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A One- and Two-Dimensional Least-Squares Smoothing and Edge-Sharpening Method for Image Processing

Mozelle R. Bell

OAK RIDGE NATIONAL LABORATORY

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Mozelle R. Bell

ABSTRACT

A rapid method is developed for two-dimensional smoothing and edge-sharpening by the least-squares fitting of a function to a limited area of the data. This convolution or matrix weighting is applied at each point of the data set to yield a smoothed or a sharpened image. Weighting matrices for 3 x 3, 5 x 5, and 7 x 7 point fitting areas are provided for polynomial function fits of all degrees up to the highest degree determinable. For the 7 x 7 point fitting area weights for fitting functions of up to the quartic in both dimensions are supplied. Application of the 5 x 5 point quadratic fit smoothing to a nuclear medicine image is shown as an example.

INTRODUCTION

Data smoothing is used extensively in nuclear medicine and other disciplines that employ images for analysis. Smoothing is needed to permit the use of isometric images, multicycle images, and color coded images, all of which suffer greatly from excessive raggedness of the data. Excess high frequency noise lying outside the frequency range defined by the system point source response reduces the readability of the image without contributing useful information. The smoothing methods generally employed in nuclear medicine are simple averages of neighboring points, of a 3 x 3 square area, or at best a simple Gaussian shaped weighting function. These methods are chosen for speed or simplicity of application and have little or no theoretical justification. The methods of least-squares two dimensional fitting give better results and have sound statistical justification but when applied in the usual straightforward manner are too time consuming for routine application to the large nuclear medicine images.

One-dimensional smoothing methods that provide least-squares fitted polynomials to noisy data are widely known. These yield good smoothing by a simple and rapid convolution or weighting method. Each entry in a short list of numbers derived from the Gram orthogonal polynomials[1] or directly from least-squares methods[2] is multiplied by successive data values. The sum of these products yields the least-squares fitted value at the mid-point of the range. The list of multipliers is then advanced along the data list by one point and the operation is repeated to provide a fitted value at the next position of the mid-point and so on. The method is rapid and well suited for use in small computers.

The method is here extended to two dimensions to provide a rapid two-dimensional smoothing method.

Another procedure, of value especially to nuclear medicine where images have necessarily both poor resolution and bad statistical fluctuation, is that of boundary sharpening. The method of sharpening an edge where there should be a sudden transition, but where the transition has been broadened by inadequate resolution, is an old one[3]. It has frequently been applied to Beta ray or scintillation spectra. It consists in the subtraction of a certain amount of the second derivative of the data curve from the curve to yield sharper transitions. Extending this method to two dimensions requires the generation of the directionally averaged second derivative of the image at each data point and the subtraction of the resultant correction image from the original to produce a resultant image with sharpened organ boundaries.

The same methods that provide the least-squares fitted value at the central point of the weighting matrix area can be extended to provide similarly the directionally averaged second derivative of the fitted two-dimensional function at the central point of the range. Weighting tables for 3 x 3, 5 x 5, and 7 x 7 point fitting regions are provided to yield smoothing and second derivative values for fitted functions of various degrees. The degree extends to a quartic in both dimensions for the 7 x 7 point area. The 7 x 7 point smoothing or second derivative procedures require about 3 minutes to process a 16,000 point nuclear medicine image on a PDP-8/E computer without EAE.

I. One Dimensional

A. Orthogonal Polynomial Method

The use of the Gram orthogonal polynomials to calculate the least-square formulas for n^{th} degree polynomials using 2M + 1 points has been expounded in great detail in F. B. Hildebrand's "Introduction to Numerical Analysis"[1] in sections 7.11 through 7.14 (see pages 288 through 302). [Formula numbers with H given in the remainder of this memo refer to this book]. Formulas are given there for the smoothed central value for cases up to $n = 5$ and $M = 3$ (i.e., fifth-degree seven-point formulas). For the sake of completeness we develop and repeat these formulas here and also include the companion formulas for the second derivative at the central point, since these will later be found to be useful for edge-sharpening of the data.

1. Five Point Formulas for Polynomials of Degree ≤ 3. For $M = 2$ (5 points) the highest order orthogonal polynomial needed is of third degree, $p_3(t,4)$; a 4th degree polynomial would fit the data exactly. Here t represents the distance from the mid-point of the range in units of the spacing.

Then $y(t) = a_0 p_0(t,4) + a_1 p_1(t,4) + a_2 p_2(t,4) + a_3 p_3(t,4)$ IA.1.1

Substituting the values for the orthogonal polynomials given by formulas 7.2.1H we have

$$y(t) = a_0 + a_1 \frac{t}{2} + \frac{a_2}{2}(t^2 - 2) + \frac{a_3}{6}(5t^3 - 17t) \qquad \text{IA.1.2}$$

whence

$$y''(t) = a_2 + 5a_3 t \qquad \text{IA.1.3}$$

For the central point, $t = 0$,

$$y(0) = a_0 - a_2 \qquad \text{IA.1.4}$$

and

$$y''(0) = a_2 \qquad \text{IA.1.5}$$

We note that at the central point the cubic term in the original equation makes no contribution. The quadratic and cubic fits give the same results at the central point.

Applying equations 7.11.14H and 7.11.13H and noting that $p_0(t,4) = 1$ and $p_2(t,4) = \frac{(t^2 - 2)}{2}$ we have

$$\gamma_0 = \sum_{t=-2}^{t=2} p_0^{\,2}(t,4) = 1^2 + 1^2 + 1^2 + 1^2 + 1^2 = 5 \qquad \text{IA.1.6}$$

$$\gamma_2 = \sum_{t=-2}^{t=2} p_2^{\,2}(t,4) = \left(\tfrac{1}{2}\right)^2 \left[(2)^2 + (-1)^2 + (-2)^2 + (-1)^2 + (2)^2\right] = \frac{7}{2} \qquad \text{IA.1.7}$$

$$a_0 = \frac{1}{\gamma_0} \sum_{t=-2}^{t=2} f(t)\, p_0(t,4) = \frac{1}{5}\left[f_{-2} + f_{-1} + f_0 + f_1 + f_2\right] \qquad \text{IA.1.8}$$

$$a_2 = \frac{1}{\gamma_2} \sum_{t=-2}^{t=2} f(t)\, p_2(t,4) = \frac{2}{7}\left[f_{-2} - 1/2\, f_{-1} - f_0 - 1/2\, f_1 + f_2\right] \qquad \text{IA.1.9}$$

Here $f_{-2}, f_{-1}, \ldots, f_2$ represent the data values at $t = -2, -1, \ldots, 2$. Hence for a polynomial fit of either degree 2 or degree 3

$$y(0) = a_0 - a_2 = \frac{1}{35}\left[-3f_{-2} + 12f_{-1} + 17f_0 + 12f_1 - 3f_2\right] \qquad \text{IA.1.10}$$

and

$$y''(0) = a_2 = \frac{2}{7}\left[f_{-2} - 1/2\, f_{-1} - f_0 - 1/2\, f_1 + f_2\right] \qquad \text{IA.1.11}$$

2. <u>Seven Point Formulas for Polynomials of Degree ≤ 5</u>. For $M = 3$ (7 points) the highest order least squares fit possible is

$$y(t) = a_0 p_0(t,6) + a_1 p_1(t,6) + a_2 p_2(t,6) + a_3 p_3(t,6) + a_4 p_4(t,6) + a_5 p_5(t,6) \qquad \text{IA.2.1}$$

Evaluating formulas 7.11.10H with M = 3 to obtain the orthogonal polynomials for this case and substituting into (2.1),

$$y(t) = a_0 + a_1 \frac{t}{3} + a_2 \left(\frac{t^2 - 4}{5}\right) + a_3 \left(\frac{t^3 - 7t}{6}\right) + a_4 \left(\frac{7t^4 - 67t^2 + 72}{36}\right) + a_5 \left(\frac{21t^5 - 245t^3 + 524t}{60}\right) \qquad \text{IA.2.2}$$

whence

$$y''(t) = \frac{2a_2}{5} + a_3 t + \frac{7}{3} a_4 t^2 - \frac{67}{18} a_4 + 7a_5 t^3 - \frac{49}{2} a_5 t \qquad \text{IA.2.3}$$

For the central point, t = 0,

$$y(0) = a_0 - \frac{4a_2}{5} + 2a_4 \qquad \text{IA.2.4}$$

and

$$y''(0) = \frac{2a_2}{5} - \frac{67}{18} a_4 \qquad \text{IA.2.5}$$

Again applying equations 7.11.14H and 7.11.13H we have

$$\gamma_0 = \sum_{t=-3}^{t=+3} (1)^2 = 7 \qquad \text{IA.2.6}$$

$$\gamma_2 = \sum_{t=-3}^{t=+3} \left[\frac{t^2 - 4}{5}\right]^2 = 1 + 0 + \frac{9}{25} + \frac{16}{25} + \frac{9}{25} + 0 + 1 = \frac{84}{25} \qquad \text{IA.2.7}$$

$$\gamma_4 = \sum_{t=-3}^{t=+3} \left[\frac{7t^4 - 67t^2 + 72}{36}\right]^2 = 1 + \frac{49}{9} + \frac{1}{9} + 4 + \frac{1}{9} + \frac{49}{9} + 1 = \frac{154}{9} \qquad \text{IA.2.8}$$

$$a_0 = \frac{1}{\gamma_0} \sum_{t=-3}^{t=+3} f(t)\,(1) = \frac{1}{7} [f_{-3} + f_{-2} + f_{-1} + f_0 + f_1 + f_2 + f_3] \qquad \text{IA.2.9}$$

$$a_2 = \frac{1}{\gamma_2} \sum_{t=-3}^{t=+3} f(t) \left[\frac{t^2 - 4}{5}\right] = \frac{25}{84} [f_{-3} + 0 - \frac{3}{5} f_{-1} - \frac{4}{5} f_0 - \frac{3}{5} f_1 + 0 + f_3] \qquad \text{IA.2.10}$$

$$a_4 = \frac{1}{\gamma_4} \sum_{t=-3}^{t=+3} f(t) \left[\frac{7t^4 - 67t^2 + 72}{36}\right] = \frac{9}{154} [f_{-3} - \frac{7}{3} f_{-2} + \frac{1}{3} f_{-1} + 2f_0 + \frac{1}{3} f_1 - \frac{7}{3} f_2 + f_3] \qquad \text{IA.2.11}$$

For a polynomial fit of degree 2 or degree 3, a_4 and a_5 do not occur and

$$y(0) = a_0 - \frac{4}{5} a_2 = \frac{1}{21} [-2f_{-3} + 3f_{-2} + 6f_{-1} + 7f_0 + 6f_1 + 3f_2 - 2f_3] \qquad \text{IA.2.12}$$

and

$$y''(0) = \frac{2a_2}{5} = \frac{5}{42} [f_{-3} - \frac{3}{5} f_{-1} - \frac{4}{5} f_0 - \frac{3}{5} f_1 + f_3] \qquad \text{IA.2.13}$$

For a polynomial fit of degree 4 or degree 5,

$$y(0) = a_0 - \frac{4}{5} a_2 + 2a_4 = \frac{1}{231} [5f_{-3} - 30f_{-2} + 75f_{-1} + 131f_0 + 75f_1 - 30f_2 + 5f_{-3}] \qquad \text{IA.2.14}$$

and

$$y''(0) = \frac{2a_2}{5} - \frac{67}{18} a_4 = \frac{1}{132} [-13f_{-3} + 67f_{-2} - 19f_{-1} - 70f_0 - 19f_1 + 67f_2 - 13f_3] \qquad \text{IA.2.15}$$

B. Least Squares Solutions Using a Symmetrical Grid with Equal Spacing

Let us determine our experimental data points in the following symmetrical types of grid:

-2 -1 0 1 2 → x-axis for 5 points

and

-3 -2 -1 0 1 2 3 → x-axis for 7 points

We then have $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} x_i^3 = \sum_{i=1}^{n} x_i^5 = \ldots = \sum_{i=1}^{n} x_i^{odd} = 0.$

As we shall now show this fact allows us to make such great simplifications in the set of least-square equations that the solutions thereof may be obtained directly. This provides an alternate method of solution in which the use and knowledge of orthogonal polynomials is not needed.

Let us represent a general fitting polynomial of degree ≤ 5 by

$$y = b_1 + b_2x + b_3x^2 + b_4x^3 + b_5x^4 + b_6x^5 \qquad \text{IB.1}$$

Then $y(0) = b_1$ IB.2

and $y''(0) = 2b_3$ IB.3

We can reduce this from a quintic to a quartic to a cubic to a quadratic by setting $b_6 = 0$, $b_5 = 0$, and $b_4 = 0$ respectively.

The least-square equations are obtained by minimizing

$$F \equiv \sum_{i=1}^{n} [f_i - (b_1 + b_2x_i + b_3x_i^2 + b_4x_i^3 + b_5x_i^4 + b_6x_i^5)]^2 \qquad \text{IB.4}$$

where f_i is the experimental data.

Differentiating F with respect to b_1, b_2, b_3, b_4, b_5, and b_6 in turn, setting each of the six equations equal to 0 and remembering that $\Sigma\, x_i^{odd} = 0$, we get the following set of least-squares equations.

$$\frac{\partial F}{\partial b_1}: \quad C_1 \equiv \Sigma f_i = nb_1 + b_3 \Sigma x_i^2 + b_5 \Sigma x_i^4 \qquad \text{IB.5}$$

$$\frac{\partial F}{\partial b_2}: \quad C_2 \equiv \Sigma f_i x_i = b_2 \Sigma x_i^2 + b_4 \Sigma x_i^4 + b_6 \Sigma x_i^6 \qquad \text{IB.6}$$

$$\frac{\partial F}{\partial b_3}: \quad C_3 \equiv \Sigma f_i x_i^2 = b_1 \Sigma x_i^2 + b_3 \Sigma x_i^4 + b_5 \Sigma x_i^6 \qquad \text{IB.7}$$

$$\frac{\partial F}{\partial b_4}: \quad C_4 \equiv \Sigma f_i x_i^3 = b_2 \Sigma x_i^4 + b_4 \Sigma x_i^6 + b_6 \Sigma x_i^8 \qquad \text{IB.8}$$

$$\frac{\partial F}{\partial b_5}: \quad C_5 \equiv \Sigma f_i x_i^4 = b_1 \Sigma x_i^4 + b_3 \Sigma x_i^6 + b_5 \Sigma x_i^8 \qquad \text{IB.9}$$

$$\frac{\partial F}{\partial b_6}: \quad C_6 \equiv \Sigma f_i x_i^5 = b_2 \Sigma x_i^6 + b_4 \Sigma x_i^8 + b_6 \Sigma x_i^{10} \qquad \text{IB.10}$$

For determining central values only the three equations B.5, B.7, and B.9 need be considered.

The solutions of the least-squares equations will be given as linear functions of C_1, C_3, and C_5, which are themselves linear functions of f_i. We will use these facts to find a set of weights, w_i, such that our answers may be written as $\sum_{i=1}^{n} w_i f_i$, an easily calculable form.

1. Five Point Formulas.

For $n = 5$: $x_1 = -2$, $x_2 = -1$, $x_3 = 0$, $x_4 = 1$, $x_5 = 2$, whence

$$\Sigma x_i^2 = 10; \ \Sigma x_i^4 = 34; \ \Sigma x_i^6 = 130; \ \Sigma x_i^8 = 514.$$

1.1. Quadratic or Cubic (highest possible degree for $n = 5$). For a quadratic or cubic ($b_5 = b_6 \equiv 0$) the set of equations to be solved becomes

$$C_1 = 5b_1 + 10b_3 \qquad \text{IB.1.1}$$

$$C_3 = 10b_1 + 34b_3 \qquad \text{IB.1.2}$$

The solution of this pair of equations gives

$$y(0) = b_1 = \frac{1}{35}(17C_1 - 5C_3) \qquad \text{IB.1.3}$$

$$y''(0) = 2b_3 = \frac{1}{7}(C_3 - 2C_1) \qquad \text{IB.1.4}$$

Applying the definitions of C_1 and C_3

$$y(0) = \frac{1}{35}[-3f_{-2} + 12f_{-1} + 17f_0 + 12f_1 - 3f_2] \qquad \text{IB.1.5}$$

and

$$y''(0) = \frac{1}{7}[2f_{-2} - f_{-1} - 2f_0 - f_1 + 2f_2] \qquad \text{IB.1.6}$$

in agreement with equations IA.1.10 and IA.1.11, where f with a subscript means the value of the data at the x point which is the subscript.

2. Seven Point Formulas.

For $n = 7$: $x_1 = -3$; $x_2 = -2$; $x_3 = -1$; $x_4 = 0$; $x_5 = 1$; $x_6 = 2$; $x_7 = 3$ whence

$$\Sigma\, x_i^{\,2} = 28;\ \Sigma\, x_i^{\,4} = 196;\ \Sigma\, x_i^{\,6} = 1588;\ \Sigma\, x_i^{\,8} = 13636.$$

2.1. Quadratic or Cubic. For a quadratic or cubic the set of equations to be solved is:

$$C_1 = 7b_1 + 28b_3 \qquad \text{IB.2.1.1}$$

$$C_3 = 28b_1 + 196b_3 \qquad \text{IB.2.1.2}$$

The solution of this pair of equations gives

$$y(0) = b_1 = \frac{1}{21}(7C_1 - C_3) \qquad \text{IB.2.1.3}$$

$$y''(0) = 2b_3 = \frac{1}{42}(C_3 - 4C_1) \qquad \text{IB.2.1.4}$$

Expressed in terms of the experimental data these are

$$y(0) = \frac{1}{21}(-2f_{-3} + 3f_{-2} + 6f_{-1} + 7f_0 + 6f_1 + 3f_2 - 2f_3) \qquad \text{IB.2.1.5}$$

a nd

$$y''(0) = \frac{1}{42}(5f_{-3} + 0 - 3f_{-1} - 4f_0 - 3f_1 + 0 + 5f_3) \qquad \text{IB.2.1.6}$$

in agreement with equations IA.2.12 and IA.2.13.

2.2. Quartic or Quintic (highest possible degree for $n = 7$). For a quartic or quintic the set of equations to be solved is

$$C_1 = 7b_1 + 28b_3 + 196b_5 \qquad \text{IB.2.2.1}$$

$$C_3 = 28b_1 + 196b_3 + 1588b_5 \qquad \text{IB.2.2.2}$$

$$C_5 = 196b_1 + 1588b_3 + 13636b_5 \qquad \text{IB.2.2.3}$$

Although the arithmetic involved is more tedious than in previous cases, the solution is straightforward and gives

$$y(0) = b_1 = \frac{524C_1 - 245C_3 + 21C_5}{924} \qquad \text{IB.2.2.4}$$

and

$$y''(0) = 2b_3 = \frac{-840C_1 + 679C_3 - 67C_5}{1584} \qquad \text{IB.2.2.5}$$

Expressed in terms of the experimental data these are

$$y(0) = \frac{1}{231}(5f_{-3} - 30f_{-2} + 75f_{-1} + 131f_0 + 75f_1 - 30f_2 + 5f_3) \qquad \text{IB.2.2.6}$$

and

$$y''(0) = \frac{1}{132}(-13f_{-3} + 67f_{-2} - 19f_{-1} - 70f_0 - 19f_1 + 67f_2 - 13f_3) \qquad \text{IB.2.2.7}$$

in agreement with equations IA.2.14 and IA.2.15.

II. Two Dimensional

1. Determination of Central Value of Function and Second Derivative.

We shall here generalize the symmetric grid procedure described in Section I, Part B.

Let us represent a general fitting polynomial of degree ≤ 5 in two dimensions by

$$\begin{aligned} f(x,y) = {} & b_1 + b_2x + b_3y + b_4x^2 + b_5x^2y^2 + b_6y^2 + b_7x^3 \\ & + b_8x^2y + b_9xy^2 + b_{10}y^3 + b_{11}x^4 + b_{12}x^3y + b_{13}x^2y^2 \\ & + b_{14}xy^3 + b_{15}y^4 + b_{16}x^5 + b_{17}x^4y + b_{18}x^3y^2 + b_{19}x^2y^3 \\ & + b_{20}xy^4 + b_{21}y^5 \end{aligned} \qquad \text{II.1.1}$$

Then

$$f(0,0) = b_1. \qquad \text{II.1.2}$$

We can reduce II.1.1 from a quintic to a quartic by setting b_{16} through $b_{21} \equiv 0$; to a cubic by additionally setting b_{11} through $b_{15} \equiv 0$; to a quadratic by additionally setting b_7 through $b_{10} \equiv 0$.

The directional derivative $\frac{df}{ds}$ at any point (x,y) taken in the direction of a straight line making an angle α with the x-axis is

$$\frac{df(x,y)}{ds} = \frac{\partial f}{\partial x} \cos \alpha + \frac{\partial f}{\partial y} \sin \alpha \equiv f_x \cos \alpha + f_y \sin \alpha \qquad \text{II.1.3}$$

The second directional derivative is

$$\frac{d^2f}{ds^2}(x,y) = \frac{\partial[f_x \cos \alpha + f_y \sin \alpha]}{\partial x} \cos \alpha + \frac{\partial[f_x \cos \alpha + f_y \sin \alpha]}{\partial y} \sin \alpha \qquad \text{II.1.4}$$

or

$$\frac{d^2f}{ds^2}(x,y) = f_{xx} \cos^2 \alpha + 2f_{yx} \sin \alpha \cos \alpha + f_{yy} \sin^2 \alpha \qquad \text{II.1.5}$$

since $f_{yx} = f_{xy}$. We take the average of $f''(x,y)$ over α by noting that $(\cos^2\alpha)_{av} = (\sin^2\alpha)_{av} = \frac{1}{2\pi}\int_0^{2\pi} \cos^2\alpha d\alpha = \frac{1}{2\pi}\int_0^{2\pi} \sin^2\alpha = \frac{1}{2}$, and $(\sin\alpha\cos\alpha)_{av}$ $= \frac{1}{2\pi}\int_0^{2\pi} \sin\alpha\cos\alpha d\alpha = 0$. Thus

$$f''(x,y)_{av} = \frac{1}{2}(f_{xx} + f_{yy}) \qquad \text{II.1.6}$$

From equation II.1.1

$$f''(0,0)_{av} = b_4 + b_6. \qquad \text{II.1.7}$$

When comparing one-dimensional answers as special cases of the two-dimensional results, note that since the two-dimensional result is an average it gives only 1/2 the one-dimensional results in the x and y directions, respectively.

2. Least-Squares Equations. The least-square equations are obtained by minimizing

$$\begin{aligned} F \equiv \sum_{i=1}^{n}\sum_{j=1}^{n} [f_{ij} - (b_1 + b_2x + b_3y + b_4x^2 + b_5xy + b_6y^2 \\ + b_7x^3 + b_8x^2y + b_9xy^2 + b_{10}y^3 + b_{11}x^4 + b_{12}x^3y + b_{13}x^2y^2 \\ + b_{14}xy^3 + b_{15}y^4 + b_{16}x^5 + b_{17}x^4y + b_{18}x^3y^2 + b_{19}x^2y^3 \\ + b_{20}xy^4 + b_{21}y^5]^2 \end{aligned} \qquad \text{II.2.1}$$

where f_{ij} is the experimental data. Differentiating F with respect to $b_1, b_2, b_3, \ldots, b_{21}$ in turn, setting each of the 21 equations equal to 0 and remembering that $\Sigma x_i^{odd} = \Sigma y_i^{odd} = 0$, we get the following set of least-square equations.

$$\frac{\partial F}{\partial b_1}: \quad k_1 \equiv \sum_i \sum_j f_{ij} = n^2 b_1 + n\Sigma x_i^{\,2} b_4 + n\Sigma y_j^{\,2} b_6 + n\Sigma x_i^{\,4} b_{11} + \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_{13}$$
$$+ n\Sigma y_j^{\,4} b_{15} \qquad \text{II.2.2}$$

$$\frac{\partial F}{\partial b_2}: \quad k_2 \equiv \sum_i \sum_j f_{ij} x_i = n\Sigma x_i^{\,2} b_2 + n\Sigma x_i^{\,4} b_7 + \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_9 + n\Sigma x_i^{\,6} b_{16}$$
$$+ \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_{18} + \Sigma x_i^{\,2} \Sigma y_j^{\,4} b_{20} \qquad \text{II.2.3}$$

$$\frac{\partial F}{\partial b_3}: \quad k_3 \equiv \sum_i \sum_j f_{ij} y_j = n\Sigma y_j^{\,2} b_3 + \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_8 + n\Sigma y_j^{\,4} b_{10} + \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_{17}$$
$$+ \Sigma x_i^{\,2} \Sigma y_j^{\,4} b_{19} + n\Sigma y_j^{\,4} b_{21} \qquad \text{II.2.4}$$

$$\frac{\partial F}{\partial b_4}: \quad k_4 \equiv \sum_i \sum_j f_{ij} x_i^{\,2} = n\Sigma x_i^{\,2} b_1 + n\Sigma x_i^{\,4} b_4 + \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_6 + n\Sigma x_i^{\,6} b_{11}$$
$$+ \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_{13} + \Sigma x_i^{\,2} \Sigma y_j^{\,4} b_{15} \qquad \text{II.2.5}$$

$$\frac{\partial F}{\partial b_5}: \quad k_5 \equiv \sum_i \sum_j f_{ij} x_i y_j = \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_5 + \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_{12} + \Sigma x_i^{\,2} \Sigma y_j^{\,4} b_{14} \qquad \text{II.2.6}$$

$$\frac{\partial F}{\partial b_6}: \quad k_6 \equiv \sum_i \sum_j f_{ij} y_j^{\,2} = n\Sigma y_j^{\,2} b_1 + \Sigma x_i^{\,2} \Sigma y_j^{\,2} b_4 + n\Sigma y_j^{\,4} b_6 + \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_{11}$$
$$+ \Sigma x_i^{\,2} \Sigma y_j^{\,4} b_{13} + n\Sigma y_j^{\,6} b_{15} \qquad \text{II.2.7}$$

$$\frac{\partial F}{\partial b_7}: \quad k_7 \equiv \sum_i \sum_j f_{ij} x_i^{\,3} = n\Sigma x_i^{\,4} b_2 + n\Sigma x_i^{\,6} b_7 + \Sigma x_i^{\,4} \Sigma y_j^{\,2} b_9 + n\Sigma x_i^{\,8} b_{16}$$
$$+ \Sigma x_i^{\,6} \Sigma y_j^{\,2} b_{18} + \Sigma x_i^{\,4} \Sigma y_j^{\,4} b_{20} \qquad \text{II.2.8}$$

$$\frac{\partial F}{\partial b_8}:\quad k_8 \equiv \sum_i \sum_j f_{ij}x_i^2 y_j = \Sigma x_i^2 \Sigma y_j^2 b_3 + \Sigma x_i^4 \Sigma y_j^2 b_8 + \Sigma x_i^2 \Sigma y_j^4 b_{10}$$
$$+ \Sigma x_i^6 \Sigma y_j^2 b_{17} + \Sigma x_i^4 \Sigma y_j^4 b_{19} + \Sigma x_i^2 \Sigma y_j^6 b_{21} \qquad \text{II.2.9}$$

$$\frac{\partial F}{\partial b_9}:\quad k_9 \equiv \sum_i \sum_j f_{ij}x_i y_j^2 = \Sigma x_i^2 \Sigma y_j^2 b_2 + \Sigma x_i^4 \Sigma y_j^2 b_7 + \Sigma x_i^2 \Sigma y_j^4 b_9$$
$$+ \Sigma x_i^6 \Sigma y_j^2 b_{16} + \Sigma x_i^4 \Sigma y_j^4 b_{18} + \Sigma x_i^2 \Sigma y_j^6 b_{20} \qquad \text{II.2.10}$$

$$\frac{\partial F}{\partial b_{10}}:\quad k_{10} \equiv \sum_i \sum_j f_{ij}y_j^3 = n\Sigma y_j^4 b_3 + \Sigma x_i^2 \Sigma y_j^4 b_8 + n\Sigma y_j^6 b_{10}$$
$$+ \Sigma x_i^4 \Sigma y_j^4 b_{17} + \Sigma x_i^2 \Sigma y_j^6 b_{19} + n\Sigma y_j^8 b_{21} \qquad \text{II.2.11}$$

$$\frac{\partial F}{\partial b_{11}}:\quad k_{11} \equiv \sum_i \sum_j f_{ij}x_i^4 = n\Sigma x_i^4 b_1 + n\Sigma x_i^6 b_4 + \Sigma x_i^4 \Sigma y_j^6 b_6$$
$$+ n\Sigma x_i^8 b_{11} + \Sigma x_i^6 \Sigma y_j^2 b_{13} + \Sigma x_i^4 \Sigma y_j^4 b_{15} \qquad \text{II.2.12}$$

$$\frac{\partial F}{\partial b_{12}}:\quad k_{12} \equiv \sum_i \sum_j f_{ij}x_i^3 y_j = \Sigma x_i^4 \Sigma y_j^2 b_5 + \Sigma x_i^6 \Sigma y_j^2 b_{12}$$
$$+ \Sigma x_i^4 \Sigma y_j^4 b_{14} \qquad \text{II.2.13}$$

$$\frac{\partial F}{\partial b_{13}}:\quad k_{13} \equiv \sum_i \sum_j f_{ij}x_i^2 y_j^2 = \Sigma x_i^2 \Sigma y_j^2 b_1 + \Sigma x_i^4 \Sigma y_j^2 b_4 + \Sigma x_i^2 \Sigma y_j^4 b_6$$
$$+ \Sigma x_i^6 \Sigma y_j^2 b_{11} + \Sigma x_i^4 \Sigma y_j^4 b_{13} + \Sigma x_i^2 \Sigma y_j^6 b_{15} \qquad \text{II.2.14}$$

$$\frac{\partial F}{\partial b_{14}}:\quad k_{14} \equiv \sum_i \sum_j f_{ij}x_i y_j^3 = \Sigma x_i^2 \Sigma y_j^4 b_5 + \Sigma x_i^4 \Sigma y_j^4 b_{12}$$
$$+ \Sigma x_i^2 \Sigma y_j^6 b_{14} \qquad \text{II.2.15}$$

$$\frac{\partial F}{\partial b_{15}}: \quad k_{15} \equiv \sum_i \sum_j f_{ij} y_j^4 = n\Sigma y_j^4 b_1 + \Sigma x_i^2 \Sigma y_j^4 b_4 + n\Sigma y_j^6 b_6 + \Sigma x_i^4 \Sigma y_j^4 b_{11}$$

$$+ \Sigma x_i^2 \Sigma y_j^6 b_{13} + n\Sigma y_j^8 b_{15} \qquad \text{II.2.16}$$

$$\frac{\partial F}{\partial b_{16}}: \quad k_{16} \equiv \sum_i \sum_j f_{ij} x_i^5 = n\Sigma x_i^6 b_2 + n\Sigma x_i^8 b_7 + \Sigma x_i^6 \Sigma y_j^2 b_9 + n\Sigma x_i^{10} b_{16}$$

$$+ \Sigma x_i^8 \Sigma y_j^2 b_{18} + \Sigma x_i^6 \Sigma y_j^4 b_{20} \qquad \text{II.2.17}$$

$$\frac{\partial F}{\partial b_{17}}: \quad k_{17} \equiv \sum_i \sum_j f_{ij} x_i^4 y_j = \Sigma x_i^4 \Sigma y_j^2 b_3 + \Sigma x_i^6 \Sigma y_j^2 b_8 + \Sigma x_i^4 \Sigma y_j^4 b_{10}$$

$$+ \Sigma x_i^4 \Sigma y_j^6 b_{21} + \Sigma x_i^8 \Sigma y_j^2 b_{17} + \Sigma x_i^6 \Sigma y_j^4 b_{19} \qquad \text{II.2.18}$$

$$\frac{\partial F}{\partial b_{18}}: \quad k_{18} \equiv \sum_i \sum_j f_{ij} x_i^3 y_j^2 = \Sigma x_i^4 \Sigma y_j^2 b_2 + \Sigma x_i^6 \Sigma y_j^2 b_7 + \Sigma x_i^4 \Sigma y_j^4 b_9$$

$$+ \Sigma x_i^8 \Sigma y_j^2 b_{16} + \Sigma x_i^6 \Sigma y_j^4 b_{18} + \Sigma x_i^4 \Sigma y_j^6 b_{20} \qquad \text{II.2.19}$$

$$\frac{\partial F}{\partial b_{19}}: \quad k_{19} \equiv \sum_i \sum_j f_{ij} x_i^2 y_j^3 = \Sigma x_i^2 \Sigma y_j^4 b_3 + \Sigma x_i^4 \Sigma y_j^4 b_8 + \Sigma x_i^2 \Sigma y_j^6 b_{10}$$

$$+ \Sigma x_i^6 \Sigma y_j^4 b_{17} + \Sigma x_i^4 \Sigma y_j^6 b_{19} + \Sigma x_i^2 \Sigma y_j^8 b_{21} \qquad \text{II.2.20}$$

$$\frac{\partial F}{\partial b_{20}}: \quad k_{20} \equiv \sum_i \sum_j f_{ij} x_i y_j^4 = \Sigma x_i^2 \Sigma y_j^4 b_2 + \Sigma x_i^4 \Sigma y_j^4 b_7 + \Sigma x_i^2 \Sigma y_j^6 b_9$$

$$+ \Sigma x_i^6 \Sigma y_j^4 b_{16} + \Sigma x_i^4 \Sigma y_j^6 b_{18} + \Sigma x_i^2 \Sigma y_j^8 b_{20} \qquad \text{II.2.21}$$

$$\frac{\partial F}{\partial b_{21}}: \quad k_{21} \equiv \sum_i \sum_j f_{ij} y_j^5 = n\Sigma y_j^6 b_3 + \Sigma x_i^2 \Sigma y_j^6 b_8 + n\Sigma y_j^{10} b_{10} + \Sigma x_i^4 \Sigma y_j^6 b_{17}$$

$$+ \Sigma x_i^2 \Sigma y_j^8 b_{19} + n\Sigma y_j^{10} b_{21} \qquad \text{II.2.22}$$

From this set of equations we see that the variables are split into the following independent groups:

b_1, b_4, b_6, b_{11}, b_{13}, b_{15} - occur only in equations 2, 5, 7, 12, 14, and 16

b_2, b_7, b_9, b_{16}, b_{18}, b_{20} - occur only in equations 3, 8, 10, 17, 19, and 21

b_3, b_8, b_{10}, b_{17}, b_{19}, b_{21} - occur only in equations 4, 9, 11, 18, 20, and 22

b_5, b_{12}, b_{14} - occur only in equations 6, 13, and 15.

Since we are interested only in central values and equations II.1.2 and II.1.7 show that these are functions of b_1, b_4, and b_6 only, we now consider only the six equations determining these values.

We again point out that - as in the one-dimensional case - all of the k values are linear combinations of f_{ij} and that our smoothing value (b_1) and second derivative value ($b_4 + b_6$) will be some linear combination of the "k's". Hence to determine a weighting factor w_{ij} at any point we need only use the contribution of that point to each of the summations involved in the "k" values in the formulas. (Another way of saying this is that to determine the weight at each point we consider f_{ij} to be a delta-function; 1 at the point and 0 elsewhere.)

3. <u>3 x 3 Point Formulas</u>. For n x n = 3 x 3: $x_1 = y_1 = -1$; $x_2 = y_2 = 0$; $x_3 = y_3 = +1$ whence $\Sigma x_i^2 = \Sigma y_j^2 = 2$.

3.1. <u>Linear</u>. For a linear fit ($b_4 = b_5 = \ldots = b_{21} = 0$) the set of equations to be solved becomes

$$k_1 = 9b_1 \qquad \text{II.3.1}$$

Hence $f(0,0) = b_1 = \frac{k_1}{9}$ and the smoothing matrix of weights is

$$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

3.2. Quadratic. For a quadratic fit ($b_7 = b_8 = \ldots = b_{21} = 0$) the set of equations to be solved becomes

$$k_1 = 9b_1 + 6b_4 + 6b_6 \qquad \text{II.3.2.1}$$

$$k_4 = 6b_1 + 6b_4 + 4b_6 \qquad \text{II.3.2.2}$$

$$k_6 = 6b_1 + 4b_4 + 6b_6 \qquad \text{II.3.2.3}$$

The solution of this set of equations gives

$$f(0,0) = b_1 = \frac{1}{9}(5k_1 - 3k_4 - 3k_6) \qquad \text{II.3.2.4}$$

and

$$f''(0,0)_{av} = b_4 + b_6 = \frac{1}{6}(3k_4 + 3k_6 - 4k_1) \qquad \text{II.3.2.5}$$

Applying the definitions of k_1, k_4, and k_6 the matrix of weights for $f(0,0)$ is

$$\frac{1}{9}\begin{bmatrix} -1 & 2 & -1 \\ 2 & 5 & 2 \\ -1 & 2 & -1 \end{bmatrix} \qquad \text{II.3.2.6}$$

and for $f''(0,0)_{av}$ the matrix is

$$\frac{1}{6}\begin{bmatrix} 2 & -1 & 2 \\ -1 & -4 & -1 \\ 2 & -1 & 2 \end{bmatrix} \qquad \text{II.3.2.7}$$

4. 5 x 5 Point Formulas. For n x n = 5 x 5: $x_1 = y_1 = -2$; $x_2 = y_2 = -1$; $x_3 = y_3 = 0$; $x_4 = y_4 = +1$; $x_5 = y_5 = +2$ whence $\Sigma\, x_i^2 = \Sigma\, y_j^2 = 10$; $\Sigma\, x_i^4 = \Sigma\, y_j^4 = 34$; $\Sigma\, x_i^6 = \Sigma\, y_j^6 = 130$; $\Sigma\, x_i^8 = \Sigma\, y_j^8 = 514$.

4.1. Linear. The linear fit gives $f(0,0) = b_1 = \frac{k_1}{25}$, a uniform weighting for each element in the smoothing matrix.

4.2. Quadratic or Cubic. For a quadratic or cubic fit ($b_{11} = b_{12} = \ldots = b_{21} = 0$) the set of equations to be solved becomes

$$k_1 = 25b_1 + 50b_4 + 50b_6 \qquad \text{II.4.2.1}$$

$$k_4 = 50b_1 + 170b_4 + 100b_6 \qquad \text{II.4.2.2}$$

$$k_6 = 50b_1 + 100b_4 + 170b_6 \qquad \text{II.4.2.3}$$

The solution of this set of equations gives

$$f(0,0) = b_1 = \frac{1}{175}(27k_1 - 5k_4 - 5k_6) \qquad \text{II.4.2.4}$$

and

$$f''(0,0)_{av} = b_4 + b_6 = \frac{1}{70}(-4k_1 + k_4 + k_6) \qquad \text{II.4.2.5}$$

Applying the definitions of k_1, k_4, and k_6 the matrix of weights for $f(0,0)$ is

$$\frac{1}{175}\begin{bmatrix} -13 & 2 & 7 & 2 & -13 \\ 2 & 17 & 22 & 17 & 2 \\ 7 & 22 & 27 & 22 & 7 \\ 2 & 17 & 22 & 17 & 2 \\ -13 & 2 & 7 & 2 & -13 \end{bmatrix} \qquad \text{II.4.2.6}$$

and for $f''(0,0)_{av}$ the matrix is

$$\frac{1}{70}\begin{bmatrix} 4 & 1 & 0 & 1 & 4 \\ 1 & -2 & -3 & -2 & 1 \\ 0 & -3 & -4 & -3 & 0 \\ 1 & -2 & -3 & -2 & 1 \\ 4 & 1 & 0 & 1 & 4 \end{bmatrix} \qquad \text{II.4.2.7}$$

4.3. Quartic or Quintic. For a quartic or quintic fit the set of equations to be solved is

$$
\begin{aligned}
k_1 &= 25b_1 + 50b_4 + 50b_6 + 170b_{11} + 100b_{13} + 170b_{15} \\
k_4 &= 50b_1 + 170b_4 + 100b_6 + 650b_{11} + 340b_{13} + 340b_{15} \\
k_6 &= 50b_1 + 100b_4 + 170b_6 + 340b_{11} + 340b_{13} + 650b_{15} \\
k_{11} &= 170b_1 + 650b_4 + 340b_6 + 2570b_{11} + 1300b_{13} + 1156b_{15} \\
k_{13} &= 100b_1 + 340b_4 + 340b_6 + 1300b_{11} + 1156b_{13} + 1300b_{15} \\
k_{15} &= 170b_1 + 340b_4 + 650b_6 + 1156b_{11} + 1300b_{13} + 2570b_{15}
\end{aligned}
\qquad \text{II.4.3.1}
$$

It is helpful to combine the above set of six equations into

$$
\begin{aligned}
k_1 &= 25b_1 + 50(b_4 + b_6) + 100b_{13} + 170(b_{11} + b_{15}) \\
(k_4 + k_6) &= 100b_1 + 270(b_4 + b_6) + 680b_{13} + 990(b_{11} + b_{15}) \\
(k_{11} + k_{15}) &= 340b_1 + 990(b_4 + b_6) + 2600b_{13} + 3726(b_{11} + b_{15}) \\
k_{13} &= 100b_1 + 340(b_4 + b_6) + 1156b_{13} + 1300(b_{11} + b_{15})
\end{aligned}
\qquad \text{II.4.3.2}
$$

Then by solving the last of this group of equations for b_{13} in terms of the other unknowns, substituting that quantity into the first three equations and simplifying we get:

$$
\begin{aligned}
289k_1 - 25k_{13} &= (5)(945)b_1 + (170)(35)(b_4 + b_6) + (2)(8315)(b_{11} + b_{15}) \\
17(k_4 + k_6) - 10k_{13} &= (5)(140)b_1 + (170)(7)(b_4 + b_6) + (2)(1915)(b_{11} + b_{15}) \\
289(k_{11} + k_{15}) - 650k_{13} &= (5)(6652)b_1 + (170)(383)(b_4 + b_6) \\
&\quad + (2)(115907)(b_{11} + b_{15})
\end{aligned}
\qquad \text{II.4.3.3}
$$

The solution of this set of equations gives

$$f(0,0) = b_1 = \frac{1}{4900}\left[2164k_1 - 1425(k_4 + k_6) + 245(k_{11} + k_{15}) + 100k_{13}\right] \qquad \text{II.4.3.4}$$

and

$$f''(0,0)_{av} = b_4 + b_6 = \frac{1}{70560}\left[-41040k_1 + 37523(k_4 + k_6) - 7595(k_{11} + k_{15}) - 1440k_{13}\right] \qquad \text{II.4.3.5}$$

Applying the definitions of k_1, k_4, k_6, k_{11}, k_{15}, and k_{13} the matrix of weights for f(0,0) is

$$\frac{1}{1225}\begin{bmatrix} 51 & -99 & 96 & -99 & 51 \\ -99 & -24 & 246 & -24 & -99 \\ 96 & 246 & 541 & 246 & 96 \\ -99 & -24 & 246 & -24 & -99 \\ 51 & -99 & 96 & -99 & 51 \end{bmatrix} \qquad \text{II.4.3.6}$$

and for $f''_{av}(0,0)$ the matrix is

$$\frac{1}{17640}\begin{bmatrix} -1734 & 2925 & -3117 & 2925 & -1734 \\ 2925 & 4344 & -2778 & 4344 & 2925 \\ -3117 & -2778 & -10260 & -2778 & -3117 \\ 2925 & 4344 & -2778 & 4344 & 2925 \\ -1734 & 2925 & -3117 & 2925 & -1734 \end{bmatrix} \qquad \text{II.4.3.7}$$

5. <u>7 x 7 Point Formulas</u>. For n x n = 7 x 7: $x_1 = y_1 = -3$; $x_2 = y_2 = -2$; $x_3 = y_3 = -1$; $x_4 = y_4 = 0$; $x_5 = y_5 = 1$; $x_6 = y_6 = 2$; $x_7 = y_7 = 3$ whence $\Sigma x_i^2 = \Sigma y_j^2 = 28$; $\Sigma x_i^4 = \Sigma y_j^4 = 196$; $\Sigma x_i^6 = \Sigma y_j^6 = 1588$; $\Sigma x_i^8 = \Sigma y_j^8 = 13636$; $\Sigma x_i^2\,\Sigma y_j^2 = 784$; $\Sigma x_i^2\,\Sigma y_j^4 = \Sigma x_i^4\,\Sigma y_j^2 = 5488$; $\Sigma x_i^2\,\Sigma y_j^6 = \Sigma x_i^6\,\Sigma y_j^2 = 44464$; $\Sigma x_i^4\,\Sigma y_j^4 = 38416$.

5.1. <u>Linear</u>. The linear fit gives $f(0,0) = b_1 = \frac{k_1}{49}$, a uniform weighting for each element in the smoothing matrix.

5.2. <u>Quadratic or Cubic</u>. For a quadratic or cubic fit ($b_{11} = b_{12} = \ldots = b_{21} = 0$) the set of equations to be solved becomes

$$\begin{aligned} k_1 &= 49b_1 + 196b_4 + 196b_6 \\ k_4 &= 196b_1 + (7)(196)b_4 + (4)(196)b_6 \\ k_6 &= 196b_1 + (4)(196)b_4 + (7)(196)b_6 \end{aligned} \qquad \text{II.5.2.1}$$

The solution of this set of equations gives

$$f(0,0) = b_1 = \frac{1}{147}(11k_1 - k_4 - k_6) \qquad \text{II.5.2.2}$$

and

$$f''(0,0)_{av} = b_4 + b_6 = \frac{1}{588}(k_4 + k_6 - 8k_1) \qquad \text{II.5.2.3}$$

Applying the definitions of k_1, k_4, and k_6 the matrix of weights for $f(0,0)$ is

$$\frac{1}{147}\begin{bmatrix} -7 & -2 & 1 & 2 & 1 & -2 & -7 \\ -2 & 3 & 6 & 7 & 6 & 3 & -2 \\ 1 & 6 & 9 & 10 & 9 & 6 & 1 \\ 2 & 7 & 10 & 11 & 10 & 7 & 2 \\ 1 & 6 & 9 & 10 & 9 & 6 & 1 \\ -2 & 3 & 6 & 7 & 6 & 3 & -2 \\ -7 & -2 & 1 & 2 & 1 & -2 & 7 \end{bmatrix} \qquad \text{II.5.2.4}$$

and for $f''(0,0)_{av}$ the matrix is

$$\frac{1}{588}\begin{bmatrix} 10 & 5 & 2 & 1 & 2 & 5 & 10 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 2 & -3 & -6 & -7 & -6 & -3 & 2 \\ 1 & -4 & -7 & -8 & -7 & -4 & 1 \\ 2 & -3 & -6 & -7 & -6 & -3 & 2 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 10 & 5 & 2 & 1 & 2 & 5 & 10 \end{bmatrix} \qquad \text{II.5.2.5}$$

5.3. Quartic or Quintic. For a quartic or quintic fit the set of equations to be solved is

$$
\begin{aligned}
k_1 &= 49b_1 + 196b_4 + 196b_6 + 1372b_{11} + 784b_{13} + 1372b_{15} \\
k_4 &= 196b_1 + 1372b_4 + 784b_6 + 11116b_{11} + 5488b_{13} + 5488b_{15} \\
k_6 &= 196b_1 + 784b_4 + 1372b_6 + 5488b_{11} + 5488b_{13} + 11116b_{15} \\
k_{11} &= 1372b_1 + 11116b_4 + 5488b_6 + 95452b_{11} + 44464b_{13} + 38416b_{15} \\
k_{13} &= 784b_1 + 5488b_4 + 5488b_6 + 44464b_{11} + 38416b_{13} + 44464b_{15} \\
k_{15} &= 1372b_1 + 5488b_4 + 11116b_6 + 38416b_{11} + 44464b_{13} + 95452b_{15}
\end{aligned}
\qquad \text{II.5.3.1}
$$

It is helpful to combine the above set of six equations into

$$
\begin{aligned}
\frac{k_1}{49} &= b_1 + 4(b_4 + b_6) + 16b_{13} + 28(b_{11} + b_{15}) \\
\frac{(k_4 + k_6)}{28} &= 14b_1 + 77(b_4 + b_6) + 392b_{13} + 593(b_{11} + b_{15}) \\
\frac{(k_{11} + k_{15})}{28} &= 98b_1 + 593(b_4 + b_6) + 3176b_{13} + 4781(b_{11} + b_{15}) \\
\frac{k_{13}}{112} &= 7b_1 + 49(b_4 + b_6) + 343b_{13} + 397(b_{11} + b_{15}).
\end{aligned}
\qquad \text{II.5.3.2}
$$

Then by solving the last of this group of equations for b_{13} in terms of the other unknowns, substituting that quantity into the first three equations, and simplifying we get:

$$
\begin{aligned}
49k_1 - k_{13} &= (147)(11)b_1 + 4116(b_4 + b_6) + (84)(271)(b_{11} + b_{15}) \\
7(k_4 + k_6) - 2k_{13} &= (147)(8)b_1 + 4116(b_4 + b_6) + (84)(325)(b_{11} + b_{15}) \\
343(k_{11} + k_{15}) - 794k_{13} &= (147)(2168)b_1 + (4116)(325)(b_4 + b_6) \\
&\quad + (84)(126337)(b_{11} + b_{15})
\end{aligned}
\qquad \text{II.5.3.3}
$$

The solution of this set of equations gives

$$f(0,0) = b_1 = \frac{1}{19404}\,[3452k_1 - 911(k_4 + k_6) + 63(k_{11} + k_{15}) + 44k_{13}] \qquad \text{II.5.3.4}$$

and

$$f''_{av}(0,0) = b_4 + b_6 = \frac{1}{(4)(38808)}\,[-14576k_1 + 5457(k_4 + k_6) - 469(k_{11} + k_{15}) - 176k_{13}] \qquad \text{II.5.3.5}$$

Applying the definitions of k_1, k_4, k_6, k_{11}, k_{15}, and k_{13} the matrix of weights for f(0,0) is

$$\frac{1}{4851}\begin{bmatrix} 206 & -174 & -24 & 89 & -24 & -174 & 206 \\ -174 & -279 & 36 & 204 & 36 & -279 & -174 \\ -24 & 36 & 450 & 651 & 450 & 36 & -24 \\ 89 & 204 & 651 & 863 & 651 & 204 & 89 \\ -24 & 36 & 450 & 651 & 450 & 36 & -24 \\ -174 & -279 & 36 & 204 & 36 & -279 & -174 \\ 206 & -174 & -24 & 89 & -24 & -174 & 206 \end{bmatrix} \qquad \text{II.5.3.6}$$

and for $f''_{av}(0,0)$ the matrix of weights is

$$\frac{1}{38808}\begin{bmatrix} -1646 & 1134 & -12 & -863 & -12 & 1134 & -1644 \\ 1134 & 2814 & 1008 & -63 & 1008 & 2814 & 1134 \\ -12 & 1008 & -1194 & -2397 & -1194 & 1008 & -12 \\ -863 & -63 & -2397 & -3644 & -2397 & -63 & -863 \\ -12 & 1008 & -1194 & -2397 & -1194 & 1008 & -12 \\ 1134 & 2814 & 1008 & -63 & 1008 & 2814 & 1134 \\ -1646 & 1134 & -12 & -863 & -12 & 1134 & -1646 \end{bmatrix} \qquad \text{II.5.3.7}$$

III. Example of Application*

The 5 x 5 point quadratic smoothing matrix was applied to a nuclear medicine image with a low counting rate area to demonstrate the effectiveness of the least-squares processing when compared with a standard gaussian weighting method. The gaussian weight used is shown below. It is a "sharp" averager with one standard deviation per element spacing.

$$\text{Gaussian Weight Matrix} = \begin{matrix} .003 & - & - & - & - \\ .013 & .060 & - & - & - \\ .022 & .101 & .162 & - & - \\ - & - & - & - & - \\ - & - & - & - & - \end{matrix}$$

The image was an ordinary clinical scan with ^{67}Ga made on an Ohio Nuclear dual 8" rectilinear scanner. Only one 4K section of this large scan is illustrated. The liver is at the upper edge of this section with the abdominal area in the lower part of the image.

Three processes were used in succession. The first pass was a bounding action in which the smoothing matrix was applied with weight 1. The smoothed value was compared with this data point. If the point lay within the smoothed value ± the square root of the smoothed value, the value was unchanged; if it lay outside the range, it was replaced by the smoothed value. The purpose is to remove bad points or statistically improbable values. Figure 1 shows Z cuts of the raw data and the least squares bounded image at the line marked in the image. After the bounding pass the images were smoothed once with weight 4 and once with weight 1. Figure 2 shows the same line on the left with the simple gaussian weight and on the right with the least square quadratic fit. Note that the least squares process produces a smoother image while at the same time the ascending colon has

*Supplied by P. R. Bell, Medical Instrumentation Group.

a greater relief from the region around it. The mean counting rate in this region is about 6 counts per picture element. Figure 3 shows a Z cut across the lower part of the liver. Note the steeper rise of the least squares lines and its rise to a higher value.

The time required for processing this image by the two methods was the same.

PHOTO B-10 31185

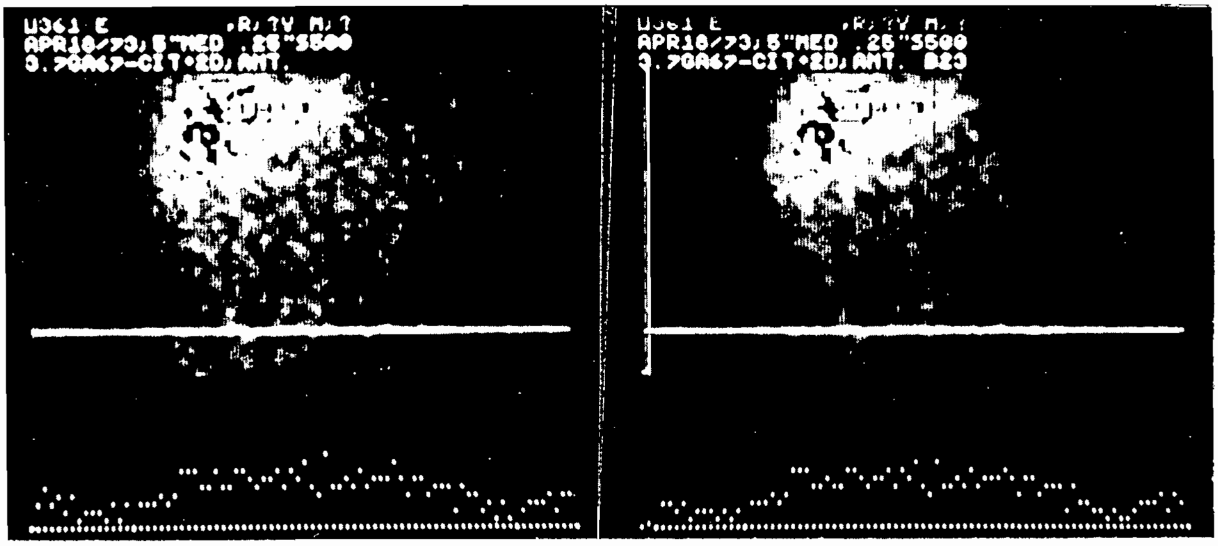

Fig. 1. Left is an unprocessed section of a ^{67}Ga image. The liver is at the top. The Z-cut crosses the ascending colon on the left central part of the image. The activity at the extreme left and right are the patient's arms. The count density near the ascending colon is about 6 counts/picture element.

The right image is that following bounding with the 5 x 5 point quadratic smoothing matrix. Note the reduction of the "sparkle" due to points with large statistical deviation in the image.

PHOTO B-10 31186

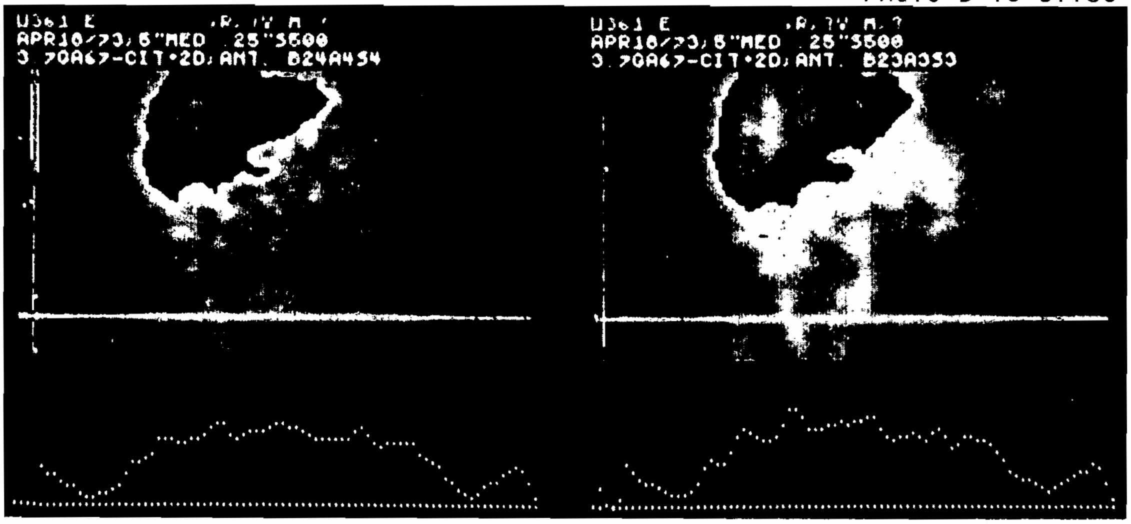

Fig. 2. Left image was produced by bounding followed by weight 4 smoothing and weight 1 smoothing all with the gaussian smoothing matrix. The right image was similarly processed using the 5 x 5 point least-squares quadratic smoothing matrix. Note the greater difference between the ascending colon and the region around it in the least-squares smoothed image. This is due to the greater suppression of this feature by the gaussian smoothing. Note the overall somewhat better smoothness of the least-squares processing.

PHOTO B-10 31187

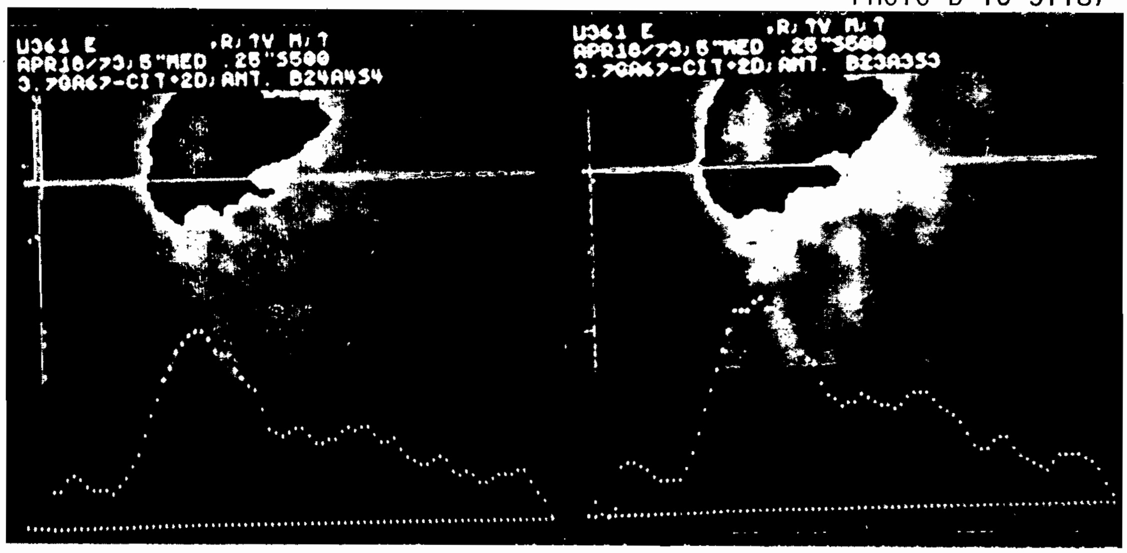

Fig. 3. Same images as in Fig. 2 with the Z-cut across the tip of the liver. Note the steeper and higher rise produced by the least-squares processing.

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APPENDIX

Once we have determined a least-squares fitting function (in either one or two dimensions) we can also give two other quantities of interest to image processing: the location and magnitude of the extreme (maximum or minimum) value of the function. We will give formulas for these quantities for quadratic fitting functions.

In the one dimensional case, $y = b_1 + b_2x + b_3x^2$ so that the location of the extremum is given by setting $y' = 0$, i.e.

$$x_{EXT} = \frac{-b_2}{2b_3} \qquad \text{A.1}$$

and the extreme value of the function is

$$y_{EXT} = b_1 - \frac{b_2^{\ 2}}{4b_3} \qquad \text{A.2}$$

If y", i.e. $2b_3$, is positive, the extremum is a minimum; if y" is negative, the extremum is a maximum. The values of b_1 and $2b_3$ are given by I.B.1.5 and I.B.1.6 for a 5 point fit and by I.B.2.5 and I.B.2.6 for a 7 point fit. From equation I.B.6 we find $b_2 = \sum_i f_i x_i / \sum_i x_i^{\ 2}$. Hence for the 5 point case

$$b_2 = \frac{1}{10}\,(-2f_{-2} - f_{-1} + f_1 + 2f_2) \qquad \text{A.3}$$

and for the 7 point case

$$b_2 = \frac{1}{28}\,(-3f_{-3} - 2f_{-2} - f_{-1} + f_1 + 2f_2 + 3f_3) \qquad \text{A.4}$$

In the two dimensional case, $f(x,y) = b_1 + b_2x + b_3y + b_4x^2 + b_5xy + b_6y^2$. The location of the extremum is given by the solution of the simultaneous equations

$$\frac{\partial f}{\partial x} = b_2 + 2b_4x + b_3y = 0 \qquad \text{A.5}$$

and

$$\frac{\partial f}{\partial y} = b_3 + b_5x + 2b_6y = 0 \qquad \text{A.6}$$

This solution is

$$X_{EXT} = \frac{-2b_2b_6 + b_3b_5}{4b_4b_6 - b_5^2} \qquad \text{A.7}$$

and

$$Y_{EXT} = \frac{-2b_3b_4 + b_2b_5}{4b_4b_6 - b_5^2} \qquad \text{A.8}$$

The extreme value of the function is then given by

$$f_{EXT} = b_1 - \frac{(b_2^2b_6 - b_2b_3b_5 + b_3^2b_4)}{(4b_4b_6 - b_5^2)} \qquad \text{A.9}$$

Call the common quantity in the denominator of the above three expressions Δ, i.e. $\Delta = 4b_4b_6 - b_5^2$. The function will have a maximum value if $\Delta > 0$ and either b_4 or $b_6 < 0$; the function will have a minimum value if $\Delta > 0$ and either b_4 or $b_6 > 0$. If $\Delta < 0$ (which is necessarily the case if b_4 and b_6 have opposite signs or are 0) the function has neither a maximum nor a minimum but rather a saddle point. Hence whenever there is the possibility of a maximum or a minimum b_4 and b_6 have the same sign.

For a 7 x 7 point fitting area for a quadratic, the value of the weighting matrix to be convolved with the experimental data to give b_1 is given by equation II.5.2.4. Equation II.5.2.3 gives $b_4 + b_6 = \frac{1}{588}(k_4 + k_6 - 8k_1)$ and it can be shown that

$$b_4 = \frac{1}{588}(k_4 - 4k_1) \qquad \text{A.10}$$

and

$$b_6 = \frac{1}{588}(k_6 - 4k_1) \qquad \text{A.11}$$

Equations II.2.3, II.2.4 and II.2.6 separately give the following solutions for b_2, b_3, and b_5.

$$b_2 = (\sum_i \sum_j f_{ij}x_i)/n \sum_i x_i^2 \qquad \text{A.12}$$

$$b_3 = (\sum_i \sum_j f_{ij}y_j)/n \sum_j y_j^2 \qquad \text{A.13}$$

$$b_5 = (\sum_i \sum_j f_{ij}x_iy_j)/\sum_i x_i^2 \sum_j y_j^2 \qquad \text{A.14}$$

The weighting matrices to give these additional values are given below

$$W \text{ for } b_2 = \frac{1}{196}\begin{bmatrix} -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \end{bmatrix}$$

$$W \text{ for } b_3 = \frac{1}{196}\begin{bmatrix} 3 & 3 & 3 & 3 & 3 & 3 & 3 \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -2 & -2 & -2 & -2 & -2 & -2 & -2 \\ -3 & -3 & -3 & -3 & -3 & -3 & -3 \end{bmatrix}$$

$$W \text{ for } b_5 = \frac{1}{784}\begin{bmatrix} -9 & -6 & -3 & 0 & 3 & 6 & 9 \\ -6 & -4 & -2 & 0 & 2 & 4 & 6 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 2 & 1 & 0 & -1 & -2 & -3 \\ 6 & 4 & 2 & 0 & -2 & -4 & -6 \\ 9 & 6 & 3 & 0 & -3 & -6 & -9 \end{bmatrix}$$

$$W \text{ for } b_4 = \frac{1}{588}\begin{bmatrix} 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \\ 5 & 0 & -3 & -4 & -3 & 0 & 5 \end{bmatrix}$$

$$W \text{ for } b_6 = \frac{1}{588}\begin{bmatrix} 5 & 5 & 5 & 5 & 5 & 5 & 5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -3 & -3 & -3 & -3 & -3 & -3 & -3 \\ -4 & -4 & -4 & -4 & -4 & -4 & -4 \\ -3 & -3 & -3 & -3 & -3 & -3 & -3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 5 & 5 & 5 & 5 & 5 & 5 \end{bmatrix}$$

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