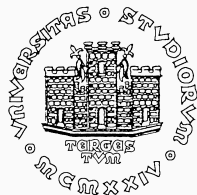


Systems Dynamics

Course ID: 267MI – Fall 2018

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Lecture 8

Least-Squares Estimation

Linear regression

- This is the typical context suited to the use of the least-squares (LS) estimator
- We have $q + 1$ variables $y(t), u_1(t), \dots, u_q(t)$ over the time-window $t = 1, 2, \dots, N$
- We want to compute (if possible) q parameters $\vartheta_1, \vartheta_2, \dots, \vartheta_q$ such that

$$y(t) = \vartheta_1 u_1(t) + \dots + \vartheta_q u_q(t), \quad t = 1, \dots, N \quad (\star)$$

- Relationship $(\star)$ is defined as the **linear regression** of the variable $y(t)$ on the variables $u_1(t), \dots, u_q(t)$

Least-Squares Estimation - Linear Regression (cont.)

- The problem can be equivalently stated in vector form letting

$$\vartheta = \begin{bmatrix} \vartheta_1 \\ \vdots \\ \vartheta_q \end{bmatrix} \quad \varphi(t) = \begin{bmatrix} u_1(t) \\ \vdots \\ u_q(t) \end{bmatrix}$$

and hence getting

$$y(t) = \varphi(t)^\top \vartheta$$

- Clearly, in case of real data, an **error** $\varepsilon(t)$ **is always present**:

$$\varepsilon(t) = y(t) - \varphi(t)^\top \vartheta$$

Least-Squares Estimation - Linear Regression (cont.)

- The goal of the linear regression problem is to minimize the error $\varepsilon(t)$ by determining an optimal vector ϑ° such that such a **minimum** is achieved
- We introduce the **quadratic cost function**:

$$J(\vartheta) = \sum_{t=1}^N [\varepsilon(t)]^2 = \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta]^2$$

- Therefore, the **Least-Squares Estimator** is given by

$$\vartheta^\circ = \arg \min_{\vartheta} J(\vartheta)$$

Least-Squares Estimation - Linear Regression (cont.)

- Denoting by ϑ_i the i -th component of the vector ϑ , one has:

$$\begin{aligned}\frac{\partial J}{\partial \vartheta_i} &= \frac{\partial}{\partial \vartheta_i} \left\{ \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta]^2 \right\} \\ &= -2 \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta] u_i(t), \quad i = 1, 2, \dots, q\end{aligned}$$

and noticing that

$$\frac{\partial J}{\partial \vartheta} = \begin{bmatrix} \frac{\partial J}{\partial \vartheta_1} & \frac{\partial J}{\partial \vartheta_2} & \cdots & \frac{\partial J}{\partial \vartheta_q} \end{bmatrix}$$

it follows that

$$\frac{\partial J}{\partial \vartheta} = -2 \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta] \varphi(t)^\top$$

Least-Squares Estimation - Linear Regression (cont.)

- Imposing $\frac{\partial J}{\partial \vartheta} = [0 \ 0 \ \dots \ 0]$ one gets:

$$\begin{aligned} -2 \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta] \varphi(t)^\top &= [0 \ 0 \ \dots \ 0] \\ \implies \sum_{t=1}^N y(t) \varphi(t)^\top &= \sum_{t=1}^N \varphi(t)^\top \vartheta \varphi(t)^\top \end{aligned}$$

and converting the equality between row-vectors into an equality between column-vectors:

$$\sum_{t=1}^N \varphi(t) y(t) = \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \vartheta$$

**Least-Squares
Normal Equations**

(q equations, q unknowns)

- If $\sum_{t=1}^N \varphi(t) \varphi(t)^\top$ is **non-singular**, it finally follows that:

$$\hat{\vartheta}_N = \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) y(t)$$

Least-Squares Formula

Least-Squares Estimation - Geometric Interpretation

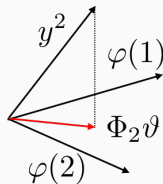
Let:

$$\varepsilon_{\vartheta}^N = \begin{bmatrix} \varepsilon_{\vartheta}(1) \\ \vdots \\ \varepsilon_{\vartheta}(N) \end{bmatrix} \quad y^N = \begin{bmatrix} y(1) \\ \vdots \\ y(N) \end{bmatrix} \quad \Phi_N = \begin{bmatrix} \varphi(1)^\top \\ \vdots \\ \varphi(N)^\top \end{bmatrix}$$

Then, we write:

$$J(\vartheta) = \sum_{t=1}^N [y(t) - \varphi(t)^\top \vartheta]^2 = \|y^N - \Phi_N \vartheta\|^2$$

Clearly $\|y^N - \Phi_N \vartheta\|$ is minimum when $y^N - \Phi_N \vartheta$ is orthogonal to $\Phi_N \vartheta$



Least-Squares Estimation (cont.)

- Let's verify that $\hat{\vartheta}_N$ is a **minimum** by evaluating the definiteness of the symmetric matrix

$$\left[\frac{d^2 J}{d\vartheta^2} \right]_{i,j} = \frac{\partial^2 J}{\partial \vartheta_i \partial \vartheta_j}, \quad i, j = 1, \dots, q$$

We have

$$\left(\frac{\partial J}{\partial \vartheta} \right)^\top = 2 \left\{ \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \vartheta - \sum_{t=1}^N \varphi(t) y(t) \right\}$$

and hence:

$$\frac{d^2 J}{d\vartheta^2} = 2 \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]$$

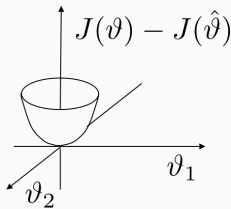
Clearly, this matrix is symmetric and positive semi-definite and thus $\hat{\vartheta}_N$ is a **local minimum** of $J(\vartheta)$.

Least-Squares Estimation (cont.)

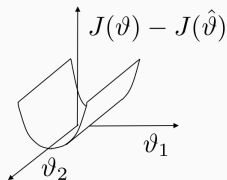
- Therefore, considering the quadratic form

$$J(\vartheta) - J(\hat{\vartheta}) = \frac{1}{2}(\vartheta - \hat{\vartheta})^\top \left. \frac{d^2 J}{d\vartheta^2} \right|_{\hat{\vartheta}} (\vartheta - \hat{\vartheta})$$

two possible scenarios may occur:



$$\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \neq 0$$



$$\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] = 0$$

Least-Squares Estimation (cont.)

- Then:

- If $\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \neq 0 \implies \hat{\vartheta}_N$ is the unique global minimum
- If $\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] = 0 \implies \hat{\vartheta}_N$ is one among the infinite global minima

- The condition

$$\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \neq 0$$

is called **Identifiability Condition**

Probabilistic Properties of the Least-Squares Estimator

- Suppose that the identifiability condition is verified:

$$\det \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right] \neq 0$$

and then

$$\hat{\vartheta}_N = \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) y(t)$$

- **Assumption:** $y(t) = \varphi(t)^\top \vartheta^\circ + \xi(t)$ where the process is uncorrelated with $u(\cdot)$ and $E[\xi(t)] = 0$

Therefore:

We are assuming that the true relationship between $y(t)$ and $u_1(t), \dots, u_q(t)$ is linear + uncorrelated zero-mean noise

Probabilistic Properties of the Least-Squares Estimator (cont.)

Bias:

$$\begin{aligned}\hat{\vartheta}_N &= \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) y(t) \\ &= \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) [\varphi(t)^\top \vartheta^\circ + \xi(t)] \\ &= \vartheta^\circ + \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) \xi(t)\end{aligned}$$

Hence:

$$\begin{aligned}\hat{\vartheta}_N - \vartheta^\circ &= \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) \xi(t) \\ \implies E \left(\hat{\vartheta}_N - \vartheta^\circ \right) &= \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) E[\xi(t)] = 0 \\ \implies E \left(\hat{\vartheta}_N \right) &= \vartheta^\circ\end{aligned}$$

The LS estimator is unbiased

Important Remark:

- In the bias analysis of the LS estimator we have considered the regression vector $\varphi(t)$ as **known and set** (not random any more).
- On the other hand, carrying out the bias analysis considering $\varphi(s, t)$ as a random vector (hence a function of the result s of a random experiment), would lead to a **biased** LS estimator for any finite value of N .

Probabilistic Properties of the Least-Squares Estimator (cont.)

Variance:

Further Assumption: $\xi(t) \sim WN(0, \lambda^2)$

Let us introduce the symmetric matrix $S(N) = \sum_{t=1}^N \varphi(t) \varphi(t)^\top$

Hence:

$$\begin{aligned} \text{var} \left(\hat{\vartheta}_N \right) &= E \left[\left(\hat{\vartheta}_N - \vartheta^\circ \right) \left(\hat{\vartheta}_N - \vartheta^\circ \right)^\top \right] \\ &= E \left\{ \left[S(N)^{-1} \sum_{t=1}^N \varphi(t) \xi(t) \right] \left[S(N)^{-1} \sum_{s=1}^N \varphi(s) \xi(s) \right]^\top \right\} \\ &= E \left\{ \left[S(N)^{-1} \sum_{t=1}^N \varphi(t) \xi(t) \right] \left[\sum_{s=1}^N \xi(s) \varphi(s)^\top S(N)^{-1} \right] \right\} \\ &= S(N)^{-1} E \left[\sum_{t=1}^N \varphi(t) \xi(t) \sum_{s=1}^N \xi(s) \varphi(s)^\top \right] S(N)^{-1} \end{aligned}$$

Probabilistic Properties of the Least-Squares Estimator (cont.)

In the product $\sum_{t=1}^N \varphi(t) \xi(t) \sum_{s=1}^N \xi(s) \varphi(s)^\top$ we have two kinds of terms:

- $\varphi(t) \xi(t)^2 \varphi(t)^\top$ if $t = s$
- $\varphi(t) \xi(t) \xi(s) \varphi(s)^\top$ if $t \neq s$

But:

$$\xi(t) \sim WN(0, \lambda^2) \implies E [\xi(t)\xi(s)] = \begin{cases} \lambda^2 & \text{if } t = s \\ 0 & \text{if } t \neq s \end{cases}$$

Hence:

$$E \left[\sum_{t=1}^N \varphi(t) \xi(t) \sum_{s=1}^N \xi(s) \varphi(s)^\top \right] = \sum_{t=1}^N \lambda^2 \varphi(t) \varphi(t)^\top = \lambda^2 S(N)$$

and thus

$$\text{var} \left(\hat{\vartheta}_N \right) = S(N)^{-1} \lambda^2 S(N) S(N)^{-1} = \lambda^2 S(N)^{-1}$$

Probabilistic Properties of the Least-Squares Estimator (cont.)

Interpretation:

Assume that ϑ° is scalar and hence also $\varphi(t)$ is scalar as well.
Then:

$$y(t) = \varphi(t) \vartheta^\circ + \xi(t) = u(t) \vartheta^\circ + \xi(t)$$

and hence:

$$\hat{\vartheta}_N = \left[\sum_{t=1}^N \varphi(t) \varphi(t)^\top \right]^{-1} \sum_{t=1}^N \varphi(t) y(t) = \frac{\frac{1}{N} \sum_{t=1}^N u(t) y(t)}{\frac{1}{N} \sum_{t=1}^N u(t)^2}$$

But:

- $\frac{1}{N} \sum_{t=1}^N u(t) y(t)$ is the sample estimate of the cross-correlation $E[u(t)y(t)]$
- $\frac{1}{N} \sum_{t=1}^N u(t)^2$ is the sample estimate of $E[u(t)^2]$ (variance if $E(u) = 0$).

Probabilistic Properties of the Least-Squares Estimator (cont.)

Moreover:

$$\text{var} \left(\hat{v}_N \right) = \lambda^2 S(N)^{-1} = \frac{1}{N} \frac{\lambda^2}{\frac{1}{N} \sum_{t=1}^N u(t)^2}$$

Therefore:

- $\text{var} \left(\hat{v}_N \right)$ grows with λ^2 . Hence, estimate's uncertainty grows with data uncertainty
- For given N and λ^2 , $\text{var} \left(\hat{v}_N \right)$ decreases when the sample variance of u increases and this is consistent with intuition: the noise influence on the signal containing the useful information decreases

Probabilistic Properties of the Least-Squares Estimator (cont.)

- $\frac{\lambda^2}{\frac{1}{N} \sum_{t=1}^N u(t)^2}$ is kind of a noise/signal ratio
- If the variance of u is bounded then

$$\lim_{N \rightarrow \infty} \text{var} \left(\hat{\vartheta}_N \right) = 0$$

and, owing to the fact that the estimator is unbiased one has:

$$\lim_{N \rightarrow \infty} E \left(\left\| \hat{\vartheta}_N - \vartheta^\circ \right\|^2 \right) = 0$$

that is, **the LS estimator converges in quadratic mean**

Probabilistic Properties of the Least-Squares Estimator (cont.)

Moreover, we can write

$$\begin{aligned}\hat{\vartheta}_N &= \frac{1}{\sum_{t=1}^N u(t)^2} \sum_{t=1}^N u(t) [u(t) \vartheta^\circ + \xi(t)] \\ &= \vartheta^\circ + \frac{\frac{1}{N} \sum_{t=1}^N u(t) \xi(t)}{\frac{1}{N} \sum_{t=1}^N u(t)^2} \longrightarrow \vartheta^\circ + \frac{E[u(t) \xi(t)]}{E[u(t)^2]}\end{aligned}$$

- If u is deterministic, one has:

$$\vartheta^\circ + \frac{E[u(t) \xi(t)]}{E[u(t)^2]} = \vartheta^\circ + u(t) \frac{E[\xi(t)]}{E[u(t)^2]} = \vartheta^\circ$$

- If u is stochastic but uncorrelated with ξ , one has:

$$\vartheta^\circ + \frac{E[u(t) \xi(t)]}{E[u(t)^2]} = \vartheta^\circ + \frac{E[u(t)] E[\xi(t)]}{E[u(t)^2]} = \vartheta^\circ$$

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Lecture 8

Least-Squares Estimation

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