Odhady kuželoseček a kvadrik a jejich přesnost

Eva Fišerová

Univerzita Palackého v Olomouci

Robust 2018
21.-26. ledna 2018, Rybník, Český les

Poděkování

Prezentované výsledky vznikly ve spolupráci se

- Sandrou Donevskou,
- Viktorem Witkovským (SAV Bratislava),
- Gejzou Wimmerem (SAV Bratislava).

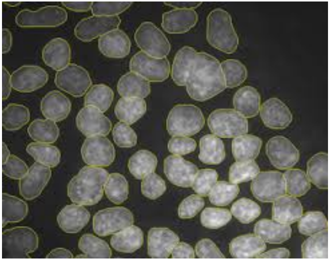
Outline

Motivation

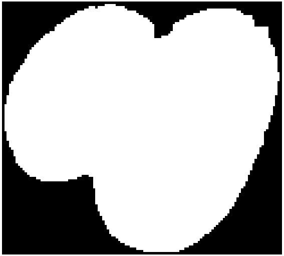
The fitting of geometric features to given 2D/3D points is desired in various fields, e.g.

- quality control (e.g. steel coils quality assurance, grain sorting)
- metrology (e.g. optical interferometers or photogrammetric measurements)
- biology (e.g. chromosome analysis, cell segmentation, tumor modelling)

Segmentation of Cell Nuclei in Microscopy Images



A microscopy image



A pair of touching nuclei

Conics Description

General conic equation

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0$$

Discriminant classification (determinant of matrix corresponding with the quadratic part)

- ellipse: $B^2 - 4AC < 0$
- circle: $A = C,\ B = 0$
- hyperbola: $B^2 - 4AC > 0$
- parabola: $B^2 - 4AC = 0$

Conics description

The general conic equation

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0$$

Assumptions for real non-degenerate conic

- $A^2 + B^2 + C^2 > 0$
- Non-zero determinant Δ of the matrix

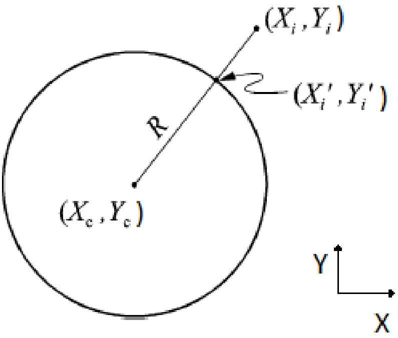
$$\begin{bmatrix} A & B/2 & D/2 \\ B/2 & C & E/2 \\ D/2 & E/2 & F \end{bmatrix},$$

- for the ellipse: $\Delta(A + C) < 0$

For the uniqueness, A, B, C, D, E, F must fulfil one linear restriction, e.g. $A = 1$, or $F = -1$.

Circle

- R radius
- (X_c, Y_c) center



Conic equation for the circle

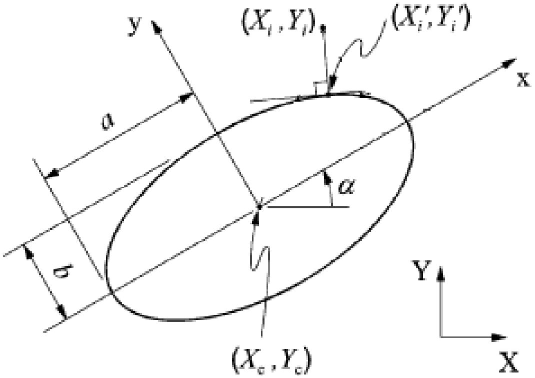
$$x^2 + y^2 + Dx + Ey + F = 0$$

Relationships between geometric and algebraic circle parameters:

$$R = \sqrt{D^2/4 + E^2/4 - F}, \quad X_c = -D/2, \quad Y_c = -E/2$$

Ellipse

Geometric description



- α rotation angle, $\alpha \in (-\pi/2, \pi/2\rangle$
- (X_c, Y_c) center
- a length of semi-major axis
- b length of semi-minor axis

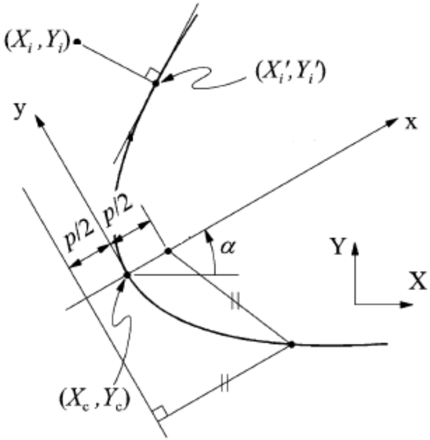
Conic equation for the ellipse

$$x^2 + Bxy + Cy^2 + Dx + Ey + F = 0, \quad B^2 - 4C < 0$$

Relationships between geometric and algebraic ellipse parameters:

$$X_c = \frac{BE - 2CD}{4C - B^2}$$
$$Y_c = \frac{BD - 2E}{4C - B^2}$$
$$a_x = \frac{2\sqrt{C}}{4C - B^2}\sqrt{CD^2 - BDE + E^2 - F(4C - B^2)}$$
$$b_y = \frac{2}{4C - B^2}\sqrt{CD^2 - BDE + E^2 - F(4C - B^2)}$$
$$\alpha = \frac{1}{2}\operatorname{arccot}\left(\frac{1 - C}{B}\right) \ \textit{for } 1 < C, \ \textit{otherwise } \alpha + \frac{\pi}{2}$$

- p focal parameter (distance from the focus to the directrix)
- α pose angle, $\alpha \in (-\pi, \pi\rangle$
- (X_c, Y_c) vertex



$$Ax^2 + 2Bxy + Cy^2 + 2Dx + 2Ey + F = 0$$

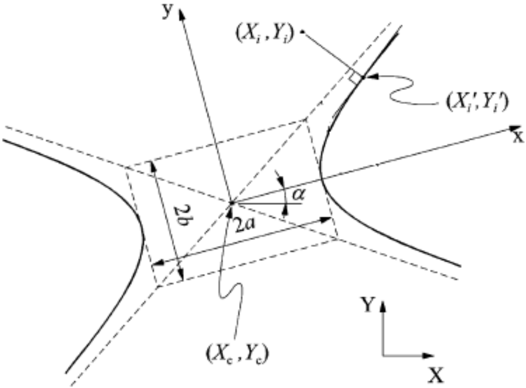
$$B^2 - AC = 0, \quad A + C - 1 = 0$$

Relationships between geometric and algebraic parabola parameters:

$$A = \sin^2\alpha, \quad B = -\sin\alpha\cos\alpha, \quad C = \cos^2\alpha,$$
$$D = -X_c\sin^2\alpha + Y_c\sin\alpha\cos\alpha - p\cos\alpha,$$
$$E = X_c\sin\alpha\cos\alpha - Y_c\cos^2\alpha - p\sin\alpha,$$
$$F = (X_c\sin\alpha - Y_c\cos\alpha)^2 + 2p(X_c\cos\alpha + Y_c\sin\alpha).$$

Hyperbola

- α pose angle, $\alpha \in (-\pi/2, \pi/2\rangle$
- (X_c, Y_c) center
- a length of semi-major axis
- b length of semi-minor axis



Unique relationships between the algebraic and geometric parameters.

Overview of Methods for Conics Fitting

- **Least-squares methods**
  - algebraic fitting - minimized error distances are deviations of the implicit equation from the zero
  - geometric fitting - minimized error distances are orthogonal (shortest) distances from given points to the geometric feature to be fitted
- **Hough transform** (Hough, 1962; Douda and Hart, 1972; Ballard, 1981)
- **Moment method** (Chaudhuri and Samanta, 1991; Safaee et. al, 1992; Voss and Süsse, 1997)
- **Maximum likelihood method** - minimize orthogonal distances
  - accurate results
  - often inadequate for many practical scenarios - time consuming and numerically unstable (Ahn, 2004; Chernov 2011)

Overview of Methods for Conics Fitting

- **Other alternative techniques** - minimize different cost functions - balance between the accuracy of the orthogonal distance regression method and the simplicity of algebraic fitting methods
  - gradient-weighted method,
  - approximate maximum likelihood (AML),
  - hyper-accurate methods,
  - etc.

Least-Squares: Algebraic Fitting

Minimizes the squares of algebraic distances

$$\min_{\theta} \sum_{i=1}^{n} (Ax_i^2 + Bx_i y_i + Cy_i^2 + Dx_i + Ey_i + F)^2$$

$$\theta = (A, B, C, D, E, F)'$$

Advantages: simple and quick calculation

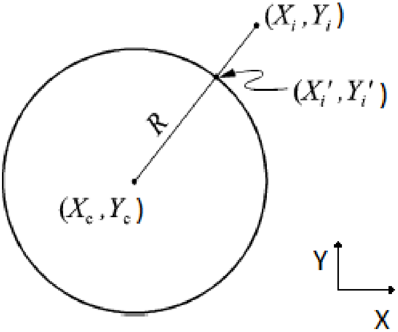
Disadvantages: biased estimators, sometimes ends in unintended geometric feature, interpretation of errors, problem with the accuracy and inference

Least-Squares: Geometric Fitting

- Minimized error distances are orthogonal distances from given points (x_i, y_i) to the geometric feature to be fitted

$$\min \sum_{i=1}^{n} \{(x_i - x_i')^2 + (y_i - y_i')^2\} \text{ w.r.t}$$

$$Ax_i'^2 + Bx_i'y_i' + Cy_i'^2 + Dx_i' + Ey_i' + F = 0$$



- X, Y random variables

Least-Squares: Geometric Fitting

- Iterative algorithms
  - Gander et al.(1994) - slow, complicated and often divergent algorithms
  - Projection algorithms - Ahn et. al (2001), Aigner et. al (2008), Sturm (2007), Wijewickrema (2010), Chernov (2012, 2014)
  - Köning et. al (2014) - ellipse fitting by a linear model with nonlinear restrictions

Geometric Fitting by Linear Model with Constraints

Statistical model

$$x_i = \mu_i + \varepsilon_{x,i}, \;\; i = 1, 2, \ldots, n,$$
$$y_i = \nu_i + \varepsilon_{y,i}, \;\; i = 1, 2, \ldots, n,$$
$$\mu_i^2 + B\mu_i\nu_i + C\nu_i^2 + D\mu_i + E\nu_i + F = 0, \; i = 1, 2, \ldots, n$$

non-linear restrictions $\nearrow$

$$\mathrm{var}(\varepsilon_{x,i}) = \mathrm{var}(\varepsilon_{y,i}) = \sigma^2, \quad \mathrm{cov}(\varepsilon_{x,i}, \varepsilon_{y,i}) = 0$$

Matrix form of a model:

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\varepsilon}_x \\ \boldsymbol{\varepsilon}_y \end{pmatrix}, \quad \mathrm{var}[\boldsymbol{\varepsilon}_x', \boldsymbol{\varepsilon}_y'] = \sigma^2 \mathbf{I}_{2n}$$

$$\mathbf{B}\boldsymbol{\theta} + \mathbf{b} = \mathbf{0},$$

where $\mathbf{B} = \left[\boldsymbol{\mu\nu} \,\vdots\, \boldsymbol{\nu}^2 \,\vdots\, \boldsymbol{\mu} \,\vdots\, \boldsymbol{\nu} \,\vdots\, \mathbf{1} \right]$, $\boldsymbol{\theta} = (B, C, D, E, F)'$, and $\mathbf{b} = \boldsymbol{\mu}^2$.

Estimation of Algebraic Parameters and Errorless Values

Results in the linearized model

- locally best linear unbiased estimators (LBLUE) of
  - the algebraic parameters B, C, D, E, F.
  - the errorless values $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$
- the covariance matrices of the estimators $\widehat{\boldsymbol{\mu}}$, $\widehat{\boldsymbol{\nu}}$ and $(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F})'$
- the cross-covariance matrix of the estimators $\widehat{\boldsymbol{\mu}}$ and $\widehat{\boldsymbol{\nu}}$
- the cross-covariance matrix of the estimators $(\widehat{\boldsymbol{\mu}}', \widehat{\boldsymbol{\nu}}')'$ and $(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F})'$

All results are data-dependent $\Longrightarrow$ need to solve it in an iterative procedure

Steps of the Iterative Procedure

1. Determine an initial guess: the conics algebraic parameters $B^{(0)}$, $C^{(0)}$, $D^{(0)}$,$E^{(0)}$, $F^{(0)}$ and the errorless recordings $\boldsymbol{\mu}^{(0)}$, $\boldsymbol{\nu}^{(0)}$ on the following way:

$$\begin{aligned} \boldsymbol{\mu}^{(0)} &= \mathbf{x} \\ \boldsymbol{\nu}^{(0)} &= \mathbf{y} \\ \boldsymbol{\theta}^{(0)} &= -\left(\mathbf{B}_0'\mathbf{B}_0\right)^{-1}\mathbf{B}_0'\mathbf{x}^2, \end{aligned}$$

where $\boldsymbol{\theta}^{(0)} = (B^{(0)}, C^{(0)}, D^{(0)}, E^{(0)}, F^{(0)})'$, $\mathbf{B}_0 = \left[\mathbf{y}^2 \vdots \mathbf{xy} \vdots \mathbf{x} \vdots \mathbf{y} \vdots \mathbf{1}\right]$.

2. For all data points $(x_i, y_i)'$, $i = 1, \ldots, n$, calculate the estimates $\widehat{\boldsymbol{\theta}}$,$\widehat{\boldsymbol{\mu}}$ and $\widehat{\boldsymbol{\nu}}$.
3. Update the initial values
4. Repeat steps 2 through 4 until estimates converge.

Properties of the Iterative Procedure

- The iterative procedure converges very quickly, and after few iterations the estimates settle down at stable values.
- If the iterative procedure converges, the resulting estimates are the same as the maximum likelihood ones.
- The iterative procedure guarantees that resulting estimates satisfy the constraints, i.e.

$$\widehat{\mu}_i^2 + \widehat{B}\widehat{\mu}_i\widehat{\nu}_i + \widehat{C}\widehat{\nu}_i^2 + \widehat{D}\widehat{\mu}_i + \widehat{E}\widehat{\nu}_i + \widehat{F} = 0$$

Geometric Parameters Estimation

Geometric parameters are functions of algebraic parameters

$$g_j = f_j(B, C, D, E, F)$$

$$\Downarrow$$

In general, plug-in estimators of geometric parameters

$$\widehat{g}_j = f_j(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F})$$

For example, for a circle we obtain:

$$\widehat{R} = \sqrt{\widehat{D}^2/4 + \widehat{E}^2/4 - \widehat{F}}, \quad \widehat{X}_c = -\widehat{D}/2, \quad \widehat{Y}_c = -\widehat{E}/2$$

Optimality properties of $\widehat{g}_j$ are in general unknown

$\rightarrow$ bootstrap, simulations

Geometric Parameters Estimation – Accuracy

In general, plug-in estimators of geometric parameters

$$\widehat{g}_j = f_j(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F})$$

Estimated variance-covariance matrix of $\widehat{\boldsymbol{g}}$

$$\widehat{\mathrm{var}}(\widehat{\boldsymbol{g}}) = \widehat{\boldsymbol{J}} \, \mathrm{var}[(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F})'] \, \widehat{\boldsymbol{J}}'$$

$$\widehat{\boldsymbol{J}}_{j1} = \frac{\partial f_j}{\partial B}, \ldots, \widehat{\boldsymbol{J}}_{j5} = \frac{\partial f_j}{\partial F}$$

- 2D conics - explicit expressions

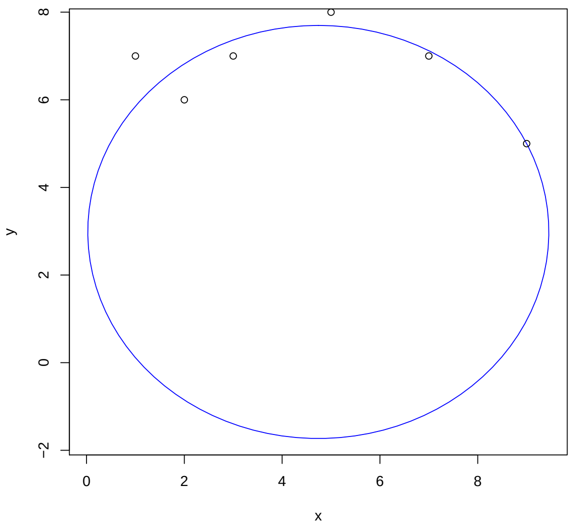
Example: Circle Fitting

- Data: Ahn (2001)
- Convergence criterion

  $\| \widehat{\beta}^{i} - \widehat{\beta}^{i-1} \|_E^2 < 10^{-6}$

- Results:
  - 19 iterations
  - estimates (std errors):
    $\widehat{X}_c = 4.740\,(0.476)$
    $\widehat{Y}_c = 2.984\,(1.543)$
    $\widehat{R} = 4.714\,(1.499)$
  - $\widehat{\sigma}^2 = 0.409$

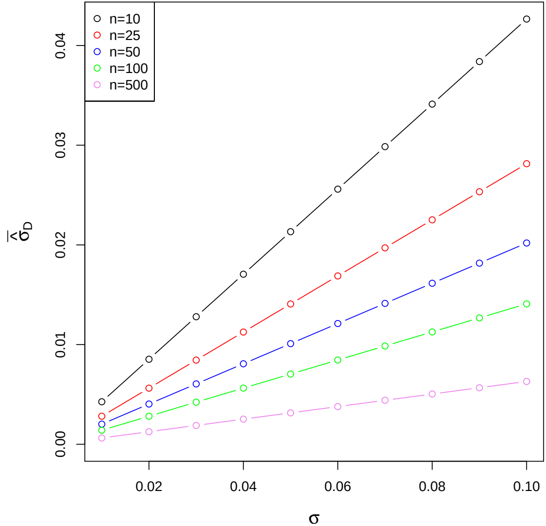
Fitted Circle



Simulation Study

- Performed for all types of conics
- Sample size of 10, 25, 50, 100, 500 given points evenly spaced around the conic
- Standard errors of measurements chosen from 0.01 to 0.1
- Convergence criterion higher than 10^{-12}
- 1000 simulations for each case

$$x^2 + y^2 + Dx + Ey + F = 0$$

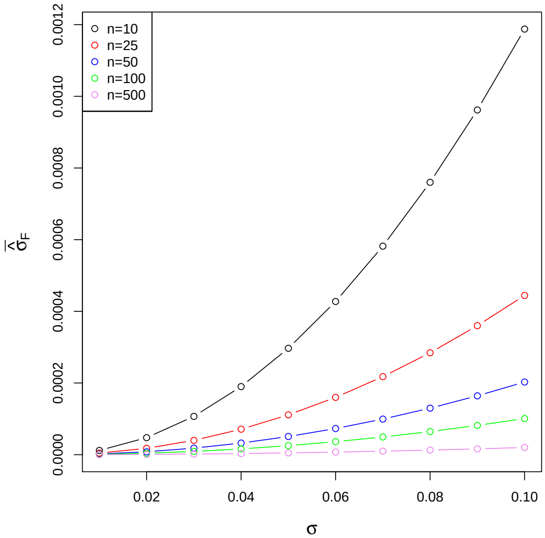


n=10
n=25
n=50
n=100
n=500
0.00
0.01
0.02
0.03
0.04
$\bar{\hat{\sigma}}_D$
0.02
0.04
0.06
0.08
0.10
σ

Circle Fitting: Accuracy for Algebraic Parameter F

Averages from 1000 simulations

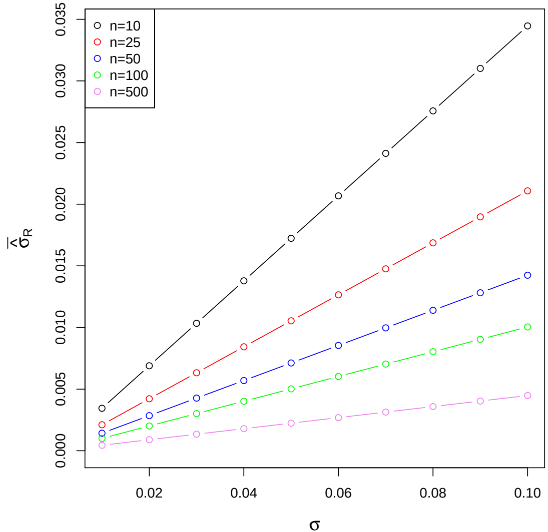
$$x^2 + y^2 + Dx + Ey + F = 0$$



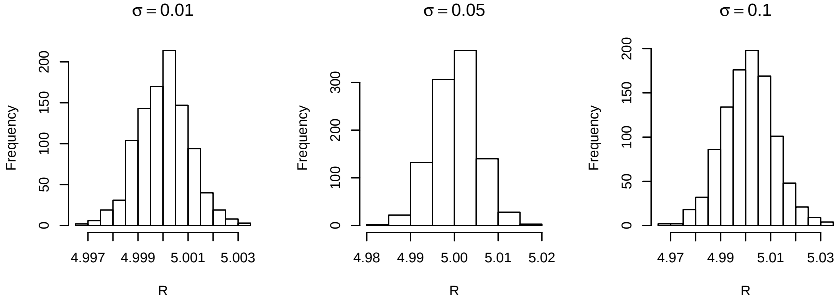
Circle Fitting: Accuracy for Geometric Parameter R

Averages from 1000 simulations

$$R = \sqrt{D^2/4 + E^2/4 - F}$$



Properties of Circle Geometric Parameters Estimators $X_c = 3,\ Y_c = 1,\ R = 5, (n = 100, \sigma = 0.01, 0.05, 0.1)$



Histograms of the estimates of the radius of the circle resulting from the simulation study

Properties of Circle Geometric Parameters Estimators $X_c = 3,\ Y_c = 1,\ R = 5$, $(n = 100, \sigma = 0.01, 0.05, 0.1)$

- Average values of the estimates

X_c	1.000	1.000	1.001
Y_c	3.000	3.000	3.000
R	5.000	5.000	5.001

- The coverage probability (in %) of 95% confidence interval

X_c	95.6	95.6	95.5
Y_c	94.3	94.3	94.3
R	94.2	93.9	94.0

- Average width of 95% confidence interval

X_c	0.006	0.028	0.056
Y_c	0.006	0.028	0.056
R	0.004	0.020	0.040

- Similar results for other types of conics

Ellipsoid description

The general ellipsoid is a second-order algebraic surface

$$Ax^2 + By^2 + Cz^2 + Dxy + Exz + Fyz + Gx + Hy + Kz + L = 0$$

Assumptions for real non-degenerate ellipsoid

- $\mathbf{M}_3$, $\mathbf{M}_4$ full rank matrices,
- $\mathbf{M}_3$ positive definite matrix,
- the determinant of the matrix $\mathbf{M}_4$ is negative

$$\mathbf{M}_3 = \begin{bmatrix} A & D/2 & E/2 \\ D/2 & B & F/2 \\ E/2 & F/2 & C \end{bmatrix}, \quad \mathbf{M}_4 = \begin{bmatrix} A & D/2 & E/2 & G/2 \\ D/2 & B & F/2 & H/2 \\ E/2 & F/2 & C & K/2 \\ G/2 & H/2 & K/2 & L \end{bmatrix}$$

For the uniqueness, $A, B, C, D, E, F, G, H, K, L$ fulfil one linear restriction, e.g. $A = 1$, or $L = -1$.

Ellipsoid Description - cont.

$$Ax^2 + By^2 + Cz^2 + Dxy + Exz + Fyz + Gx + Hy + Kz + L = 0$$

$$\Updownarrow$$

$$(\mathbf{x} - \mathbf{x}_c)'\mathbf{M}_3(\mathbf{x} - \mathbf{x}_c) = \kappa, \quad \kappa = \mathbf{x}_c'\mathbf{M}_3\mathbf{x}_c - L, \quad \mathbf{x} = (x, y, z)'$$

Centre $\mathbf{x}_c = (x_c, y_c, z_c)'$

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = -\frac{1}{2}\mathbf{M}_3^{-1} \begin{pmatrix} G \\ H \\ K \end{pmatrix}$$

The semi-axis length in the direction of the eigenvector $\mathbf{v}_i$ of $\mathbf{M}_3$

$$r_i = \sqrt{\kappa/\lambda_i}, \quad i = 1, 2, 3$$

Ellipsoid Parametrization

- r_x, r_y, r_z semi-axes lengths in the direction of x-, y-, z-axis
- θ_x, θ_y, θ_z angles of rotations around $x-$, $y-$, $z-$axes
- a right-handed Cartesian coordinate system

Rotation of θ_x radians in a counter-clockwise direction when looking towards origin about the x-axis

$$\mathbf{R}_x(\theta_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_x) & -\sin(\theta_x) \\ 0 & \sin(\theta_x) & \cos(\theta_x) \end{pmatrix}$$

Rotation of θ_y radians about the y-axis:

$$\mathbf{R}_y(\theta_y) = \begin{pmatrix} \cos(\theta_y) & 0 & \sin(\theta_y) \\ 0 & 1 & 0 \\ -\sin(\theta_x) & 0 & \cos(\theta_y) \end{pmatrix}$$

Rotation of θ_z radians about the z-axis:

$$\mathbf{R}_z(\theta_z) = \begin{pmatrix} \cos(\theta_z) & -\sin(\theta_z) & 0 \\ \sin(\theta_z) & \cos(\theta_z) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Ellipsoid Parametrization - cont.

Rotations in 3D do not commute $\longrightarrow$ it depends in which order multiple rotations are performed

Assume rotation firstly about z-axis, then about y-axis, and, finally, about x-axis (Turner et al., 1999):

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \mathbf{R}_x(\theta_x)\mathbf{R}_y(\theta_y)\mathbf{R}_z(\theta_z) \begin{pmatrix} r_x \cos(u)\cos(v) \\ r_y \sin(u)\cos(v) \\ r_z \sin(v) \end{pmatrix} + \begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix}$$

$$-\pi \le u < \pi, \quad -\pi/2 \le v < \pi/2$$

Ellipsoid Geometric Parameters - Particular Solution

- the centre $\mathbf{x}_c = (x_c, y_c, z_c)'$ - uniquely defined
- a class of rotations angles and semi-axes lengths triplets reproducing the same algebraic parameters
- semi-axes lengths: $(r_x, r_y, r_z) = (r_1, r_2, r_3)$, $r_1 \geq r_2 \geq r_3$

The eigenvectors of $\mathbf{M}_3$ form the rotation matrix $\mathbf{R} \longrightarrow \phi_x, \phi_y, \phi_z$

- $\phi_y \neq \pm\frac{\pi}{2}$, i.e. $R_{13} \neq \pm 1$: 2 triplets of angles

$$
\begin{aligned}
\phi_y^1 &= \arcsin(R_{13}), \quad \phi_y^2 = \pi - \arcsin(R_{13}) \\
\phi_x^j &= \arctan 2[-R_{23}/\cos(\phi_y^j), R_{33}/\cos(\phi_y^j)], \\
\phi_z^j &= \arctan 2[-R_{12}/\cos(\phi_y^j), R_{11}/\cos(\phi_y^j)], \quad j = 1, 2
\end{aligned}
$$

- $\phi_y = \pm\frac{\pi}{2}$, i.e. $R_{13} = \pm 1$: infinite number of solutions

$$
\begin{aligned}
\phi_x &= -\phi_z + \arctan 2(R_{21}, R_{22}) \quad \text{for} \quad \phi_y = \frac{\pi}{2}, \\
\phi_x &= \phi_z - \arctan 2(R_{21}, R_{22}) \quad \text{for} \quad \phi_y = -\frac{\pi}{2}
\end{aligned}
$$

One possible solution - set $\phi_z = 0$ and to evaluate the corresponding value of ϕ_x.

Ellipsoid Geometric Parameters - Number of Equivalent Solutions

Lemma 1. 576 triplets (ϕ_x, ϕ_y, ϕ_z) under the assumption that the second rotation in the sequence of rotations about principal axes is not $\pm pi/2$.
Proof: $2 \times 6 \times 6 \times 8 = 576$

- 2 particular solutions
- 6 possible ordering of eigenvectors
- 6 possible sequences of rotations
- the multiplication of eigenvectors by -1 results in 8 options for each triplet of eigenvectors

Lemma 2. 6 triplets (r_x, r_y, r_z)
Proof: No relationship between eigenvalues and x-, y, z-axis $\longrightarrow$ 6 triplets (r_x, r_y, r_z)

Theorem 3. $6 \times 576 = 3454$ sextuplets $(r_x, r_y, r_z, \phi_x, \phi_y, \phi_z)$

Fitting Ellipsoid to Correlated Data

Statistical model

$$x_i = \mu_i + \varepsilon_{x,i},\ \ i = 1, 2, \ldots, n,$$
$$y_i = \nu_i + \varepsilon_{y,i},\ \ i = 1, 2, \ldots, n,$$
$$z_i = \xi_i + \varepsilon_{z,i},\ \ i = 1, 2, \ldots, n,$$

non-linear restrictions:

$$\mu_i^2 + B\nu_i^2 + C\xi_i^2 + D\mu_i\nu_i + E\mu_i\xi_i + F\nu_i\xi_i + G\mu_i + H\nu_i + K\xi_i + L = 0$$

$$\mathrm{var}(\varepsilon_{x,i}) = \mathrm{var}(\varepsilon_{y,i}) = \mathrm{var}(\varepsilon_{z,i}) = \sigma^2,$$

$$\mathrm{cov}(\varepsilon_{x,i}, \varepsilon_{y,i}) = \varrho_{x,y}\sigma^2,\ \mathrm{cov}(\varepsilon_{x,i}, \varepsilon_{z,i}) = \varrho_{x,z}\sigma^2,\ \mathrm{cov}(\varepsilon_{y,i}, \varepsilon_{z,i}) = \varrho_{y,z}\sigma^2$$

Matrix form of a model:

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \\ \mathbf{z} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\nu} \\ \boldsymbol{\xi} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\varepsilon}_x \\ \boldsymbol{\varepsilon}_y \\ \boldsymbol{\varepsilon}_z \end{pmatrix}$$

$$\mathrm{var}[(\boldsymbol{\varepsilon}'_x, \boldsymbol{\varepsilon}'_y, \boldsymbol{\varepsilon}'_z)'] = \boldsymbol{\Sigma} = \sigma^2 \begin{pmatrix} \mathbf{I}_{n,n} & \varrho_{x,y}\mathbf{I}_{n,n} & \varrho_{x,z}\mathbf{I}_{n,n} \\ \varrho_{x,y}\mathbf{I}_{n,n} & \mathbf{I}_{n,n} & \varrho_{y,z}\mathbf{I}_{n,n} \\ \varrho_{x,z}\mathbf{I}_{n,n} & \varrho_{y,z}\mathbf{I}_{n,n} & \mathbf{I}_{n,n} \end{pmatrix} = \sum_{i=1}^{4} \vartheta_i \mathbf{V}_i$$

$$\mathbf{B}\boldsymbol{\theta} + \mathbf{b} = \mathbf{0},$$

where

$$\mathbf{B} = \left[\boldsymbol{\nu}^2 \vdots \boldsymbol{\xi}^2 \vdots \boldsymbol{\mu}\boldsymbol{\nu} \vdots \boldsymbol{\mu}\boldsymbol{\xi} \vdots \boldsymbol{\nu}\boldsymbol{\xi} \vdots \boldsymbol{\mu} \vdots \boldsymbol{\nu} \vdots \boldsymbol{\xi} \vdots \mathbf{1} \right]$$

$\boldsymbol{\theta} = (B, C, D, E, F, G, H, K, L)'$, and $\mathbf{b} = \boldsymbol{\mu}^2$.

Estimation of Variance Components

The variance-covariance matrix of random errors

$$\mathrm{var}[(\varepsilon_x', \varepsilon_y', \varepsilon_z')'] = \sigma^2 \begin{pmatrix} \mathbf{I}_{n,n} & \varrho_{x,y}\mathbf{I}_{n,n} & \varrho_{x,z}\mathbf{I}_{n,n} \\ \varrho_{x,y}\mathbf{I}_{n,n} & \mathbf{I}_{n,n} & \varrho_{y,z}\mathbf{I}_{n,n} \\ \varrho_{x,z}\mathbf{I}_{n,n} & \varrho_{y,z}\mathbf{I}_{n,n} & \mathbf{I}_{n,n} \end{pmatrix} = \sum_{i=1}^{4} \vartheta_i \mathbf{V}_i$$

where

$$\vartheta_1 = \sigma^2, \quad \vartheta_2 = \sigma^2 \varrho_{x,y}, \quad \vartheta_3 = \sigma^2 \varrho_{x,z}, \quad \vartheta_4 = \sigma^2 \varrho_{y,z}$$

In the linearized model, locally minimum norm quadratic unbiased estimator (LMINQUE) of $\vartheta_1, \ldots, \vartheta_4$ based on Rao's procedure (Rao and Kleffe, 1988) can be determined.

Results are data-dependent $\Longrightarrow$ need to solve it in an iterative procedure

Steps of the Iterative Procedure

1. Determine an initial guess: the ellipsoid algebraic parameters $\boldsymbol{\theta}^{(0)}$, the errorless recordings $\boldsymbol{\mu}^{(0)}$, $\boldsymbol{\nu}^{(0)}$, $\boldsymbol{\xi}^{(0)}$ and variance components $\boldsymbol{\vartheta}_0$ in the following way:

$$
\begin{aligned}
\vartheta_1^{(0)} &= \sigma^{2(0)} = 1,\ \vartheta_2^{(0)} = \sigma^{2(0)}\varrho_{x,y} = 0 \\
\vartheta_3^{(0)} &= \sigma^{2(0)}\varrho_{x,z} = 0,\ \vartheta_4^{(0)} = \sigma^{2(0)}\varrho_{y,z} = 0 \\
\boldsymbol{\mu}^{(0)} &= \mathbf{x},\ \boldsymbol{\nu}^{(0)} = \mathbf{y},\ \boldsymbol{\xi}^{(0)} = \mathbf{z} \\
\boldsymbol{\theta}^{(0)} &= -\left([\mathbf{B}^{(0)}]'\mathbf{B}^{(0)}\right)^{-1}[\mathbf{B}^{(0)}]'\mathbf{x}^2, \\
\mathbf{B}^{(0)} &= \left[\boldsymbol{y}^2 \vdots \boldsymbol{z}^2 \vdots \boldsymbol{xy} \vdots \boldsymbol{xz} \vdots \boldsymbol{yz} \vdots \boldsymbol{x} \vdots \boldsymbol{y} \vdots \boldsymbol{z} \vdots \mathbf{1}\right].
\end{aligned}
$$

2. For all data points $(x_i, y_i, z_i)'$, $i = 1, \ldots, n$, calculate the estimates $\widehat{\boldsymbol{\theta}}$,$\widehat{\boldsymbol{\mu}}$, $\widehat{\boldsymbol{\nu}}$ and $\widehat{\boldsymbol{\xi}}$.
3. Calculate the estimates of variance components $\boldsymbol{\vartheta}$.
4. Update the initial values
5. Repeat steps 2 through 5 until estimates converge.

Geometric Parameters Estimation - Quadric Surfaces, e.g. Ellipsoid

- **The centre** is uniquely determined by the algebraic parameters (there exists explicite function)

- **Other geometric parameters** relate with the sequence of axes rotations and their orientation $\Rightarrow$ a class of rotations angles and semi-axes lengths triplets reproducing the same algebraic parameters
  - choice of particular solution

- Accuracy of estimators

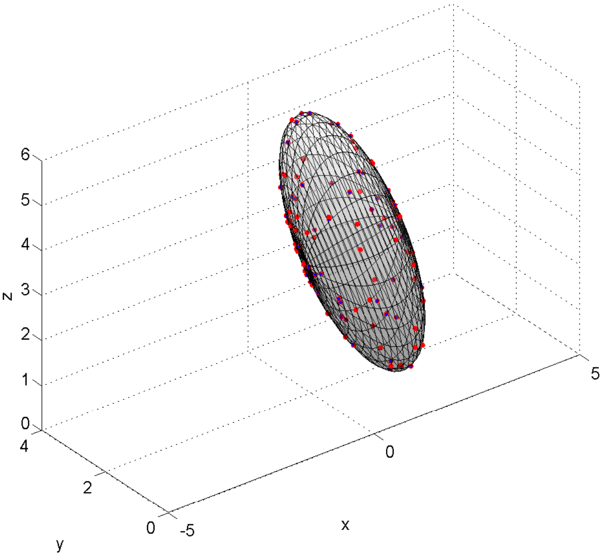
$$\widehat{\mathrm{var}}(\widehat{\boldsymbol{g}}) = \widehat{\boldsymbol{J}}\,\mathrm{var}[(\widehat{B}, \widehat{C}, \widehat{D}, \widehat{E}, \widehat{F}, \widehat{G}, \widehat{H}, \widehat{K}, \widehat{L})']\,\widehat{\boldsymbol{J}}'$$

  - numerical differentiation should be used for estimating derivatives w.r.t algebraic parameters

Example: Ellipsoid Fitting

Similated data

- $n = 100$
- $(X_c, Y_c, Z_c) = (1, 2, 3)$
- $(r_x, r_y, r_z) = (3, 2, 1)$
- $(\theta_x, \theta_y, \theta_z) = (-0.7, 1.18, 0.7)$
- $\sigma^2 = 0.01$
- $\rho = 0$



Example: Ellipsoid Fitting - Results

Param.	True	Est.	Stand. error	Lower 95%CI	Upper 95%CI
X_c	1	1.000	0.0014	0.997	1.003
Y_c	2	2.001	0.0021	1.997	2.005
Z_c	3	2.998	0.0026	2.993	3.003
r_x	3	2.999	0.0034	2.993	3.006
r_y	2	1.993	0.0029	1.988	1.999
r_z	1	1.000	0.0014	0.997	1.002
θ_x	-0.7	-0.699	0.0039	-0.707	-0.692
θ_y	1.18	1.182	0.0014	1.179	1.184
θ_z	0.7	-0.701	0.0046	-0.710	-0.692

- similar accuracy for correlated data

Conclusions

Conics and quadric surfaces fitting

- currently very topical issue
- many algorithms - problem with accuracy, time computing, statistical inference, not include correlations between coordinates
- proposed solution via linear model with restrictions avoid these problems:
  - estimators of geometric parameters (together with their uncertainties)
  - possible to perform statistical inference
  - high accuracy of algebraic and geometric parameters
  - for data spaced around a small part of conic/quadric surface, the correction for bias should be used (see e.g. Schaffrin and Snow, 2010)

Key References

- Chernov, N. (2010). Circular and Linear Regression: Fitting Circles and Lines by Least Squares. Chapman&Hall/CRC.
- Donevska, S., Fišerová, E., Hron, K. (2011) On the Equivalence between Orthogonal Regression and Linear Model with Type-II Constraints. Acta Univ. Palacki. Olomuc., Mathematica 50, 19-–27.
- Fišerová, E., Donevska, S (2015) Conics fitting by least squares. In: Souvenir Booklet of the 24th IWMS, 98-104.
- Kubáček, L., Kubáčková, L., Volaufová, J. (1995) Statistical models with linear structures. Veda, Bratislava.
- Köning, R., Wimmer, G., Witkovský, V. (2014) Ellipse fitting by linearized nonlinear constraints to demodulate quadrature homodyne interferometer signals and to determine the statistical uncertainty of the interferometric phase. Meas. Sci. Technol. 25, 115001.
- Rao, C.R., Kleffe, J. (1988) Estimation of Variance Components and Applications.
- Schaffrin, B., Snow, K. (2010) Total Least-Squares regularization of Tykhonov type and an ancient racetrack in Corinth. Linear Algebra and its Applications 432, 2061-–2076.
- Turner, D.A., Anderson, I.J., Mason, J.C., Cox, M.G. (1999) An algorithm for fitting an ellipsoid to data.

References: List of methods

- Aigner, M. and Jüttler, B. (2008). Gauss-Newton type techniques for robustly fitting implicitly defined curves and surfaces to unorganized data points, *Shape Modeling International.*, 121–130.
- Ahn, S. J., Rauh, W. and Warnecke, H.J. (2001). Least-squares orthogonal distances fitting of circle, sphere, ellipse, hyperbola, and parabola, *Pattern Recog.*, 34, 2283–2303.
- Ahn, S. J. (2004). *Least Squares Orthogonal Distance Fitting of Curves and Surfaces in Space*, Springer, Berlin.
- Berman, M. (1989). Large sample bias in least squares estimators of a circular arc center and its radius, *CVGIP*, 45, 126-128.
- Chan, N. N. (1965). On circular functional relationships, *J. R. Statist. Soc. B.*, 27, 45-56.
- Chernov, N., Lesort, C. (2004). Statistical efficiency of curve fitting algorithms, *Comp. Stat. Data Anal.*, 47, 713-728.
- Chernov, N. and Ma, H. (2011). Least squares fitting of quadratic curves and surfaces, *Computer Vision*, (Yoshida, S. R., eds.), Nova Science Publishers, 285-302.
- Gander, W., Golub, G. H. and Strebel, R. (1994). Least-squares fitting of circles and ellipses, *BIT Numer. Math.*, 34, 34-558.

References: List of methods

- K. Kanatani, K., (1994) Statistical bias of conic fitting and renormalization, *IEEE Trans. PAMI*, 16, 320-326.
- Rosin, P.L. (1993). A note on the least squares fitting of ellipses, *Pattern Recognition Lett.*, 14, 799-808.
- Rosin, P.L. (1996). Assessing error of fit functions for ellipses, *Graphical Models Image Process.*, 58, 494-502.
- Safaee-Rad, R., Tchoukanov, I., Benhabib, B. and Smith, K.C. (1991). Accurate parameter estimation of quadric curves from grey-level images, *CVGIP: Image Understanding*, 54, 259-274.