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The Inertia Matrix in Least-Squares Linear Fitting

ABSTRACT Least squares fitting of point sets to lines, planes, curves and surfaces is carried out using eigenvalues and eigenvectors to find the major principal moment of inertia axis of a point set taken as representing the mass distribution of a rigid body. This engineering geometric approach produces identical results when compared to methods of conventional minimization using partial derivatives with respect to linear equation coefficients. Extending the approach to the fitting of conics and quadrics achieves great computational advantage over conventional leastsquares optimization of *Euclidean*, as opposed to *algebraic* distance. The results, though imperfect, provide a starting point for iterations that will converge rapidly. Often, if enough points are given and these do not deviate wildly from the fit shape type selected, the result is satisfactory without resorting to further improvement.

Keywords: Fitting, Curves, Surfaces, Linear, Algebra, Inertia, Moment, Grassmann, Geometry

1 INTRODUCTION

The importance and utility of extracting underlying simple functional relations and geometric shape features from experimental data, acquired either as images or numbers, are evident. So it is deemed unnecessary to give examples and reasons in this regard. Rather, fitting a line to three given planar points by means of first partial derivatives of the sum of points' squared distances to a line y = ax + b, where a and b are unknown, will be compared to the novel method exposed herein where the moments and products of inertia of the points about Cartesian axes lead to principal moment of inertia axes, in the plane, via the eigenvalues and eigenvectors of the inertia matrix. The line of best fit will be seen to lie on the centroid of the point triangle and normal to the eigenvector associated with the larger eigenvalue of the planar inertia matrix. This latter concept will then be applied to fitting a plane to spatial points and finally to fitting a conic, using the inertia notion in the context of a five dimensional Euclidean point space of quadratic forms. A special conic, a circle fit to four points, is used to illustrate a preliminary result and to point out the essential shortcoming of our pseudo-linear approach. Although familiarity with elementary calculus, linear algebra and mechanics is assumed, [1], [2] and [3], respectively, provide all the relevant background necessary.

2 A LINE TO THREE POINTS

The proposed inertia matrix method, elaborated upon in Section 4, will now be introduced using the numerical example in Fig. 1 with points

$$_{1}P(1,2), _{2}P(3,4), _{3}P(5,3)$$

The first moment is calculated to yield G the centroid on the fit line.

$$[(1+3+5)/3, (2+4+3)/3] \to G(3,3)$$

The inertia matrix is referred to this origin so

$$_{1}P'(-2,-1), _{2}P'(0,1), _{3}P'(2,0)$$

replaces $_{i}P$ above. Then the second moments and product are obtained as

$$I_{xx} = (-1)^2 + 1^2 + 0^2 = 2, \quad I_{yy} = (-2)^2 + 0^2 + 2^2 = 8$$

 $I_{xy} = (-2)(-1) + 0(1) + 2(0) = 2$

Eigenvalues are found as follows.

$$\begin{bmatrix} I_{xx} - \lambda & -I_{xy} \\ -I_{xy} & I_{yy} - \lambda \end{bmatrix} \begin{bmatrix} e_x \\ e_y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\rightarrow \begin{vmatrix} 2 - \lambda & -2 \\ -2 & 8 - \lambda \end{vmatrix} = 0 \rightarrow \frac{\lambda^2 - 10\lambda + 12 = 0}{\lambda = 5 \pm \sqrt{13}}$$

$$(1)$$

Then the eigenvector **e** associated with the greater eigenvalue is given by either one of Eq. 1. E.g., this eigenvector, normal to the sought line on G, has a slope of e_y/e_x , i.e., given by

$$[2 - (5 + \sqrt{13})]e_x - 2e_y = 0$$

This line on G represents the axis in the plane about which the moment of inertia of the three points is greatest. The line on G parallel to the other eigenvector is the axis of minimum inertia. One must not confuse these axes with I_{zz} , encountered in elementary planar mechanics, which is mutually orthogonal to them. The inertia matrix approach clearly reveals the underlying geometric structure of this simple fitting problem. Now consider a conventional alternative. Examining the upper diagram in Fig. 1 one may easily formulate the sum of the three squared normal distances Δn_i in terms of line coefficients a and b. By induction and taking first partial derivatives with respect to a and b one quickly arrives at a quadratic in a and a linear equation relating b = b(a).

$$a^{2} + \frac{\left[\sum_{ik}(x_{i}^{2} - x_{k}^{2})\right] - \left[\sum_{ik}(y_{i}^{2} - y_{k}^{2})\right]}{\sum_{ik}[(x_{i} - x_{k})(y_{i} - y_{k})]}a - 1 = 0$$
(2)

$$nb = \sum_{i} y_i - (\sum_{i} x_i)a \tag{3}$$

Note that n is the number of points and that all possible differences and differences of squares must be taken in the sums. Two solutions for a, the slope of the fitted line, appear. One is the actual slope the other is its normal. Eq. 3 provides the corresponding values of b. The lines intersect on G, the centroid of the given points. There is no way *a-priori* to tell which line is which ... unless one is prepared to examine second derivatives; a procedure that becomes quite inconvenient in problems of higher dimension. Least Squares Line Fit to Three Given Points

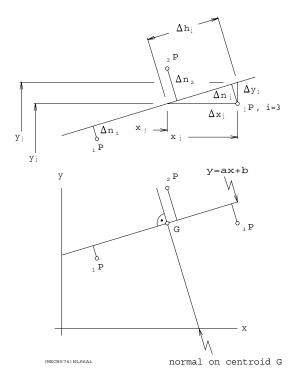


Figure 1: Three Point Line Fit

3 A PLANE TO SIX POINTS

This time an example where six given random points will be fit to a plane is presented and the singular matrix appears in Eq. 4.

$$\begin{bmatrix} I_{xx} - \lambda & -I_{xy} & -I_{xz} \\ -I_{xy} & I_{yy} - \lambda & -I_{yz} \\ -I_{xz} & -I_{yz} & I_{zz} - \lambda \end{bmatrix} \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$
(4)

The six given points ${}_{i}P({}_{i}p_{x,i} p_{y,i} p_{z})$ appear below.

$${}_{1}P(4,3,2), {}_{2}P(7,1,4), {}_{3}P(2,8,1), {}_{4}P(9,6,7), {}_{5}P(1,4,6), {}_{6}P(12,-3,-5)$$

The homogeneous coordinates of the centroid are $G\{g_0 : g_1 : g_2 : g_3\} \equiv \{6 : 35 : 19 : 15\}$. To obtain the elements of the inertia matrix $_iP$ are first multiplied by 6 and g_1, g_2, g_3 are subtracted from $_iP$ to produce

$${}_{4}P'(-11,-1,-3), {}_{2}P'(7,-13,9), {}_{3}P'(-23,29,-9), \\ {}_{4}P'(19,17,27), {}_{5}P'(-29,5,21), {}_{6}P'(37,-37,-45)$$

Notice that all six of the following sums of products contain the common divisor 6. Inertia matrix element magnitude is irrelevant because we seek only the *direction* of eigenvector \mathbf{e} associated with greatest eigenvalue λ .

$$\begin{split} &I_{xx} = \{[(-1)^2 + (-3)^2] + [(-13)^2 + 9^2] \\ &+ [29^2 + (-9)^2] + [17^2 + 27^2] + [5^2 + 21^2] \\ &+ [(-37)^2 + (-45)^2]\}/6 = 1010 \\ &I_{yy} = \{[(-3)^2 + (-11)^2] + [9^2 + 7^2] \\ &+ [(-9)^2 + (-23)^2] + [27^2 + 19^2] \\ &+ [21 + (-29)^2] + [(-45)^2 + 37^2]\}/6 = 1106 \\ &I_{zz} = \{[(-11)^2 + (-1)^2] + [7^2 + (-13)^2] \\ &+ [(-23)^2 + 29^2] + [19^2 + 17^2] + [(-29)^2 + 5^2] \\ &+ [37^2 + (-37)^2]\}/6 = 994 \\ &I_{xy} = \{[(-11)(-1)] + [(7)(-13)] + [(-23)(9)] \\ &+ [(19)(17)] + [(-29)(5)] + [(37)(-37)]\}/6 = 323 \\ &I_{xz} = \{[(-3)(-11)] + [(9)(7)] + [(-9)(23)] \\ &+ [(27)(19)] + [(21)(-29)] + [(-45)(37)]\}/6 = 243 \\ &I_{yz} = \{[(-1)(-3)] + [(-13)(9)] + [(29)(-9)] \\ &+ [(17)(27)] + [(5)(21)] + [(-37)(-45)]\}/6 = -309 \end{split}$$

The cubic characteristic equation becomes

$$\lambda^3 - 3110\lambda^2 + 2961505\lambda - 796404408 = 0$$

which has three real roots, ignoring small imaginary residues returned by numerical solution.

 $\lambda = 453.1092563, 1244.042205, 1412.84854$

Using the third, greatest one in the expansion of Eq. 4 yields a set of three linearly dependent equations in the elements of \mathbf{e} , the associated eigenvector.

$$\begin{array}{l} (1010-1412.84854)e_x+323e_y+243e_z=0\\ 323e_x+(1106-1412.84854)e_y-309e_z=0\\ 243e_x-309e_y+(994-1412.84854)e_z=0 \end{array}$$

Solving, say, the first two homogeneously produces three direction numbers normal to the desired plane.

$$e_x = -25242.80478, e_y = -45991.1989, e_z = 19284.4863$$

These, together with the homogeneous coordinates of G, yield the plane equation.

$$G_{1}x + G_{2}y + G_{3}z + G_{0} = 0 \rightarrow$$

$$g_{0}e_{x}x + g_{0}e_{y}y + g_{0}e_{z}z - (g_{1}e_{x} + g_{2}e_{y} + g_{3}e_{z}) = 0$$

$$\rightarrow$$

$$(6)(-25242.80478)x + (6)(-45991.1989)y$$

$$(6)(19284.4863)z - [(35)(-25242.80478) + (19)(-45991.1989) + (15)(19284.4863)] = 0$$

Fig. 2 shows top and front view of the array of six spatial points as well as *all three* mutually orthogonal eigenvector *directions*. The remaining two were computed with the other two eigenvalues. The one labelled λ_3 is associated with the greatest eigenvalue. It does not *appear* as the longest because the direction numbers were plotted as calculated. Vectors were not normalized and assigned inertial magnitudes represented by the respective eigenvalues.

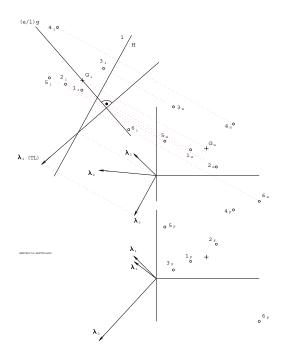


Figure 2: Six Point Plane Fit

4 CONIC GRASSMANNIAN

The coefficients of a conic on five given points are provided by the top row minor 5×5 determinants of the singular matrix, Eq. 5.

$$\begin{bmatrix} w^2 & wx & wy & x^2 & xy & y^2 \\ w_1^2 & w_1x_1 & w_1y_1 & x_1^2 & x_1y_1 & y_1^2 \\ w_2^2 & w_2x_2 & w_2y_2 & x_2^2 & x_2y_2 & y_2^2 \\ w_3^2 & w_3x_3 & w_3y_3 & x_3^2 & x_3y_3 & y_3^2 \\ w_4^2 & w_4x_4 & w_4y_4 & x_4^2 & x_4y_4 & y_4^2 \\ w_5^2 & w_5x_5 & w_5y_5 & x_5^2 & x_5y_5 & y_5^2 \end{bmatrix} = 0$$

$$(5)$$

Therefore the conic is represented in a six dimensional homogeneous vector space of quadratic point form variables q_i , derived from point coordinates p_i , Eq. 6.

$$P\{p_0: p_1: p_2: p_3\} \equiv \{w: x: y: z\} \rightarrow Q\{q_0: q_1: q_2: q_3: q_4: q_5\} \\ \equiv \{w^2: wx: wy: x^2: xy: y^2\}$$
(6)

For a brief but excellent introduction relating homogeneous coordinates and projective geometry to modern linear algebra a recent text by Pottmann and Wallner [4] is highly recommended. When fitting a conic to more than five given points, for the purpose of pattern recognition, *e.g.*, in unsupervised automated inspection of industrial production [5], digital image pixels often constitute the point set. Hence, after pre-processing, the spatial point set P is assumed to lie in the Euclidean plane of the curve it must represent. For this reason Eq. 5 contains only six planar quadratic forms (columns) rather than ten needed to define a three dimensional quadric surface in space. One may set $p_0 = w = 1$ for points in the Euclidean plane to obtain the usual Cartesian coordinates

$$P(p_1, p_2) \equiv (x, y) \to Q(q_1, q_2, q_3, q_4, q_5)$$

$$\equiv (x, y, x^2, xy, y^2)$$
(7)

Now first moments (centres of "gravity") and second moments (moments and products of "inertia") of the numerous given points, assumed to be of equal unit weight, in a five dimensional Euclidean space, will be defined. But first, consider what is in hand and what will be done with it.

• There are n given points

$$_{i}Q(_{i}q_{1}, _{i}q_{2}, _{i}q_{3}, _{i}q_{4}, _{i}q_{5}), i = 1, \ldots, n$$

• The first moment is defined with respect to a point G about which the sum of all point moments vanishes. Conversely G is the point where all n points may concentrate their weight so as to exert the same moment, anywhere, as do the n points in their actual position.

$$G\{g_0: g_1: g_2: g_3: g_4: g_5\} \equiv \{n: \sum_{i=1}^n {}_iq_1: \sum_{i=1}^n {}_iq_2: \sum_{i=1}^n {}_iq_3: \sum_{i=1}^n {}_iq_4: \sum_{i=1}^n {}_iq_5\}$$
(8)

- A hyperplane $g\{G_0: G_1: G_2: G_3: G_4: G_5\}$ on G is sought such that the sum of the squares of the normal "distances" from $_iQ$ to g is minimized.
- This will occur, at least in the context of this geometric model, when the hyperplane normal direction numbers $G_1: G_2: G_3: G_4: G_5$ are in the same ratio as those of the point cloud inertia matrix eigenvector $e\{0: E_1: E_2: E_3: E_4: E_5\}$ associated with the eigenvalue of greatest magnitude, say, $\lambda_{max} = \lambda_5$. The reason for this choice is evident. The sum of the squares of the distances to unit mass points in all directions normal to an axis is maximized if that axis is the principal axis of greatest inertia of a rigid body whose mass is composed exclusively of unit masses on $_iQ$. This observation proceeds directly from the definition of mass moment of inertia about an axis of rotation.

- $G_0 = 0$ if $G \in g$. *I.e.*, if one chooses G as origin. Then g is identical to e, except for some non-zero real multiplier.
- A little thought experiment may help to clarify the two arguments above.
 - 1. Imagine a massless rectangular wire-frame "box" with edge lengths a > b > c. On each of the eight vertices is located a unit point mass. Since 8 > 3, these points are redundant in defining a unique plane. However it is obvious that G is at the centre of the box, g bisects the four edges of length c and the normal to g on G is the principal axis of greatest inertia. Finally, $2c^2$ is the sum, of the distances squared, from vertex points $_iP$ to g. It is obviously minimal.
 - 2. It must be pointed out that, as regards fitting planes to points, this geometric model is perfect. However the analogy between points and quadratic point forms is not and neither is the fit it produces.

This "point cloud" then, for a conic, is in five dimensional Euclidean space. The inertia matrix can be written as a symmetric array of sums of squares (along the diagonal) and negative product (off diagonal) terms in Eq. 9.

$$\mathbf{I} = \begin{bmatrix} I_{11} & -I_{12} & -I_{13} & -I_{14} & -I_{15} \\ -I_{12} & I_{22} & -I_{23} & -I_{24} & -I_{25} \\ -I_{13} & -I_{23} & I_{33} & -I_{34} & -I_{35} \\ -I_{14} & -I_{24} & -I_{34} & I_{44} & -I_{45} \\ -I_{15} & -I_{25} & -I_{35} & -I_{45} & I_{55} \end{bmatrix}$$
(9)

Rather than fitting six or more points to a general conic an example to fit four points to a circle is chosen because the simpler calculation can be demonstrated in detail and this special case will illustrate some intricacy not otherwise evident.

5 CIRCLE ON FOUR POINTS

Fitting a circle to an over-determined system of four given points ${}_{i}P\{{}_{i}p_{0}:{}_{i}p_{1}:ip_{2}\} \equiv \{w:x:y\}$ begins with a table of their homogeneous point coordinates.

This is represented in a table containing only *four* quadratic point forms, rather than six of a general conic, because the circle's invariance under rotation would fill the column under xy with zeros. Similarly, another circle characteristic, identical coefficients of x^2 and y^2 , require that these two columns be combined as a sum. Thus these four appear in a 5×5 matrix, of rank deficiency two, whose determinant expresses the circle equation. Additional given points would simply add

more zero columns on the left, further increasing rank deficiency, *i.e.*, expanding the null space of the matrix.

$$\begin{bmatrix} 0 & w^2 & wx & wy & x^2 + y^2 \\ 0 & _1p_0^2 & _1p_0 & _1p_1 & _1p_0 & _1p_2 & _1p_1^2 + _1p_2^2 \\ 0 & _2p_0^2 & _2p_0 & _2p_1 & _2p_0 & _2p_2 & _2p_1^2 + _2p_2^2 \\ 0 & _3p_0^2 & _3p_0 & _3p_1 & _3p_0 & _3p_2 & _3p_1^2 + _3p_2^2 \\ 0 & _4p_0^2 & _4p_0 & _4p_1 & _4p_0 & _4p_2 & _4p_1^2 + _4p_2^2 \end{bmatrix} = 0$$

These quadratic point forms

$$\{w^2 : wx : wy : x^2 + y^2\} \equiv \{ip_0^2 : ip_0 \ ip_1 : ip_0 \ ip_2 : ip_1^2 + ip_2^2\}$$
$$\equiv \{iq_0 : iq_1 : iq_2 : iq_3\}$$

and their sum and their average are tabulated below.

	q_0	q_1	q_2	q_3
	1	4	2	20
	1	9	5	106
	1	14	5	221
	1	18	4	340
Σ	4	45	16	687
$G=\overline{q}$	1	11.25	4	171.75

5.1 Centroid, Inertia Matrix & Elements

Subtracting the coordinates of G, the "centre of gravity", produces the next table.

Now the inertia matrix characteristic equation is given by

$$\begin{vmatrix} I_{11} - \lambda & -I_{12} & -I_{13} \\ -I_{12} & I_{22} - \lambda & -I_{23} \\ -I_{13} & -I_{23} & I_{33} - \lambda \end{vmatrix} = 0$$

where

$$I_{11} = \sum_{i=1}^{4} \left(iq_{2}^{\prime 2} + iq_{3}^{\prime 2} \right), \quad I_{12} = \sum_{i=1}^{4} \left(iq_{1}^{\prime i}q_{2}^{\prime 2} \right)$$
$$I_{13} = \sum_{i=1}^{4} \left(iq_{1}^{\prime i}q_{3}^{\prime } \right), \quad I_{22} = \sum_{i=1}^{4} \left(iq_{1}^{\prime 2} + iq_{3}^{\prime 2} \right)$$
$$I_{23} = \sum_{i=1}^{4} \left(iq_{2}^{\prime i}q_{3}^{\prime } \right), \quad I_{33} = \sum_{i=1}^{4} \left(iq_{1}^{\prime 2} + iq_{2}^{\prime 2} \right)$$

$q_2'^2 + q_3'^2$	$q_1'q_2'$	$q_1'q_3'$
$\begin{array}{c} 23032.0625 \\ 4324.0625 \end{array}$	$14.5 \\ -2.25$	$1100.1875 \\ 147.9375$
2426.5625	2.75	135.4375
28308.0625		1135.6875
$q_1'^2 + q_3'^2$ 23080.625	$q_{2}'q_{3}'$ 303.5	$q_1'^2 + q_2'^2$ 56.5625
$\begin{array}{c} 4328.125 \\ 2433.125 \end{array}$	-65.75 49.25	6.0625 8.5625
2455.125 28353.625	49.25 0	$8.5625 \\ 45.5625$
I 58000 75	T 15	I 9510.95
$I_{11} = 58090.75, I_{22} = 58195.5,$		10

and

5.2 Eigenvalues and Eigenvectors

The characteristic equation determinant yields the following cubic

 $\lambda^3 - 116403\lambda^2 + 3387767447\lambda - 20536062200 = 0$

with eigenvalues

 $\lambda = 58201.40932, 58195.52759, 6.063090633$

The greatest, first eigenvalue produces the following three dependent equations when it is substituted into the matrix that pre-multiplies column eigenvector \mathbf{e} .

Solving the first two equations homogeneously reveals the eigenvector normal to the "best" fitting "plane".

	e_1		-10582.05441
$\mathbf{e} =$	e_2	=	6029.52516
	e_3		428.9213329

5.3 The "Plane" & the Circle

Recall the centroid

 $G\{g_0: g_1: g_2: g_3\} = \{1: 11.25: 4: 171.75\}$

on which g the pseudo-plane of best fit must lie.

$$g\{G_0: G_1: G_2: G_3\}$$

$$= \{-(g_1e_1 + g_2e_2 + g_3e_3): g_0e_1: g_0e_2: g_0e_3\}$$

$$= g\{21262.77253: -10582.05441:$$

$$6029.52516: 428.9213329\}$$
(10)

Recall, also, the circle equation whose coefficients are the elements of g, thus.

$$21262.77253w^2 - 10582.05441wx$$
$$+6029.52516wy + 428.9213329(x^2 + y^2) = 0$$

Rearranging this in more familiar, Euclidean form and dividing by G_3 produces something that looks like a circle equation

$$(x^2 + y^2) - 24.67131755x + 14.05741496y + 49.57266263 = 0$$

that can easily be interpreted as

$$(x^{2} + y^{2}) - 2x_{c}x - 2y_{c}y + (x_{c}^{2} + y_{c}^{2} - r^{2}) = 0$$

Solving for centre coordinates $C(x_c, y_c)$ and radius r gives the following circle parameters.

$$x_c = 12.33565878, \ y_c = -7.02870748, \ r = 12.32876895$$

Examine Fig. 3. This result is quite encouraging when compared to a rigorous least squares distance fit described below. However the downward-convex circular arc centred on C' is the result of invoking the second eigenvalue, less than the greatest by only 0.01%! This inertial fit appears to be very sensitive in this regard.

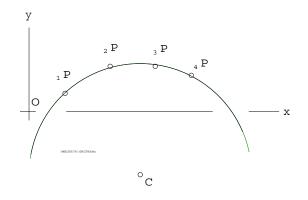


Figure 3: Four Point Circle Fit

5.4 Least Squares Distance

Consider the minimization of the following sum.

$$D = \sum_{i=1}^{4} \left[\sqrt{(x_c - x_i)^2 + (y_c - y_i)^2} - r \right]^2$$

Taking the derivatives

$$\frac{\partial D}{\partial x_c} = 0, \quad \frac{\partial D}{\partial y_c} = 0, \quad \frac{\partial D}{\partial r} = 0$$

Removing the common factor 2 from all three derivatives and the common reciprocal factor

$$\prod_{i=1}^{4} \sqrt{(x_c - x_i)^2 + (y_c - y_i)^2}$$

from the first two yields three simultaneous equations. Note that u = x, y to account for the first two of similar form.

$$(4u_c - \sum u_i)a_{1234} - [(u_c - u_1)a_{234} + (u_c - u_2)a_{134} + (u_c - u_3)a_{124} + (u_c - u_4)a_{123}]r = 0$$

$$a_1 + a_2 + a_3 + a_4 - 4r = 0$$
(11)

Multiple subscripts indicate products, *e.g.*, $a_{1234} = a_1 a_2 a_3 a_4$ and

$$a_i = \sqrt{(x_c - x_i)^2 + (y_c - y_i)^2}$$

Eliminating r leaves the two following equations.

$$\begin{aligned} & 3(4u_c - \sum u_i)a_{1234} \\ & -a_1^2[(u_c - u_2)a_{34} + (u_c - u_3)a_{24} + (u_c - u_4)a_{23}] \\ & -a_2^2[(u_c - u_1)a_{34} + (u_c - u_3)a_{14} + (u_c - u_4)a_{13}] \\ & -a_3^2[(u_c - u_1)a_{24} + (u_c - u_2)a_{14} + (u_c - u_4)a_{12}] \\ & -a_4^2[(u_c - u_1)a_{23} + (u_c - u_2)a_{13} + (u_c - u_3)a_{12}] \end{aligned} = 0$$

Solving these explicitly seems impractical. However inserting the exact values obtained with the inertial model leaves residues of about -695 and -97, respectively. After a few iterative perturbations these are reduced to about 2.1 and -3.8. To achieve still greater precision is probably not worthwhile. The centre coordinates of C are now

$$x_c = 12.32503412, \quad y_c = -7.02685$$

Substituting these into the third partial derivative, Eq. 11, produces r = 12.32552238. When these improved values are used to construct a circle in Fig. 3 this and the original arc are virtually coincident.

6 CONCLUSION

It is anticipated that the novel geometric approach, based on a moment of inertia interpretation, described here could, with further development, become a powerful image processing and pattern recognition tool. The immediate extension of its currently modest capacities will be focused on recognition of other shapes which can be represented by quadratic forms, *i.e.*, other specific conics as well as quadric surfaces.

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