Estimation of an Ellipsoid from Observation of Points on its Boundary

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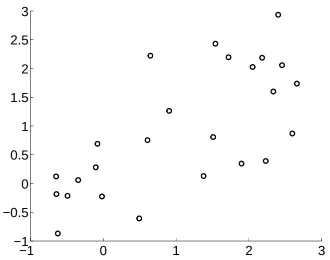
Given some points in the plane,



what is the ellipsoid that best matches them?

Quadratic measurement error model

a second order surface in $\mathbb{R}^n$ is the set

$$S(A,b,d) := \{\, x \in \mathbb{R}^{n\times 1} \;:\; x^T A x + b^T x + d = 0 \,\}$$

where $A \in \mathbb{S}$, $b \in \mathbb{R}^{n\times 1}$, and $d \in \mathbb{R}$ are parameters of the surface
($\mathbb{S}$ is the set of $n \times n$ symmetric matrices)

special cases:

- if $A = 0$ and $b \neq 0$, then $S(0,b,d)$ is a hyperplane
- if $A = A_{\mathsf{e}} > 0$ and $4d < b^T A^{-1} b$, then $S(A_{\mathsf{e}}, b, d)$ is an elliptic surface

$$E(A_{\mathsf{e}}, c) := \{\, x \in \mathbb{R}^{n\times 1} \;:\; (x-c)^T A_{\mathsf{e}} (x-c) = 1 \,\}$$

$c \in \mathbb{R}^{n\times 1}$ is the center of the elliptic surface

let $\bar{x}^l$, for $l = 1,\dots,m$, lie on the surface $S(\bar{A}, \bar{b}, \bar{d})$, i.e.,

$$(\bar{x}^l)^T \bar{A} \bar{x}^l + \bar{b}^T \bar{x}^l + \bar{d} = 0, \qquad \text{for } l = 1,\dots,m$$

let $x^l \in \mathbb{R}^{n\times 1}$, $l = 1,\dots,m$ be observations of the points $\bar{x}^l$, $l = 1,\dots,m$, i.e.,

$$x^l = \bar{x}^l + \tilde{x}^l, \qquad \text{for } l = 1,\dots,m$$

$\tilde{x}^l$, $l = 1,\dots,m$ are measurement errors

assumption: $\{\tilde{x}^l\}_{l=1}^m$ form an i.i.d. sequence and $\tilde{x}^l \sim \mathrm{N}(0, \bar{\sigma}^2 I_n)$

$\bar{A} \in \mathbb{S}$, $\bar{b} \in \mathbb{R}^{n\times 1}$, and $\bar{d} \in \mathbb{R}$ are the true values of the parameters

normalizing condition: $||\bar{A}||_F^2 + ||\bar{b}||^2 + \bar{d}^2 = 1$

estimation problem: given $\{x^l\}_{l=1}^m$ and $\bar{\sigma}$, estimate $\bar{A}$, $\bar{b}$, and $\bar{d}$

Least squares estimation

the model is linear in the parameters $\Rightarrow$ ordinary least squares (OLS)

$q_{\mathsf{ols}}(A,b,d;x) := \left(x^T A x + b^T x + d - 1\right)^2$ — elementary OLS cost function

measures the discrepancy of the single measurement x from the model $S(A,b,d)$

$Q_{\mathsf{ols}}(A,b,d) := \sum_{l=1}^m q_{\mathsf{ols}}(A,b,d;x^l)$ — OLS cost function

$$\min_{A,b,d} Q_{\mathsf{ols}}(A,b,d) \quad \text{s.t.} \quad ||\bar{A}||_F^2 + ||\bar{b}||^2 + \bar{d}^2 = 1 \qquad \text{(OLS)}$$

quadratically constraint least squares problem

let $\mathsf{vec}_{\mathsf{s}}(A)$ be the vector of the elements in the lower triangular part of A

define $x \otimes_{\mathsf{s}} x$ by

$$x^T A x = (x \otimes x)^T \mathsf{vec}(A) =: (x \otimes_{\mathsf{s}} x)^T \mathsf{vec}_{\mathsf{s}}(A)$$

denote $\beta := [\mathsf{vec}_{\mathsf{s}}(A)^T \; b^T \; 1]^T$, we have

$$Q_{\mathsf{ols}}(\beta) = \sum_{l=1}^m \Bigg(\underbrace{\left[(x^l \otimes_{\mathsf{s}} x^l)^T \; (x^l)^T \; 1\right]}_{f^l} \begin{bmatrix} \mathsf{vec}_{\mathsf{s}}(A) \\ b \\ 1 \end{bmatrix} \Bigg)^2 = \Bigg|\Bigg| \underbrace{\begin{bmatrix} f^1 \\ \vdots \\ f^m \end{bmatrix}}_{F} \beta \Bigg|\Bigg|^2$$

the (OLS) problem becomes

$$\min_{\beta} ||F\beta||^2 \quad \text{s.t.} \quad ||\beta||^2 = 1$$

and the solution is obtained from the SVD of F (or from the EVD of $F^T F$)

take the right singular vector corresponding to the smallest singular value

the OLS estimator $\hat{\beta}_{\mathsf{ols}}$ is inconsistent

Adjusted least squares estimation

define an auxiliary function $q_{\mathsf{als}}(\beta; x)$, such that

$\mathbf{E}\, q_{\mathsf{als}}(A,b,d;\bar{x}+\tilde{x}) = q_{\mathsf{ols}}(A,b,d;\bar{x})$ for all $A \in \mathbb{S}$, $b \in \mathbb{R}^{n\times 1}$, $d \in \mathbb{R}$, $\bar{x} \in \mathbb{R}^{n\times 1}$

the ALS estimator is a normalized eigenvector of $\Psi_{\mathsf{als}} := \sum_{i=1}^m q'_{\mathsf{als}}(x_i)$ corresponding to the minimum eigenvalue

we have

$$\Psi_{\mathsf{als}} = \Psi_{\mathsf{ols}} + \Delta\Psi_{\mathsf{als}}, \qquad \Psi_{\mathsf{ols}} := \sum_{i=1}^m q'_{\mathsf{ols}}(x_i)$$

for an appropriate correction $\Delta\Psi_{\mathsf{als}}$

we show the necessary correction for the two-dimensional case ($n = 2$)

in the space $\mathbb{R}^{(n+1)n/2+n+1}$, the operator Ψ_{ols} is represented by the matrix $F^T F$, i.e., a sum of matrices of the type (symmetric elements are shown with $*$)

$$\begin{bmatrix}
x_1^4 & 2x_1^3x_2 & x_1^2x_2^2 & x_1^3 & x_1^2x_2 & x_1^2 \\
* & 4x_1^2x_2^2 & 2x_1x_2^3 & 2x_1^2x_2 & 2x_1x_2^2 & 2x_1x_2 \\
* & * & x_2^4 & x_1x_2^2 & x_2^3 & x_2^2 \\
* & * & * & x_1^2 & x_1x_2 & x_1 \\
* & * & * & * & x_2^2 & x_2 \\
* & * & * & * & * & 1
\end{bmatrix}$$

the necessary correction matrix for the one above is

$$\begin{bmatrix}
3\bar{\sigma}^4 - 6\bar{\sigma}^2x_1^2 & -6\bar{\sigma}^2x_1x_2 & \bar{\sigma}^4 - \bar{\sigma}^2(x_1^2+x_2^2) & -3\bar{\sigma}^2x_1 & -\bar{\sigma}^2x_2 & -\bar{\sigma}^2 \\
* & 4\bar{\sigma}^4 - 4\bar{\sigma}^2(x_1^2+x_2^2) & -6\bar{\sigma}^2x_1x_2 & -2\bar{\sigma}^2x_2 & -2\bar{\sigma}^2x_1 & 0 \\
* & * & 3\bar{\sigma}^4 - 6\bar{\sigma}^2x_2^2 & -\bar{\sigma}^2x_1 & -3\bar{\sigma}^2x_2 & -\bar{\sigma}^2 \\
* & * & * & -\bar{\sigma}^2 & 0 & 0 \\
* & * & * & * & -\bar{\sigma}^2 & 0 \\
* & * & * & * & * & 0
\end{bmatrix}$$

because of the linearity the total correction is the sum of the corrections for all x^l

thus the operator Ψ_{als} is represented by $F^T F + \sum_{l=1}^m$ (correction matrix for x^l)

Orthogonal regression

define the distance from a point $x \in \mathbb{R}^n$ to a set $Y \subset \mathbb{R}^n$ by

$$\text{dist}(x, Y) := \min_{y \in Y} ||x - y||$$

the elementary orthogonal regression cost function is the distance from the data point x to the second order surface $S(A, b, d)$

$$q_{\text{orth}}(A, b, d; x) := \text{dist}\big(x, S(A, b, d)\big)$$

the orthogonal regression cost function is the sum of these distances for all data points

$$Q_{\text{orth}}(A, b, d) := \sum_{l=1}^{m} q_{\text{orth}}(A, b, d; x^l)$$

the orthogonal regression estimator is defined as a global minimum point of Q_{orth} subject to the normalizing condition

$$\min_{A,b,d} Q_{\text{orth}}(A, b, d) \quad \text{s.t.} \quad ||A||_F^2 + ||b||^2 + d^2 = 1$$

in general this is a non-convex optimization problem

- expensive to solve
- no guarantee that global minimum is found

the orthogonal regression cost function has geometric meaning:
sum of distances from the data points to the estimated surface

Q_{orth} is intuitively appealing cost function but defines an inconsistent estimator

advantage: gives good results for small sample size (only a few data points)

for small sample size ALS estimator is unstable

Ellipsoid estimation with ALS

suppose that the true surface belongs to the class of surfaces

$$E(A_e, c) = \{\, x \in \mathbb{R}^{n \times 1} : (x - c)^T A_e (x - c) = 1 \,\}, \quad \text{with } A_e > 0$$

the defining equation is quadratic in x but nonlinear in the parameters

$$x^T A_e x - (A_e c)^T x + c^T A_e c - 1 = 0$$

we normalize by dividing with $\lambda := \sqrt{||A_e||_F^2 + ||A_e c||^2 + (c^T A_e c - 1)^2}$

$$x^T (A_e/\lambda) x - (A_e c/\lambda)^T x + (c^T A_e c - 1)/\lambda = 0$$

and define the new parameters

$$A := \frac{A_e}{\lambda}, \quad b := -\frac{A_e c}{\lambda}, \quad d := \frac{c^T A_e c - 1}{\lambda}$$

that satisfy the normalizing condition

we can renew c and A_e from A, b, d by

$$c = -A^{-1} b, \qquad \text{and} \qquad A_e = \frac{1}{c^T A c - d} A$$

the estimator of the true parameters $\bar{A}_e$ and $\bar{c}$ is

$$\hat{c} = -(\hat{A})^{-1} \hat{b} \qquad \text{and} \qquad \hat{A}_e = \frac{1}{\hat{c}^T \hat{A} \hat{c} - \hat{d}} \hat{A}$$

for small sample size $\hat{A}_e$ might not be positive definite; we do the following additional step, let

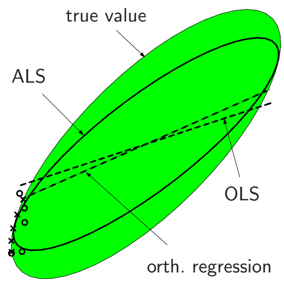
$$\hat{A}_e = \sum_{i=1}^{n} \hat{\lambda}_i \hat{v}_i^T \hat{v}_i$$

be the EVD of $\hat{A}_e$, then we redefine $\hat{A}_e$ by $\hat{A}_e := \sum_{i:\hat{\lambda}_i \geq 0} \hat{\lambda}_i \hat{v}_i^T \hat{v}_i$

Simulation examples with known center

the results depend on the error realization; for example:

ALS works, OLS and orthogonal regression fail



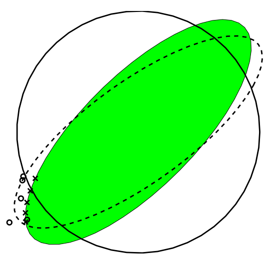
$$\bar{A} = \begin{bmatrix} 1.0000 & -0.7500 \\ -0.7500 & 1.0000 \end{bmatrix}$$

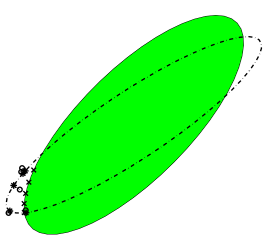
$$\hat{A}_{\text{ALS}} = \begin{bmatrix} 1.5740 & -1.6606 \\ -1.6606 & 2.4552 \end{bmatrix}$$

$$\hat{A}_{\text{OLS}} = \begin{bmatrix} 0.3289 & 0.3464 \\ 0.3464 & -0.6118 \end{bmatrix}$$

$$\hat{A}_{\text{ORTH}} = \begin{bmatrix} 0.1038 & 0.7480 \\ 0.7480 & -1.2612 \end{bmatrix}$$

ALS fails, OLS and orthogonal regression work





$$\hat{A}_{\text{ALS}} = \begin{bmatrix} 0.378 & -0.000 \\ 0.000 & 0.378 \end{bmatrix}, \; \hat{A}_{\text{OLS}} = \begin{bmatrix} 0.914 & -0.913 \\ -0.913 & 1.511 \end{bmatrix}, \; \hat{A}_{\text{ORTH}} = \begin{bmatrix} 1.588 & -2.047 \\ -2.047 & 3.313 \end{bmatrix}$$

Simulation examples with known center, cont.

we need to look at the average performance of the estimator

average performance for $m = 5$ points

for 1000 repetitions of the estimation (with different noise realization),
define the average relative error of estimation by

$$e := \frac{1}{N} \sum_{i=1}^{N} \frac{||\hat{A} - A_0||_F}{||A_0||_F}$$

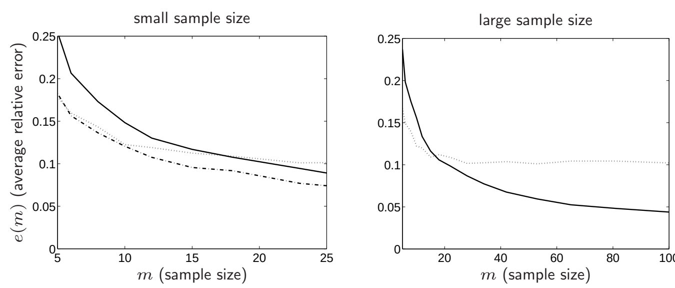
for the experiment shown above

$$e_{\text{ALS}} = 0.2375, \qquad e_{\text{OLS}} = 0.1715, \qquad e_{\text{ORTH}} = 0.1782$$

so ALS is indeed worse then OLS and orthogonal regression

asymptotic average performance

plot average performance as a function of the sample size

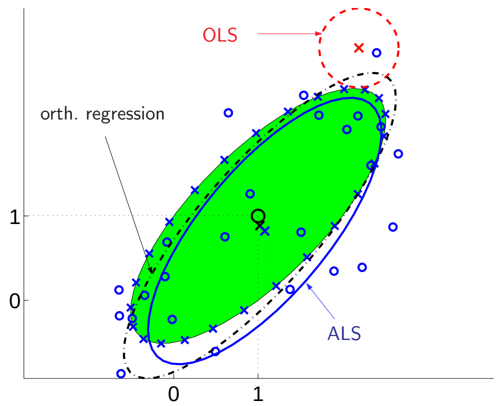


solid — ALS, dotted — OLS, dashed-dotted — orthogonal regression

OLS is biased, ALS is consistent

Simulation examples with unknown center

true ellipsoid, OLS, ALS, and orth. regression estimates



$$A_{\text{als}} = \begin{bmatrix} 1.146 & -0.739 \\ -0.739 & 0.877 \end{bmatrix},\ A_{\text{orth}} = \begin{bmatrix} 1.220 & -0.899 \\ -0.899 & 0.966 \end{bmatrix},\ c_{\text{als}} = \begin{bmatrix} 1.078 \\ 0.821 \end{bmatrix},\ c_{\text{orth}} = \begin{bmatrix} 1.020 \\ 0.886 \end{bmatrix}$$

relative errors: $e(A_{\text{als}}) = 0.108$, $e(A_{\text{orth}}) = 0.173$, $e(c_{\text{als}}) = 0.137$, $e(c_{\text{orth}}) = 0.081$

asymptotic average error of estimation