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Relaxation Technique for the Fitting of Numerical Data

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Abstract

Data, in particular that generated through successive computer approximations, may not always follow the smooth curve it is suppose to. Approximations in input data, round off error, and estimations made in the mathematical formulas, are just some of the things that could cause this problem. In any respect, this data must somehow be smoothed or fitted for publication. One way of fitting such data sets is the relaxation method. This method does not rely on the data conforming to a specific mathematical shape, as opposed to other programs that require the data to be fitable by some mathematically generated curve. Instead, the relaxation method uses the values of the points surrounding the current one to determine the new value at that location. This provides a curve independent method for fitting the data.

1 INTRODUCTION

The relaxation method was originally used in determining electrical field distributions. The field was mapped out as a two dimensional grid of estimated potentials. The potentials would then be better approximated by passing the grid through the relaxation process. The idea behind the method was to take a potential U_0 and calculate a new potential based on its value and the values of the four potentials, U_1, U_2, U_3, and U_4, surrounding it. This would be done for every point in the grid, producing a new grid with better approximations for the actual potentials. Then, by repeating the process for each new grid, the error of determining the potential for a given point is reduced.

Taking this idea into one dimensional work simplifies the matter down to only two surrounding potentials, U_2 and U_4, in which to calculate a new U_0 potential. This method can now be applied to xy curves. Defining the potential at each point to be equal to its y value, the method will relax these y values into a smooth curve. It is this process that we hope to apply towards our data curves.

2 THEORY

The calculations start with the two dimensional case as defined in figure (1)[1]. Each

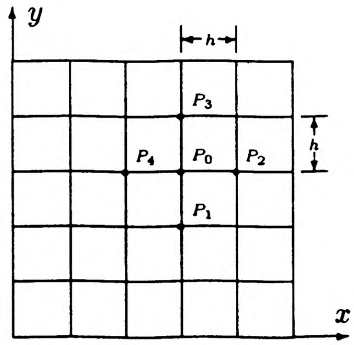

Figure 1: Computational lattice for the relaxation technique

point P_i corresponds to a potential value U_i used in the following U_0-dependent equations given by Paszkowski[1].

$$U_1 = U_0 - \left(\frac{\partial U}{\partial y}\right)_0 h + \frac{1}{2}\left(\frac{\partial^2 U}{\partial y^2}\right)_0 h^2 - \frac{1}{6}\left(\frac{\partial^3 U}{\partial y^3}\right)_0 h^3 + \cdots \quad (1)$$

$$U_2 = U_0 + \left(\frac{\partial U}{\partial x}\right)_0 h + \frac{1}{2}\left(\frac{\partial^2 U}{\partial x^2}\right)_0 h^2 + \frac{1}{6}\left(\frac{\partial^3 U}{\partial x^3}\right)_0 h^3 + \cdots \quad (2)$$

$$U_3 = U_0 + \left(\frac{\partial U}{\partial y}\right)_0 h + \frac{1}{2}\left(\frac{\partial^2 U}{\partial y^2}\right)_0 h^2 + \frac{1}{6}\left(\frac{\partial^3 U}{\partial y^3}\right)_0 h^3 + \cdots \quad (3)$$

$$U_4 = U_0 - \left(\frac{\partial U}{\partial x}\right)_0 h + \frac{1}{2}\left(\frac{\partial^2 U}{\partial x^2}\right)_0 h^2 - \frac{1}{6}\left(\frac{\partial^3 U}{\partial x^3}\right)_0 h^3 + \cdots \quad (4)$$

Each of these equations, when summed together, give us equation (5).

$$\sum_{n=1}^{4} U_n = 4U_0 + \left[\left(\frac{\partial^2 U}{\partial x^2}\right)_0 + \left(\frac{\partial^2 U}{\partial y^2}\right)_0\right] h^2 + \cdots \quad (5)$$

Since it is the one dimensional case needed as a fitting routine, only the U_2 and U_4 potentials are summed together, as follows

$$U_2 + U_4 = 2U_0 + \left(\frac{\partial^2 U}{\partial x^2}\right)_0 h^2 + \cdots \quad (6)$$

so that the terms containing the partial y will drop out. If the "terms of higher order (small value of h) are neglected"[1], equation (6) becomes

$$U_2 + U_4 - 2U_0 - h^2\nabla^2 U_0 = 0 \quad (7)$$

and when there is "no space charge ($\nabla^2 U_0 = 0$)"[1] then

$$U_2 + U_4 - 2U_0 = 0 \quad (8)$$

"Since values are assumed at the beginning of the calculations, equation (8) may not be satisfied and there may be a residue"[1], where

$$U_2 + U_4 - 2U_0 = R_0 \quad (9)$$

If "the value of R_0 is a measure of the deviation from the proper potential at point P_0, U_0 must be changed so that the residue (R_0) vanishes."[1] This correction being

$$\triangle U_0 = \frac{1}{2} R_0 \tag{10}$$

Finally, combining the previous two equations (9) and (10) to get the formula for the change in U_0,

$$\triangle U_0 = \frac{1}{2}[U_2 + U_4 - 2U_0] \tag{11}$$

Then if $U = y$ then for $i = 1$ to n,

$$\triangle y_i = \frac{1}{2}[y_{i+1} + y_{i-1} - 2y_i] \tag{12}$$

where i is the index into the set of points and n is the number of points in that set. The formula in equation (12) provides a starting point for a simple relaxation routine to do curve fitting. To get a better degree of smoothing, just pass each new data set back through the algorithm.

3 RESULTS

The relaxation method was tested on modifications of two plots, a *sin* curve and a $1/x$ curve. Theses curves were modified to test the fitting of distortion on a relatively gentle slope area, a steep slope area, and a sharp peak or arc. Each of these effects can be found in amplitude curves intended to be fitted.

This first plot is a modified $1/x$ curve where a few points were selectively distorted to see if the relaxation method could produce a $1/x$ fit. The original curve is being represented

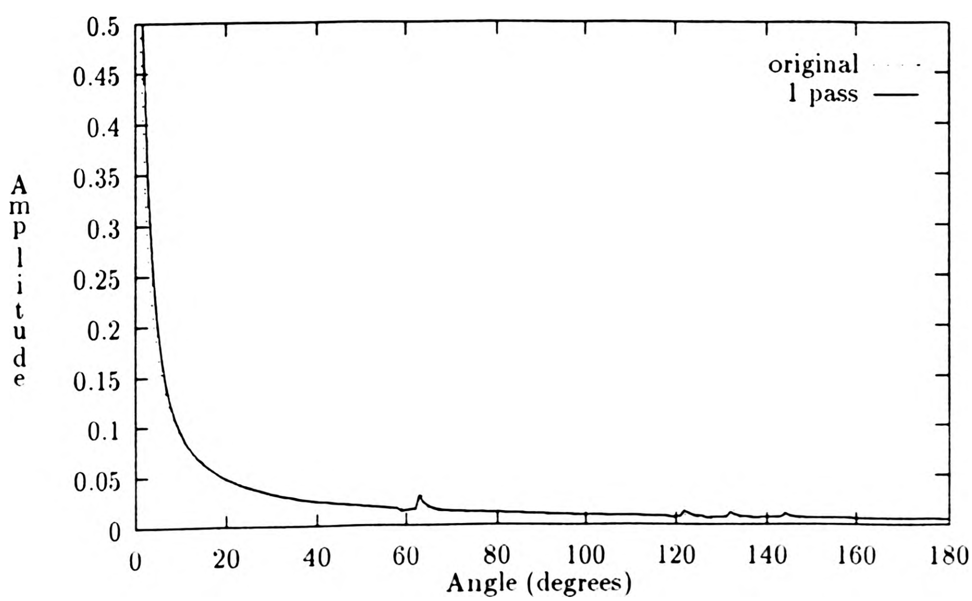

Figure 2: $1/x$ with some points distorted

with a dotted line, and a single pass through this data with the relaxation technique has produced the solid line shown in figure (2). As you can see, the distortion around 60 and 130 degrees has been partially smoothed out by only one pass through the algorithm. By making more passes through this data, these spikes were further relaxed, as shown by the thicker line and thicker dots of figure (3), representing three and five passes respectively.

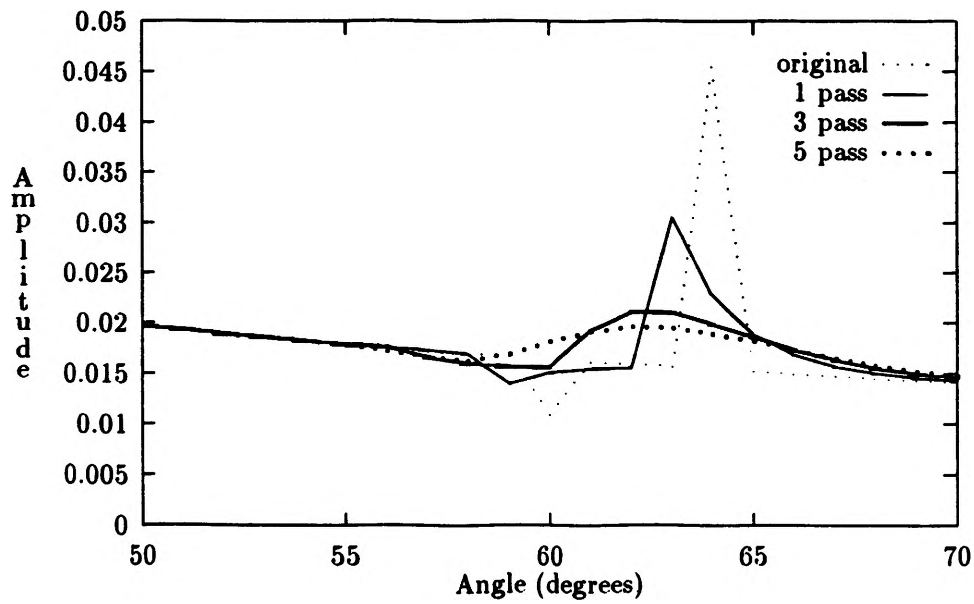

Figure 3: Comparison of multiple relaxation passes on gentle slope

Unfortunately, not all effects were good. Figure (2) shows that the fit for steeper slopes are effected more, producing a shift slightly to the right. With more passes through the algorithm, this effect becomes more exaggerated.

To see how the relaxation method would effect relatively sharp peaks and valleys, a modification of a *sin* curve was chosen. Figure (4) shows this *sin* curve, with distortion in a peak around 60 degrees and distortion in the steep slope area around 130 degrees. Again the original curve is represented with a dotted line, and a single pass through the relation algorithm is represented by the solid line. As you can see, just a single pass has relaxed the data around the peak at 60 degrees, and straightened the steep slope at 130 degrees.

As in figure (2), more passes through the *sin* data has made the distortions virtually disappear in both areas of interest. These two areas are represented in a plot of both arcs in figure (5). Unfortunately with the increase of the number of passes, a shift or decrease in the amplitudes around 60 and 120 degrees can again be seen.

One example of an amplitude curve that must be fitted is shown in figure (6). This plot displays the original data with dots, where the distortion is in the larger angles. It took five passes through the data to produce the smooth line fit. The distorted data has been smoothed, but at the expense of the decrease in amplitude around 30 degrees. This curve follows the same patterns seen with the previous two curves, where the resulting curve is more relaxed, but the steep slope area and sharp peaks experience a shift from the original data.

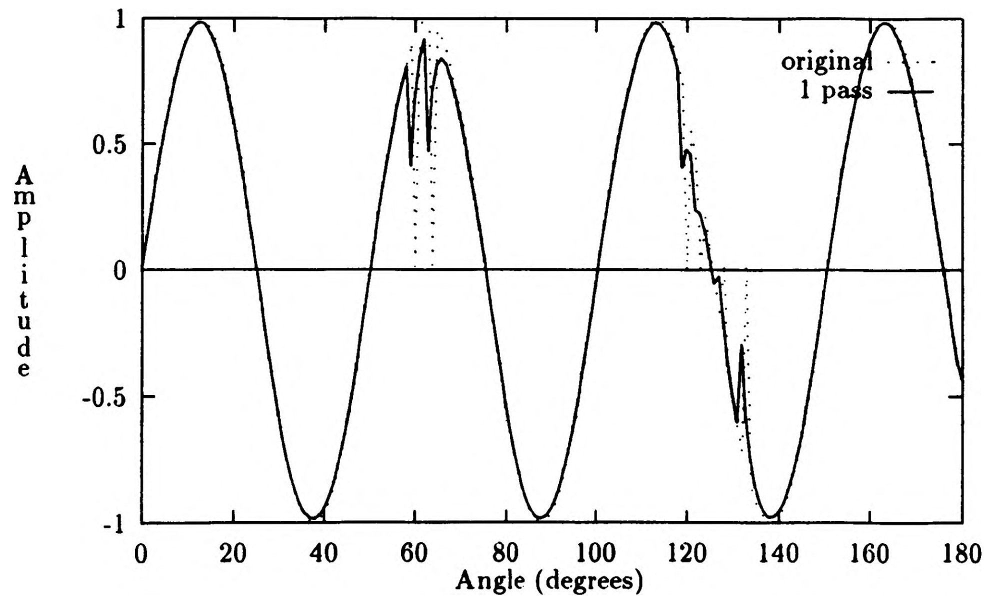

Figure 4: $Sin(x)$ with some points distorted

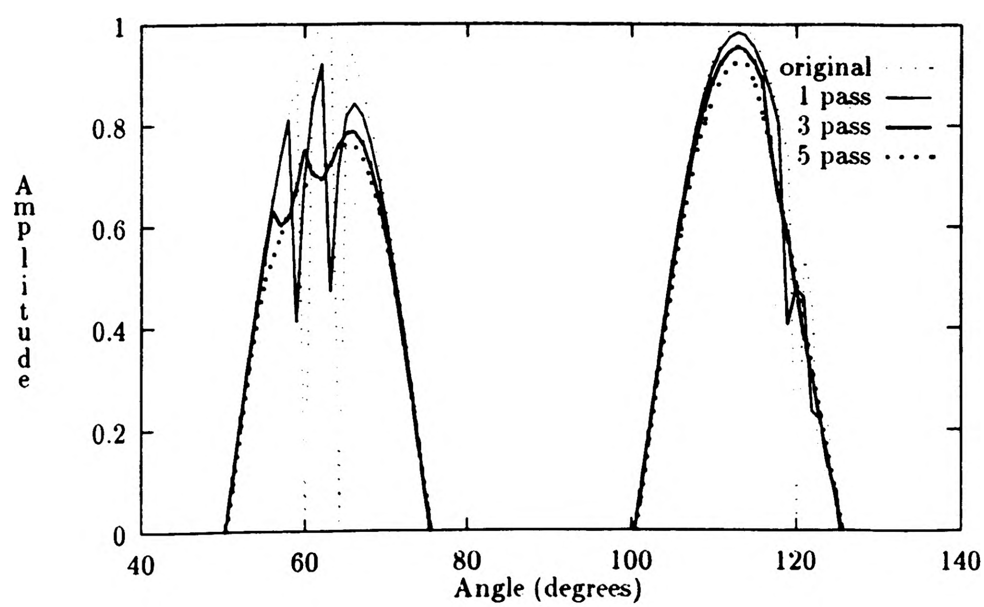

Figure 5: Comparison of multiple relaxation passes on sharp peak

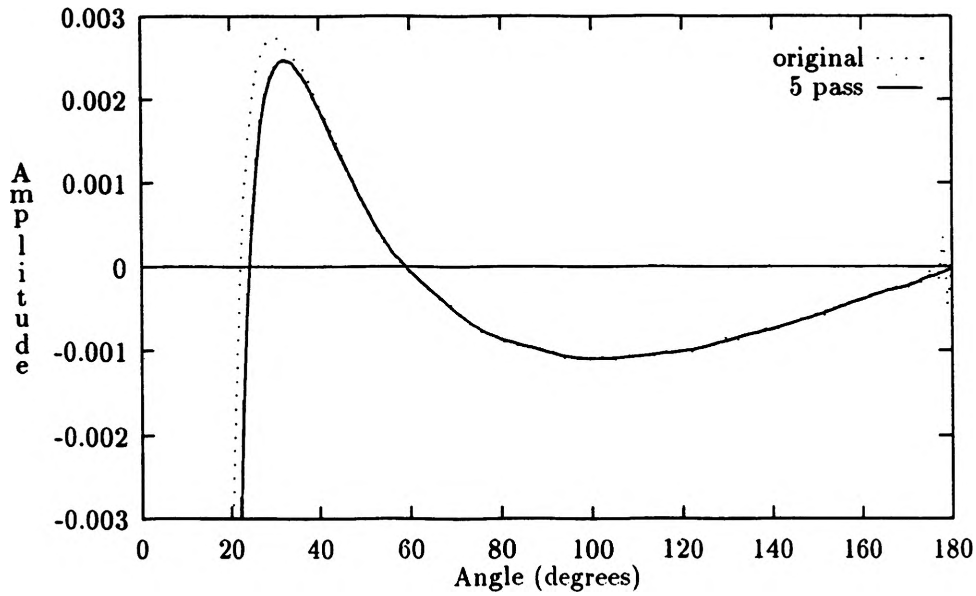

Figure 6: Amplitude curve

4 CONCLUSIONS

Areas of gentle slopes produce great results with very few passes through the algorithm; however, the shifts in the area of steep and rapidly changing slopes is a serious problem. These changes seem to be related to the slope and arc of the curve at a specific point. Several variables must be taken into account to improve this method of fitting. These would include the range on the y axis, the slope of the curve at a point, and the arc of the curve at each point. The y axis range should be considered, because the relation of the axis range to the range of the distortion that needs to be fitted tends to vary among the amplitude curves. The arc and amplitude of the arc could provide vital information on whether the curve area is gentle wiggles to be fitted or a peak to be left alone. Initial studies into a slope dependent factor being used to adjust the Δy from equation (12), has proven to lessen the effects of the amplitude shifting.

Further study is required to produce an algorithm which would work in the general case of curve fitting. Based on the results of the initial studies of a slope dependent factor, it seems possible to produce dampening routines or an intelligent algorithm to make use of the above variables, and lessen the effects to those areas where relaxation is not needed or desired.

5 ACKNOWLEDGEMENTS

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6 REFERENCES

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