_{i-1}}{h_{i-1}+h_i}} & \text{otherwise } i = 2,\ldots,n-1 \end{cases} \tag{12}$$

with end conditions

$$d_1 = \begin{cases} 0 & \text{if} \quad \Delta_1 = 0 \text{ or } \Delta_{3,1} = 0 \\ \Delta_1^{\left(1+\frac{h_1}{h_2}\right)} \Delta_{3,1}^{\left(-\frac{h_1}{h_2}\right)} & \text{otherwise} \end{cases} \tag{13}$$

$$d_n = \begin{cases} 0 & \text{if} \quad \Delta_{n-1} = 0 \text{ or } \Delta_{n.n-2} = 0 \\ \Delta_{n-1}^{\left(1+\frac{h_{n-1}}{h_{n-2}}\right)} \Delta_{n,n-2}^{\left(-\frac{h_{n-1}}{h_{n-2}}\right)} & \text{otherwise} \end{cases} \tag{14}$$

where

$$\Delta_{3,1} = \frac{(f_3 - f_1)}{(x_3 - x_1)}, \qquad \Delta_{n,n-2} = \frac{(f_n - f_{n-2})}{(x_n - x_{n-2})}.$$

The geometric mean approximation is suitable for monotonic data and convex data because its satisfy inequality

$$0 \le d_1 < \Delta_1 < d_2 < \ldots < \Delta_{i-1} < d_i < \Delta_i < \ldots < d_n \tag{15}$$

For given bounded data, the derivatives are bounded. Hence, for bounded values of shape parameters: $v_i, w_i, i = 1,2,\ldots,n-1$ the interpolant is bounded and unique. We can conclude as the following theorem

Theorem 1: For bounded $v_i, w_i \forall i$ and the derivative approximation given in section 2.2.1 and 2.2.2 there exist a unique C^1 spline solution to the interpolant (6).

For illustration we have the following data extracted from Srafraz (2000,2002) for the curve fitting.

Table 1: Monotonic data

i	1	2	3	4	5
x_i	0	6	10	29.5	30
f_i	0.01	15	15	25	30

Table 2: Convex data

i	1	2	3	4	5
x_i	1	2	4	5	10
f_i	10	2.5	0.625	0.4	0.1

Table 3: Positive data

i	1	2	3	4	5	6	7
x_i	0	2	4	10	28	30	32
f_i	20.8	8.8	4.2	0.5	3.9	6.2	9.6

The followings are the fitting curves using the given data.

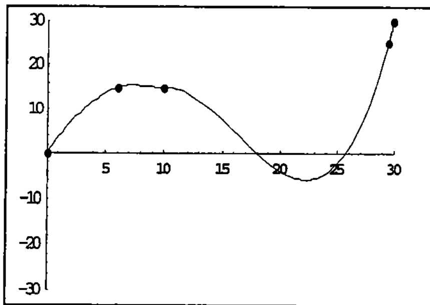

Figure 1(a): Default curve with method 1 for monotonic data in Table 1.

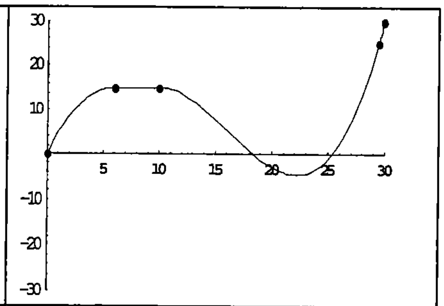

Figure 1(b): Default curve with method 2 for monotonic data in Table 1.

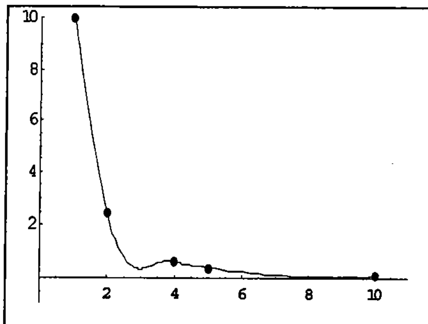

Figure 2(a): Default curve with method 1 for convex data in Table 2.

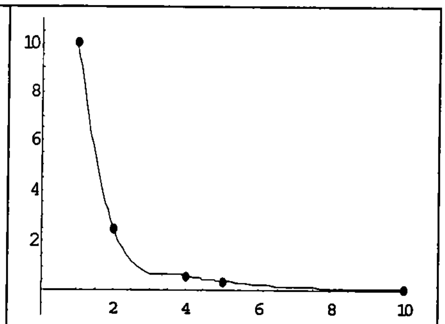

Figure 2(b): Default curve with method 2 for convex data in Table 2.

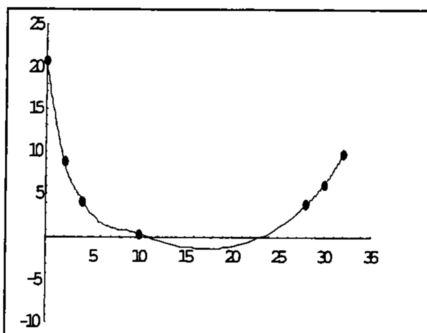

Figure 3(a): Default curve with method 1 for positive data in Table 3.

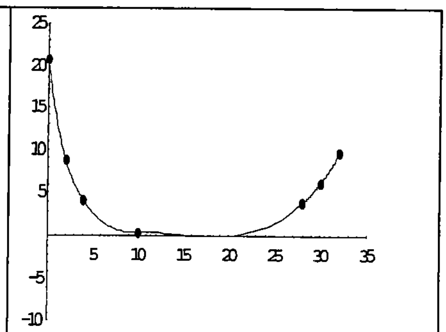

Figure 3(b): Default curve with method 2 for positive data in Table 3.

3. Spline interpolation

In order to achieve the shape preserving interpolant the shape parameters v_i 's and w_i ;s can be modified by trial-and-error basis, in the regions of the spline where shape violations are found. This is not a quick and efficient way to manipulate curves for shape preserving.. A more effective and useful is the automatic generation of shape preserving curve. This requires computation of suitable shape parameters and derivatives at the knots. To proceed with this strategy, we discussed some mathematical treatment for three types of shape preserving; monotone, convex and positive splines

3.1. Monotone spline interpolation.

For simplicity of presentation, we assume monotonic increasing set of data so that

$$f_1 \le f_2 \le \ldots \le f_n \tag{16}$$

or equivalently

$$\Delta_i \ge 0, \qquad i = 1,2,\ldots,n-1 \tag{17}$$

For a monotonic data interpolant s(x), it is then necessary that the derivative parameters should be such that

$$d_i \ge 0 \qquad i = 1,2,\ldots,n \tag{18}$$

Now, s(x) is monotonic increasing if and only if

$$s^{(1)}(x) \ge 0 \tag{19}$$

for all $x \in [x_1, x_n]$. For $x \in [x_i, x_{i+1}]$ the first derivative after some simplification is

$$s^{(1)}(x) = \frac{[\sum_{j=1}^{6} A_{j,i}\theta^{j-1}(1-\theta)^{6-j}]}{[Q_i(x)]^2} \tag{20}$$

where

$$A_{1,i} = d_i,$$

$$A_{2,i} = 2w_i(\Delta_i - \frac{1}{w_i}d_{i+1}) + d_i,$$

$$A_{3,i} = 3\Delta_i + 2w_i(\Delta_i - \frac{1}{w_i}d_{i+1}) + v_i w_i(\Delta_i - \frac{1}{v_i}d_i - \frac{1}{w_i}d_{i+1}),$$

$$A_{4,i} = 3\Delta_i + 2v_i(\Delta_i - \frac{1}{v_i}d_i) + v_i w_i(\Delta_i - \frac{1}{v_i}d_i - \frac{1}{w_i}d_{i+1}),$$

$$A_{5,i} = 2v_i(\Delta_i - \frac{1}{v_i}d_i) + d_{i+1},$$

$$A_{6,i} = d_{i+1},$$

Since the denominator in (20), is positive, therefore the sufficient condition for monotnicity on $[x_i, x_{i+1}]$ are

$$A_{j,i} \ge 0, \qquad j = 1,2,\ldots,6 \tag{21}$$

where d_i dan d_{i+1} are assumed positive. If $\Delta_i > 0$ then the following are sufficient conditions to satisfy (21):

$$\Delta_i - \frac{1}{v_i}d_i \ge 0$$

$$\Delta_i - \frac{1}{w_i}d_{i+1} \ge 0$$

$$\Delta_i - \frac{1}{v_i}d_i - \frac{1}{w_i}d_{i+1} \ge 0 \tag{22}$$

which gives

$$v_i = \frac{r_i d_i}{\Delta_i}, \qquad w_i = \frac{q_i d_{i+1}}{\Delta_i} \tag{23}$$

where r_i and q_i are some positive quantities satisfying

$$\frac{1}{r_i}+\frac{1}{q_i}\le 1 \tag{24}$$

This, together with (23) leads to the following sufficient conditions for the freedom over the choice of r_i and q_i

$$r_i \ge 1+\frac{d_{i+1}}{d_i}, \qquad q_i \ge 1+\frac{d_i}{d_{i+1}}. \tag{25}$$

We choose r_i and q_i as follows:

$$r_i = 1+\frac{d_{i+1}}{d_i}, \qquad q_i = 1+\frac{d_i}{d_{i+1}}. \tag{26}$$

This choice satisfies (24) and it provides visually pleasant result. It should be noted that if $\Delta_i = 0$, then it is necessary to set $d_i = d_{i+1} = 0$ and thus

$$s(x) = f_i = f_{i+1} \tag{27}$$

is a constant on $[x_i, x_{i+1}]$. For the case where the data is monotonic but not strictly monotonic (i.e. when some $\Delta_i = 0$), it would be necessary to divide the data strictly into monotonic parts.

The above discussion can be summarized as:

Theorem 2: Given conditions (18) on the derivatives, (23) and (26) are the sufficient conditions for interpolant (6) to be monotonic increasing.

3.2. Convex spline interpolation

By assuming a strictly convex set of data then

$$\Delta_1 < \Delta_2 < \ldots < \Delta_{n-1}. \tag{28}$$

For a convex interpolant s(x), it is necessary that the derivative parameters to be

$$d_1 < \Delta_1 < \ldots \Delta_{i-1} < d_i < \Delta_i \ldots < \Delta_{n-1} < d_n, \tag{29}$$

Now s(x) is convex if and only if

$$s^{(2)}(x) \ge 0 \tag{30}$$

for all $x \in [x_1, x_n]$. For $x \in [x_i, x_{i+1}]$, the first and second derivatives are respectively given by

$$s^{(1)}(x) = \frac{[\sum_{j=1}^{6} A_{j,i}\theta^{j-1}(1-\theta)^{6-j}]}{[Q_i(x)]^2},$$

and

$$s^{(2)}(x) = \frac{[\sum_{j=1}^{8} B_{j,i}\theta^{j-1}(1-\theta)^{8-j}]}{h_i[Q_i(x)]^3}, \tag{31}$$

$A_{j,i}$ and $B_{j,i}$ are the expression involving d_i's, Δ_i's, v_i's dan w_i's. Since the denominator for positive v_i, w_i is positive, then the sufficient conditions for convexity on $[x_i, x_{i+1}]$ are

$$B_{j,i} \ge 0, \ j = 1,2,\ldots,8, \tag{32}$$

After some simplifications, we have

$$B_{1,i} = 2\{(w_i - v_i)\Delta_i + v_i(\Delta_i - d_i) - (d_{i+1} - d_i)\},$$
$$B_{8,i} = 2\{(w_i - v_i)\Delta_i + w_i(d_{i+1} - \Delta_i) - (d_{i+1} - d_i)\}. \tag{33}$$

If $\Delta_i - d_i > 0$ and $d_{i+1} - \Delta_i > 0$ then the following conditions will be sufficient to satisfy (33)

$$v_i = w_i,$$
$$v_i(\Delta_i - d_i) - (d_{i+1} - d_i) \ge 0,$$

$$w_i(d_{i+1}-\Delta_i)-(d_{i+1}-d_i)\geq 0 . \qquad (34)$$

Since

$$\frac{d_{i+1}-\Delta_i}{\Delta_i-d_i}+\frac{\Delta_i-d_i}{d_{i+1}-\Delta i}\geq \max(\frac{d_{i+1}-d_i}{\Delta_i-d_i},\frac{d_{i+1}-d_i}{d_{i+1}-\Delta i}). \qquad (35)$$

The choice of weight parameters

$$v_i=w_i=\max(\frac{d_{i+1}-d_i}{\Delta_i-d_i},\frac{d_{i+1}-d_i}{d_{i+1}-\Delta_i}) \qquad (36)$$

will be considered for the practical implementation of default curve design. The weights can be further modified by adding some positive values to (36).

If $\Delta_i-d_i=0$ or $d_{i+1}-\Delta_i=0$, then it is necessary to set $d_i=d_{i+1}=\Delta_i$. The interpolant then will be linear in that region, i.e.,

$$s(x)=(1-\theta)f_i+\theta f_{i+1} . \qquad (37)$$

If $\Delta_i=0$, then it is necessary to set $d_i=d_{i+1}=0$ and thus

$$s(x)=f_i=f_{i+1} \qquad (38)$$

is a constant on $[x_i,x_{i+1}]$. For the case, where the data are convex but not strictly convex, the data has to be divided into strictly convex parts. If we set $d_i=d_{i+1}=0$ whenever $\Delta_i=0$, then the resulting interpolant will be C^0 at break points.

The above discussion can be summarized as:

Theorem 3: Given conditions (11) on the derivative parameters and the convex data, the constraints (36) are the sufficient conditions for the interpolant (6) to be convex.

3.3. Positive spline interpolation

Let assume positive set of data $(x_1,f_1),(x_2,f_2),...,(x_n,f_n)$ for

$$x_1<x_2<...<x_n, \qquad (39)$$

and

$$f_1>0,f_2>0,...,f_n>0 . \qquad (40)$$

Since $v_i,w_i>0$ implies that $Q_i(\theta)>0$, then the interpolant (6) will be positive if the cubic polynomial $P_i(\theta)$ is positive. Hence the problem reduces to determination suitable values of v_i,w_i so that the polynomial $P_i(\theta)$ is positive. Thus to ensure that $P_i(\theta)>0$ then

$$V_i>0,W_i>0 . \qquad (41)$$

Which gives

$$v_i>m_i,w_i>M_i \qquad (42)$$

where

$$m_i=\max\{0,\frac{-h_id_i}{f_i}\} , \qquad M_i=\max\{0,\frac{h_id_{i+1}}{f_{i+1}}\} . \qquad (43)$$

The above discussion can be summarized as:

Teorem 4: For a strictly positive data, the rational cubic interpolant (6) preserves positivity if and only if (43) is satisfied.

The weights can be futher modified to incorporate both shape preserving and shape control features. Thus one can give parameters r_i dan q_i

$$r_i,q_i\geq 1 \qquad (44)$$

such that

$$v_i=(1+m_i)r_i , \qquad w_i=(1+M_i)q_i . \qquad (45)$$

As default curve we set $r_i,q_i=1$, and

$$v_i=w_i=1+\max(m_i,M_i) . \qquad (46)$$

Figures 5 and 6 illustrate the default and shape preserving spline.

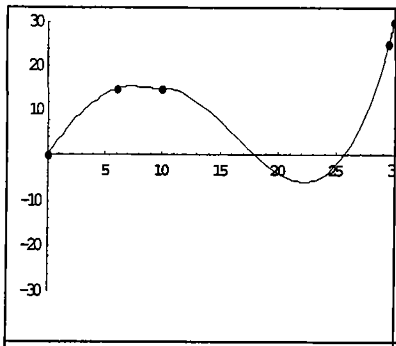

Figure 5(a): Default curve with method 1 for monotonic data in Table 1.

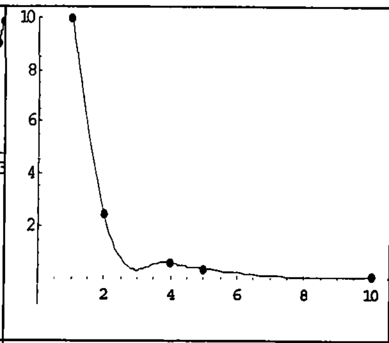

Figure 5(b): Default curve with method 1 for convex data in Table 2.

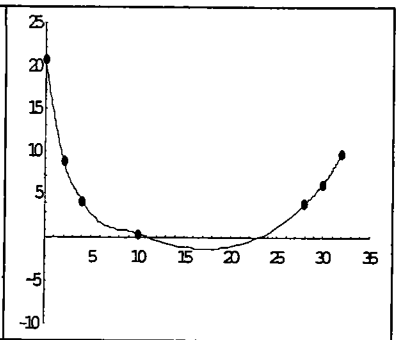

Figure 5(c): Default curve with method 1 for positive data in Table 3.

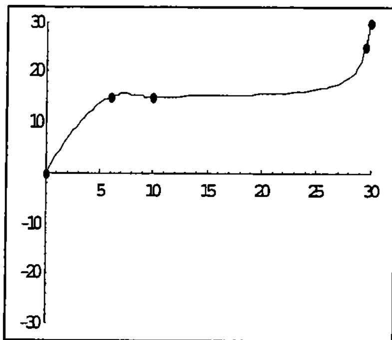

Figure 6(a): The shape preserving spline for the monotone data. .

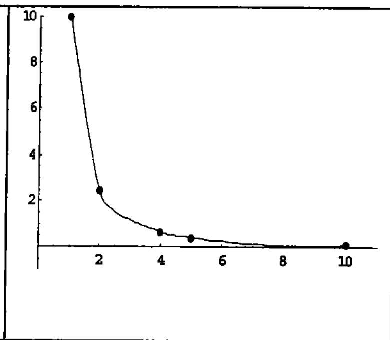

Figure 6(b): The shape preserving spline for the convex data..

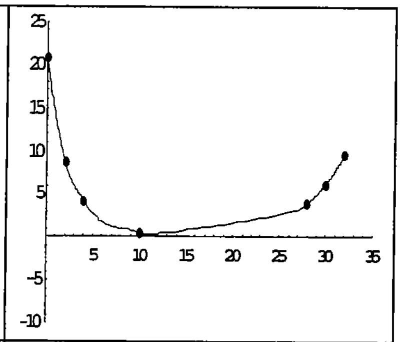

Figure 6(c): The shape preserving spline for positive data

4. Shape preserving spline for mosquito data set

For further illustration the mosquito data set is used, (Ahmad, 2004). Shape preserving methods that has been described will be applied and also the method of 'trial and error'.

Week, 1991, x_i	Rainfall	Egg	Aedes
1	3.3	835	147
2	0.5	1122	75
3	0.0	331	85
4	11.6	379	335
5	2.2	124	38

Table 4: Mosquito data

The following figures illustrate visually the data in Table 4.

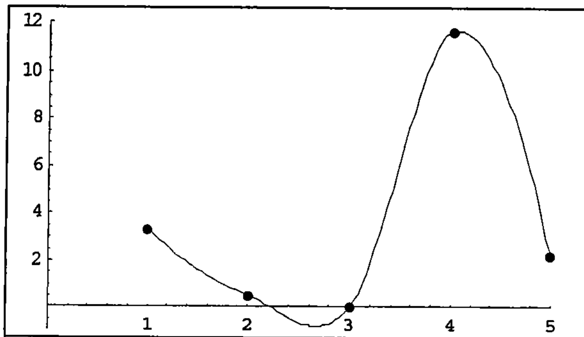

Figure 7(a): The default rational cubic spline for the Rainfall data.

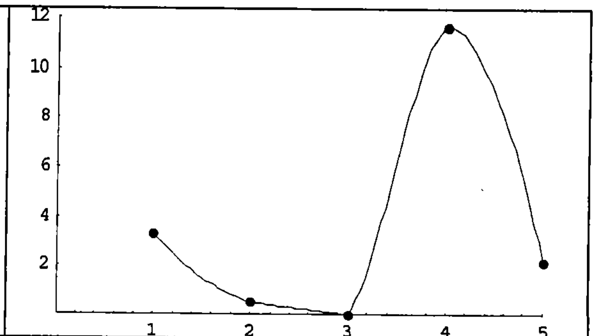

Figure 7b): The shape preserving spline for the Rainfall data .

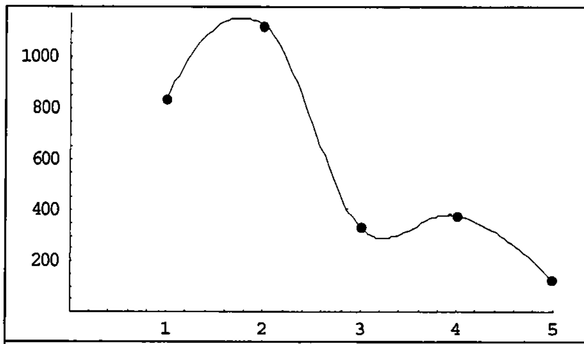

Figure 8(a): The default rational cubic spline for the Egg data .

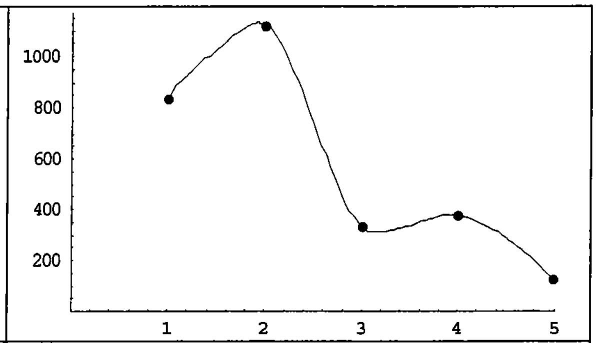

Figure 8(b): The shape preserving spline for the Egg data.

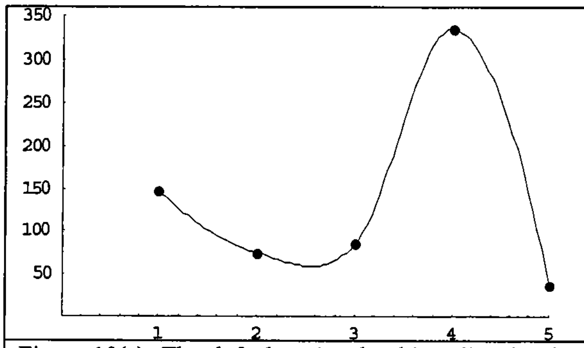

Figure 10(a): The default rational cubic spline for the Aedes data .

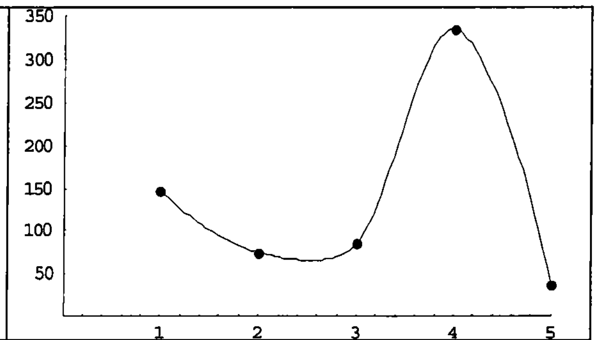

Figure 10(b): The shape preserving spline for the Aedes data.

The following figure illustrates visually the rainfall data and Aedes data.

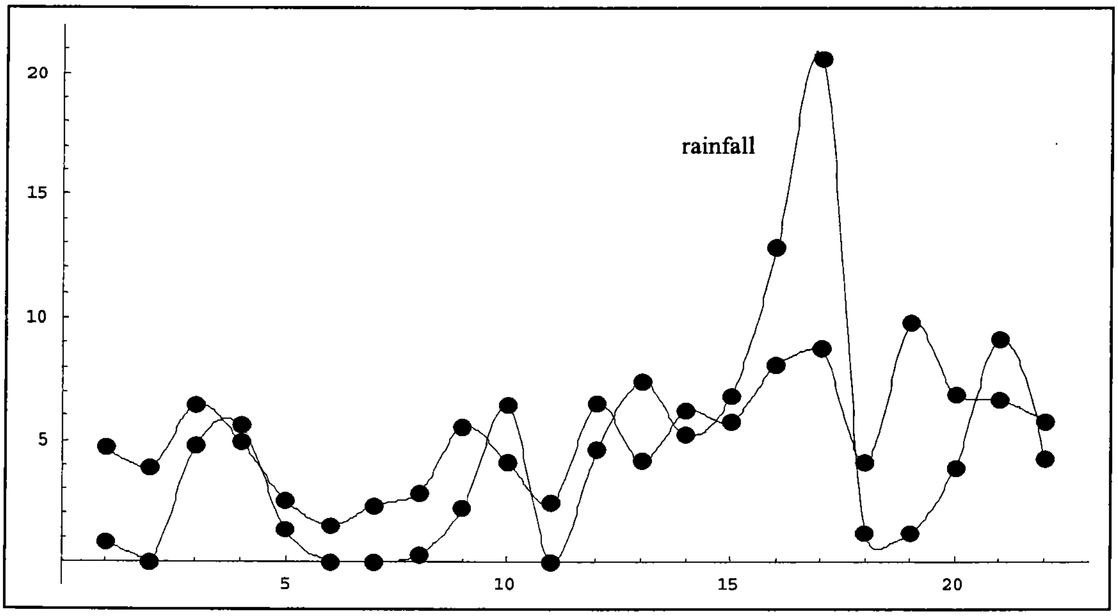

Fig. 12. Shape presering splines for data taken from the first week of January until Mei 1989. To make comparison the data values for Aedes is scaled down.

5. Conclusion

The rational spline scheme has been implemented successfully and it demonstrates a nice visually pleasant results. The user can automatically get the curves using the techniques of shape preserving. In some cases the user can manipulate the curve manually by 'trial and error ' method in regions of unreasonable shape. By visualizing the data a better interpretation about the phenomena can be made. For example in Figure 12, a simple conclusion can be made, that is the number of aedes increases about two weeks after the rainfall. Then a certain action can be made to overcome the problem of aedes.

References

Ahmad, A. H. (2004). (private communication).

Ball, A.A. (1974), CONSURF, Part 1. Introduction to conic lofting title. *Computer Aided Design* **6**, 243-249.

.Delbourgo, R. & Gregory, J.A. (1985). Shape preserving piecewise rational interpolation. *SIAM Journal of Scientific and Satistical Computing* **6**, 967-976.

Fritsch, F.N. & Butland J.A. (1984). A method for constructing local monotone piecewise cubic interpolants. *SIAM Journal of Scientific and Satistical Computing* **5**, 300-304.

Gregory, J. A. & Delbourgo, R. (1982). Piecewise rational quadratic interpolation to monotonic data. *IMA Journal of Numerical Analysis* **2**, 123-130.

McAllister, D. F., Passow, E. & Roulier, J.A. (1977). Algorithms for computing shape preserving spline interpolations to data. *Mathematical Computing* **31**, 717-725.

Passow, E. & Roulier, J.A. (1977). Monotone and convex spline interpolation. *SIAM Journal of Numerical Analysis* **14**, 904-909.

Sarfraz, M. (1992). Interpolatory rational cubic spline with biased, point and interval tension. *Computer and Graphics* **16** (4), 427-430.

Sarfraz, M. (1997). Preserving monotone shape of the data using piecewise rational cubic functions. *Computers and Graphics* **21** (1), 5-14.

Sarfraz, M. (2000). A rational cubic spline for the visualization of monotonic data. *Computers and Graphics* **24** (4), 509-516.

Sarfraz, M. (2002). Visualization of positive and convex data by a rational cubic spline interpolation. *Information Sciences* **146**, 239-254.