JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 54 (2021)

Supporting information for article:

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for Journal of Applied Crystallography article

Constrained geometrical analysis of complete K-line patterns for calibrationless auto-indexing

by

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Contents

Introduction

The geometry of Kossel lines can be described with cones having a common apex at the source point. The normal to each set of lattice planes defines a cone axis. The opening angle of a cone is related to the Bragg angle defined by the wavelength of the radiation producing the Kossel lines and the given lattice plane spacing. If one intercepts this radiation field emerging along the generatrices of these cones with a planar detector, will obtain conic sections, i.e. ellipses, hyperbolas or parabolas. These are the typical experimental manifestation of the Kossel lines.

Here we provide useful mathematical formulae and a specific parameter set to describe both the conic sections and the cones themselves, and define the quantities to be minimized when optimizing the parameters of this geometry to obtain the best fit to an experimental Kossel pattern.

Coordinate system and parameters

Without posing any restriction we can choose our coordinate system, such that the planar detector and hence the conic sections lie in the xy plane. The origin can also be chosen arbitrarily in this plane (conveniently either the corner or center point of the detector). Then we must place our source point i.e. the common apex of the cones in a general $\mathbf{s}=(s_x, s_y, s_z)$ point (Figure S1).

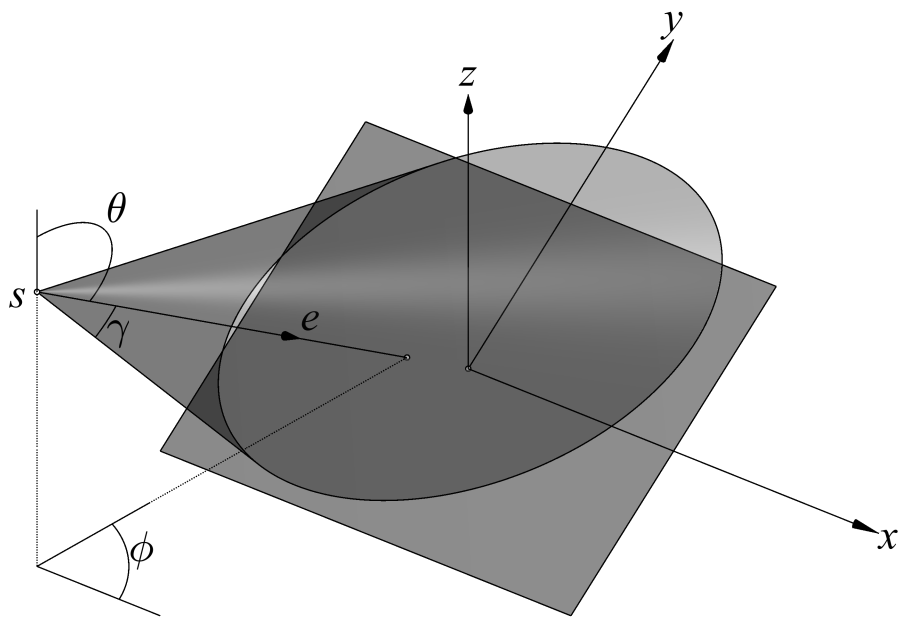

Figure S1. Coordinate system, parameters of the cone and the conic section in the base plane.

A cone has 6 (=3+2+1) independent parameters, the position of its apex, $\mathbf{s}=(s_x, s_y, s_z)$, direction of its axis $\mathbf{e}=(e_x, e_y, e_z)$; $|\mathbf{e}|=1$, and its half opening angle, γ. For the axis direction we choose polar parameters in the physical convention (θ polar and ϕ azimuthal angles), to eliminate the unit vector condition i.e. $\mathbf{e}=(\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$.

In the following we describe various problems and derive their solutions using our parameter set of $(s_x, s_y, s_z, \theta, \phi, \gamma)$. The need for and application of these results are explained in the manuscript.

Use case 1 - Cone parameters from apex and 3 points

3 points are given in the xy plane, $\mathbf{u}=(u_x, u_y, 0)$, $\mathbf{v}(v_x, v_y, 0)$ and $\mathbf{w}=(w_x, w_y, 0)$ and the apex of a cone is at $\mathbf{s}=(s_x, s_y, s_z)$. Determine (θ, ϕ, γ) parameters of the cone whose conic section crosses the 3 points (in the same branch, if it is a hyperbola)!

We could substitute $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ into the general cone equation (see below) and solve the set of 3 equations for (θ, ϕ, γ) while treating (s_x, s_y, s_z) as known parameters. However, this would lead to a complicated system of equations. Instead, we follow a solution based on geometry (Figure S2).

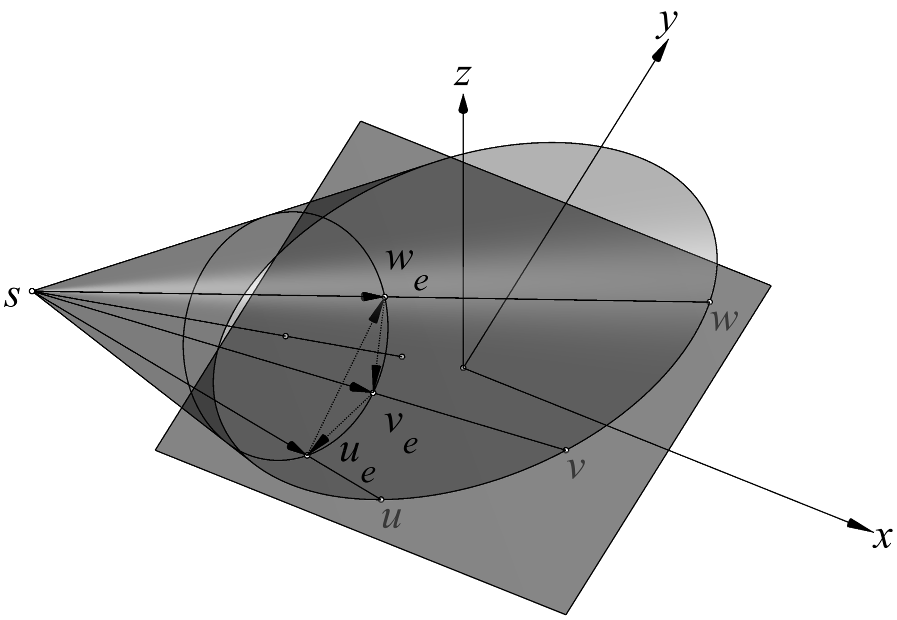

Figure S2. Determination of cone parameters from apex and 3 points.

The $\mathbf{u}-\mathbf{s}$, $\mathbf{v}-\mathbf{s}$, $\mathbf{w}-\mathbf{s}$ vectors are all generatrices of the cone. The points defined by the corresponding unit vectors originated from the apex of the cone can be written as:

$$\mathbf{u_e}=\mathbf{s}+\frac{\mathbf{u}-\mathbf{s}}{|\mathbf{u}-\mathbf{s}|}, \quad \mathbf{v_e}=\mathbf{s}+\frac{\mathbf{v}-\mathbf{s}}{|\mathbf{v}-\mathbf{s}|}, \quad \mathbf{w_e}=\mathbf{s}+\frac{\mathbf{w}-\mathbf{s}}{|\mathbf{w}-\mathbf{s}|}$$

These points lie on a circle, whose plane is perpendicular to the axis of the cone, $\mathbf{e}=(e_x, e_y, e_z)$. Then the direction of the axis can be determined from the cross product of any two vectors between these points on the circle:

$$\mathbf{e} = \frac{(\mathbf{u_e}-\mathbf{v_e})\times(\mathbf{v_e}-\mathbf{w_e})}{|(\mathbf{u_e}-\mathbf{v_e})\times(\mathbf{v_e}-\mathbf{w_e})|} = \frac{(\mathbf{v_e}-\mathbf{w_e})\times(\mathbf{w_e}-\mathbf{u_e})}{|(\mathbf{v_e}-\mathbf{w_e})\times(\mathbf{w_e}-\mathbf{u_e})|} = \frac{(\mathbf{w_e}-\mathbf{u_e})\times(\mathbf{u_e}-\mathbf{v_e})}{|(\mathbf{w_e}-\mathbf{u_e})\times(\mathbf{u_e}-\mathbf{v_e})|}$$

Substituting the $\mathbf{u}=(u_x, u_y, 0)$, $\mathbf{v}=(v_x, v_y, 0)$, $\mathbf{w}=(w_x, w_y, 0)$ and $\mathbf{s}=(s_x, s_x, s_z)$ coordinates we obtain $\mathbf{e}=(e_x, e_y, e_z)$. For the cone axis vector we can freely choose either $\mathbf{e}$ or $-\mathbf{e}$. The sign is selected such, that the cone axis vector points towards the base detector plane, i.e. $sign(e_z) = -sign(s_z)$.

From the components of this $\mathbf{e}$ we obtain the polar angles:

$$\theta = \arccos(e_z), \ \phi = \arctan 2(e_y, e_x)$$

The half opening angle of the cone is obtained from the scalar products of the axis with any of the generatrices:

$$\gamma = \arccos\left(\frac{\mathbf{e}(\mathbf{u}-\mathbf{s})}{|\mathbf{e}(\mathbf{u}-\mathbf{s})|}\right) = \arccos\left(\frac{\mathbf{e}(\mathbf{v}-\mathbf{s})}{|\mathbf{e}(\mathbf{v}-\mathbf{s})|}\right) = \arccos\left(\frac{\mathbf{e}(\mathbf{w}-\mathbf{s})}{|\mathbf{e}(\mathbf{w}-\mathbf{s})|}\right)$$

Use case 2 - Conic section from parameters

6 parameters of a cone, $(s_x, s_y, s_z, \theta, \phi, \gamma)$ are given. Determine the equation of the conic section in the xy plane!

The cone's equation for a general $\mathbf{p} = (p_x, p_y, p_z)$ point can be derived from the condition that the angle between the cone axis ($\mathbf{e}$ unit vector) and a generatrix ($\mathbf{p}-\mathbf{s}$ vector) is the half opening angle, γ (Figure S3):

$$\mathbf{e}(\mathbf{p}-\mathbf{s}) = |\mathbf{p}-\mathbf{s}| \cos\gamma$$

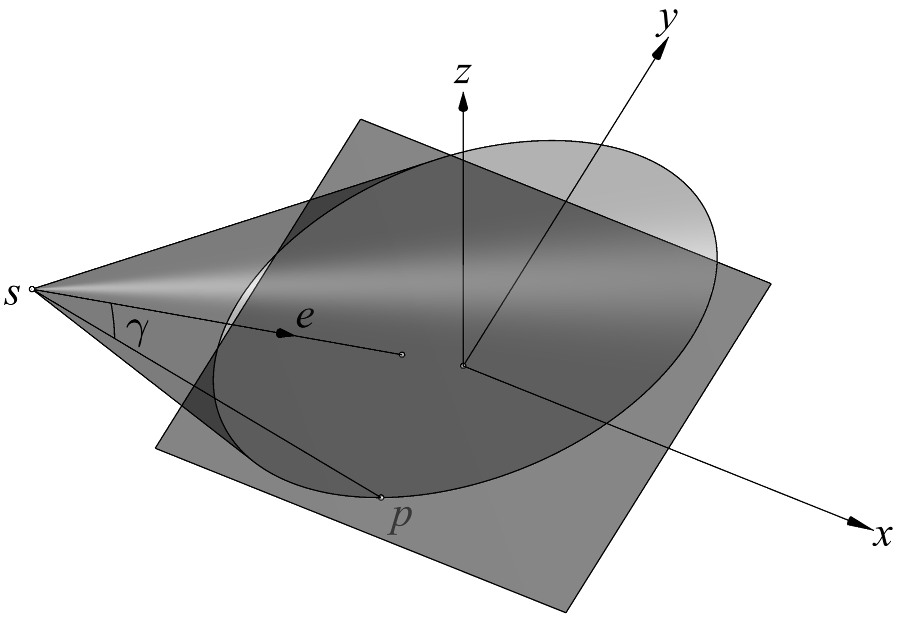

Figure S3. Determination of conic section from parameters.

If we substitute the vectors with their parameters, square the equation and collect powers of the elements of the general point $\mathbf{p}$, we arrive at:

$$\begin{aligned}
&\left(\cos^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)p_x^2\\
&+\left(\sin^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)p_y^2\\
&+\left(\cos^2(\theta)-\cos^2(\gamma)\right)p_z^2\\
&+\left(\sin(2\phi)\sin^2(\theta)\right)p_x p_y\\
&+\left(\sin(2\theta)\cos(\phi)\right)p_x p_z\\
&+\left(\sin(2\theta)\sin(\phi)\right)p_y p_z\\
&+\left(\left(2\cos^2(\gamma)-2\cos^2(\phi)\sin^2(\theta)\right)s_x+\left(-\sin(2\phi)\sin^2(\theta)\right)s_y+\left(-\sin(2\theta)\cos(\phi)\right)s_z\right)p_x\\
&+\left(\left(-\sin(2\phi)\sin^2(\theta)\right)s_x+\left(2\cos^2(\gamma)-2\sin^2(\phi)\sin^2(\theta)\right)s_y+\left(-\sin(2\theta)\sin(\phi)\right)s_z\right)p_y\\
&+\left(\left(-\sin(2\theta)\cos(\phi)\right)s_x+\left(-\sin(2\theta)\sin(\phi)\right)s_y+\left(2\cos^2(\gamma)-2\cos^2(\theta)\right)s_z\right)p_z\\
&+\left(\cos^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)s_x^2+\left(\sin(2\phi)\sin^2(\theta)\right)s_x s_y+\left(\sin(2\theta)\cos(\phi)\right)s_x s_z\\
&+\left(\sin^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)s_y^2+\left(\sin(2\theta)\sin(\phi)\right)s_y s_z+\left(\cos^2(\theta)-\cos^2(\gamma)\right)s_z^2=0
\end{aligned}$$

This is the general equation of the cone in our specific parameter set. Now, in the current problem we also know that $\mathbf{p}=(p_x,p_y,p_z)$ is in the xy plane, i.e. we can substitute $p_z=0$. Then the general cone equation simplifies to a quadratic form of p_x and p_y only, the equation of the desired conic section:

$$A\,p_x^2+B\,p_x p_y+C\,p_y^2+D\,p_x+E\,p_y+F=0$$

The coefficients can be matched from the general equation:

$$\begin{aligned}
&A=\cos^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\\
&B=\sin(2\phi)\sin^2(\theta)\\
&C=\sin^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\\
&D=\left(2\cos^2(\gamma)-2\cos^2(\phi)\sin^2(\theta)\right)s_x+\left(-\sin(2\phi)\sin^2(\theta)\right)s_y+\left(-\sin(2\theta)\cos(\phi)\right)s_z\\
&E=\left(-\sin(2\phi)\sin^2(\theta)\right)s_x+\left(2\cos^2(\gamma)-2\sin^2(\phi)\sin^2(\theta)\right)s_y+\left(-\sin(2\theta)\sin(\phi)\right)s_z\\
&F=\left(\cos^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)s_x^2+\left(\sin(2\phi)\sin^2(\theta)\right)s_x s_y+\left(\sin(2\theta)\cos(\phi)\right)s_x s_z\\
&\quad+\left(\sin^2(\phi)\sin^2(\theta)-\cos^2(\gamma)\right)s_y^2+\left(\sin(2\theta)\sin(\phi)\right)s_y s_z+\left(\cos^2(\theta)-\cos^2(\gamma)\right)s_z^2
\end{aligned}$$

Use case 3 - Nearest point of a conic section

6 coefficients of a conic section equation, (A,B,C,D,E,F) are given (see above) and there is a point in the xy plane, $\mathbf{m}=(m_x,m_y,0)$. Determine the nearest point of the conic section $\mathbf{n}=(n_x,n_y,0)$ and calculate its distance!

We find the closest point in 2 steps. First we determine points of the conic section, where the tangent line of the conic section is perpendicular to the line to the given point. As the conic sections have no inflection points, these will have extreme distances, either local minimum or maximum. As several such points may exist, we calculate their distances and select the closest one (Figure S4).

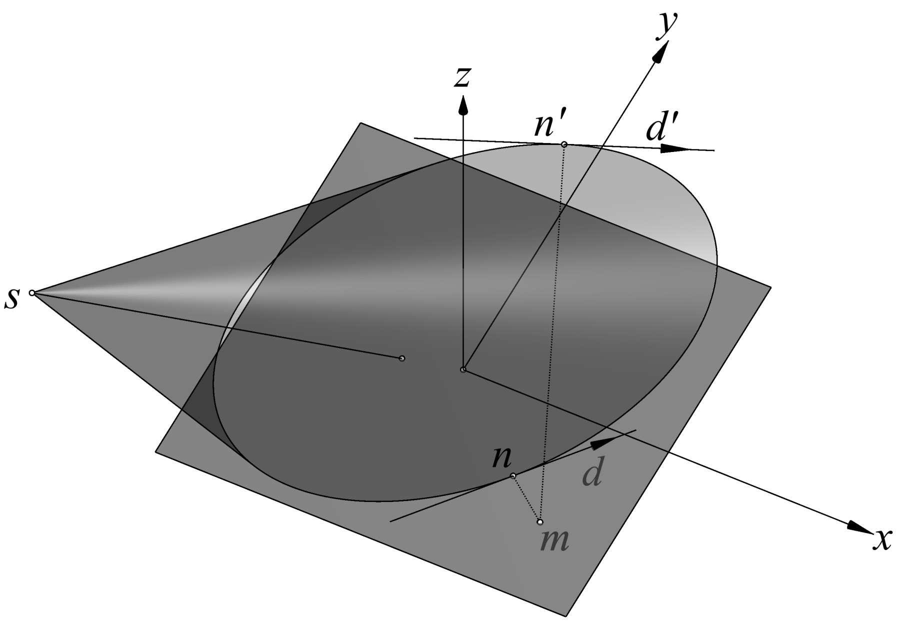

Figure S4. Determination of the nearest (and also the farthest) point of a conic section.

Since $\mathbf{n}=(n_x, n_y, 0)$ is a point of the conic section, it satisfies the equation:

$$A n_x^2 + B n_x n_y + C n_y^2 + D n_x + E n_y + F = 0 \ .$$

If $\mathbf{d}=(d_x, d_y, 0)$ is a tangent vector of the conic section at $\mathbf{n}=(n_x, n_y, 0)$, then $\mathbf{n}+\varepsilon\,\mathbf{d}$, where $\varepsilon \to 0$, is also on the conic section and satisfies a similar equation. Subtracting the two equations, then dividing by ε and omitting the terms with ε^2 we formally differentiate the above equation and obtain:

$$(2 A n_x + B n_y + D) d_x + (2 C n_y + B n_x + E) d_y = 0$$

The condition that $\mathbf{d}$ and $\mathbf{n}-\mathbf{m}$ should be perpendicular is expressed by their scalar product:

$$(n_x - m_x) d_x + (n_y - m_y) d_y = 0$$

From the latter 2 equations we obtain:

$$(n_x - m_x)(2 C n_y + B n_x + E) = (n_y - m_y)(2 A n_x + B n_y + D)$$

This equation expands to another quadratic form of the components of $\vec{n}(n_x, n_y, 0)$:

$$(B) n_x^2 + (2C - 2A) n_x n_y + (-B m_x + 2 A m_y + E) n_x + (-B) n_y^2 + (-2 C m_x + B m_y - D) n_y + (D m_y - E m_x) = 0$$

Now we have to solve this and the first given conic section equation for n_x and n_y. Since both equations are quadratic, that in general can have 4 intersections, we can expect a quartic equation for the kept component. After eliminating either n_x or n_y we obtain a single equation for the remaining variable, and vice versa:

$$a^{(x)} n_x^4 + b^{(x)} n_x^3 + c^{(x)} n_x^2 + d^{(x)} n_x + e^{(x)} = 0 \quad \text{and} \quad a^{(y)} n_y^4 + b^{(y)} n_y^3 + c^{(y)} n_y^2 + d^{(y)} n_y + e^{(y)} = 0$$

After lengthy, but simple calculations the 2×5 coefficients are as follows:

$$
\begin{aligned}
a^{(x)} &= 4A^3C-A^2B^2-8A^2C^2+6AB^2C+4AC^3-B^4-B^2C^2\\
b^{(x)} &= (8A^2C^2-6AB^2C-8AC^3+B^4+2B^2C^2)m_x\\
&\quad +(4A^2BC-AB^3+4ABC^2-B^3C)m_y\\
&\quad +(8DA^2C-2EA^2B-DAB^2+8EABC-12DAC^2-3EB^3+5DB^2C-2EBC^2+4DC^3)\\
c^{(x)} &= (4AC^3-B^2C^2)m_x^2\\
&\quad +(B^3C-4ABC^2)m_x m_y\\
&\quad +(3EB^3-5DB^2C+4EBC^2-8AEBC-8DC^3+12ADC^2)m_x\\
&\quad +(4A^2C^2-AB^2C)m_y^2\\
&\quad +(4EA^2C-3EAB^2+4DABC-2EB^2C+4DBC^2)m_y\\
&\quad +(4FA^2C-3ABDE-8FAC^2+5ACD^2+2ACE^2+4FB^2C-3B^2E^2+6BCDE+4FC^3-4C^2D^2-C^2E^2)\\
d^{(x)} &= (4C^3D-2BC^2E)m_x^2\\
&\quad +(2B^2CE-4BC^2D)m_x m_y\\
&\quad +(3B^2E^2-4FB^2C-6BCDE-8FC^3+4C^2D^2+2C^2E^2+8AFC^2-2ACE^2)m_x\\
&\quad +(4AC^2D-2ABCE)m_y^2\\
&\quad +(FB^3-B^2DE+4FBC^2+BCD^2-BCE^2-2ABE^2+4ACDE)m_y\\
&\quad +(FB^2D+4FBCE-BD^2E-BE^3-2AFBE-4FC^2D+CD^3+CDE^2+4AFCD)\\
e^{(x)} &= (4C^3F-C^2E^2)m_x^2\\
&\quad +(BCE^2-4BC^2F)m_x m_y\\
&\quad +(4DFC^2-DCE^2-4BFCE+BE^3)m_x\\
&\quad +(FB^2C-EBCD+C^2D^2)m_y^2\\
&\quad +(FB^2E-BDE^2+CD^2E)m_y\\
&\quad +(B^2F^2-EBDF+CD^2F)
\end{aligned}
$$

and

$$
\begin{aligned}
a^{(y)} &= 4A^3C-A^2B^2-8A^2C^2+6AB^2C+4AC^3-B^4-B^2C^2\\
b^{(y)} &= (4A^2BC-AB^3+4ABC^2-B^3C)m_x\\
&\quad +(2A^2B^2-8A^3C+8A^2C^2-6AB^2C+B^4)m_y\\
&\quad +(4EA^3-2DA^2B-12EA^2C+5EAB^2+8DABC+8EAC^2-3DB^3-EB^2C-2DBC^2)\\
c^{(y)} &= (4A^2C^2-AB^2C)m_x^2\\
&\quad +(AB^3-4A^2BC)m_x m_y\\
&\quad +(4EA^2B-2DAB^2+4EABC+4DAC^2-3DB^2C)m_x\\
&\quad +(4A^3C-A^2B^2)m_y^2\\
&\quad +(4DA^2B-8EA^3+12CEA^2-5EAB^2-8CDAB+3DB^3)m_y\\
&\quad +(4FA^3-8FA^2C-A^2D^2-4A^2E^2+4FAB^2+6ABDE+4FAC^2+2ACD^2+5ACE^2-3B^2D^2-3BCDE)\\
d^{(y)} &= (4A^2CE-2ABCD)m_x^2\\
&\quad +(2AB^2D-4A^2BE)m_x m_y\\
&\quad +(4FA^2B-ABD^2+ABE^2+4CADE+FB^3-B^2DE-2CBD^2)m_x\\
&\quad +(4A^3E-2A^2BD)m_y^2\\
&\quad +(2A^2D^2-8FA^3+4A^2E^2+8CFA^2-4FAB^2-6ABDE-2CAD^2+3B^2D^2)m_y\\
&\quad +(4FABD-4FA^2E+AD^2E+AE^3+4CFAE+FB^2E-BD^3-BDE^2-2CFBD)\\
e^{(y)} &= (A^2E^2+FAB^2-DABE)m_x^2\\
&\quad +(ABD^2-4A^2BF)m_x m_y\\
&\quad +(FB^2D-BD^2E+ADE^2)m_x\\
&\quad +(4A^3F-A^2D^2)m_y^2\\
&\quad +(4EFA^2-EAD^2-4BFAD+BD^3)m_y\\
&\quad +(B^2F^2-DBEF+AE^2F)
\end{aligned}
$$

Either of the above quartic equations can be solved analytically by several methods [https://en.wikipedia.org/wiki/Quartic_function#Solution_methods, http://mathworld.wolfram.com/QuarticEquation.html], that is not detailed here. Following both solution paths redundantly, we obtain 4 general solutions each, $n_x^{(1)}, n_x^{(2)}, n_x^{(3)}, n_x^{(4)}$ and $n_y^{(1)}, n_y^{(2)}, n_y^{(3)}, n_y^{(4)}$. These are not necessarily solution coordinate pairs. For each of these, we obtain the other coordinate from any of the original equations. Since these were quadratic, we obtain 2 solutions for each, labeled with a and b , and such the 2×4×2 candidate solutions are as follows:

$$(n_x^{(1)}, n_y^{(1a)}), (n_x^{(1)}, n_y^{(1b)}),\ (n_x^{(2)}, n_y^{(2a)}), (n_x^{(2)}, n_y^{(2b)}),\ (n_x^{(3)}, n_y^{(3a)}), (n_x^{(3)}, n_y^{(3b)}),\ (n_x^{(4)}, n_y^{(4a)}), (n_x^{(4)}, n_y^{(4b)})$$
$$(n_x^{(1a)}, n_y^{(1)}), (n_x^{(1b)}, n_y^{(1)}),\ (n_x^{(2a)}, n_y^{(2)}), (n_x^{(2b)}, n_y^{(2)}),\ (n_x^{(3a)}, n_y^{(3)}), (n_x^{(3b)}, n_y^{(3)}),\ (n_x^{(4a)}, n_y^{(4)}), (n_x^{(4b)}, n_y^{(4)})$$

Some of these coordinates are not real, but complex, some of the solutions are false solutions due to squaring equations, some of them are on the conic section but have maximal distance and they are also doubled due to the redundant solution of the equations. Therefore the coordinate of the nearest point and the minimal distance is simply selected from this set of potential solutions after numerical evaluation of $(n_x - m_x)^2 + (n_y - m_y)^2$.