Systems Dynamics

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Lecture 9
Bayes Estimation

Lecture 9: Table of Contents

Introduction to the Bayes Estimation

Bayes Estimation

Considerations

- We look for an estimation method allowing to embed the possible a-priori knowledge on the unknown quantity to be estimated
- In the framework of Bayes estimation also the unknown vector is interpreted as a random vector
- The probability density function $p(\vartheta)$ in absence of observed data is the a-priori probability density function embedding the available information on ϑ before collecting the data.
- Hence, in the absence of data, the a-priori estimator could be

$$\hat{\vartheta} = E(\vartheta) = \int \vartheta \, p(\vartheta) \, d\vartheta$$

and the uncertainty $\mathrm{var}(\vartheta)$ of the estimate would be the a-priori estimate

Bayes Estimation (cont.)

- Clearly, as soon as new data are collected, the probability density function $p(\vartheta)$ changes.
- As a consequence, $E(\vartheta)$ and $\mathrm{var}(\vartheta)$ change as well.
- In particular, we expect $\mathrm{var}(\vartheta)$ to decrease
- Summing up, the basic idea is to consider a joint random experiment with respect to d and ϑ and this is the conceptual peculiarity of the Bayes estimation approach.

The Optimal Bayes Estimator

Bayes Estimation (cont.)

- Consider the generic estimator as function of the data

$$\hat{\vartheta} = h(d)$$

and define the cost functional

$$J[h(\cdot)] = E\left[\|\vartheta - h(d)\|^2\right]$$

- The goal is to determine an estimator $h^\circ(\cdot)$ such that $J[h(\cdot)]$ is minimised, that is we have to determine

$$h^\circ(\cdot) \; : \; E\left[\|\vartheta - h^\circ(d)\|^2\right] \le E\left[\|\vartheta - h(d)\|^2\right], \quad \forall\, h(\cdot)$$

where the expected values are computed with reference to the joint random experiment

Bayes Estimation (cont.)

- Assume for simplicity that d and ϑ are scalar:

$$E\left[\|\vartheta - h(d)\|^2\right] = E\left[\vartheta^2 - 2\vartheta\, d + h(d)^2\right]$$

and setting $f(d,\vartheta) = \vartheta^2 - 2\vartheta\, d + h(d)^2$ one gets:

$$E\left[f(d,\vartheta)\right] = \int_{x,y} f(x,y)\, p(x,y)\, dxdy$$

where x and y are the current values taken on by d and ϑ and $p(d,\vartheta)$ is the joint probability density of d and ϑ

- Recall the Bayes formula (of very general validity):

$$p(x,y) = p(y\,|x)\, p(x)$$

Bayes Estimation (cont.)

- Hence:

$$E\,[f(d,\vartheta)] = \int_{x,y} f(x,y)\,p(y\,|x)\,p(x)\,dxdy$$
$$= \int_x \left[\int_y f(x,y)\,p(y\,|x)\,dy\right] p(x)\,dx$$

- On the other hand, by definition one has:

$$\int_y f(x,y)\,p(y\,|x)\,dy = E\,[\,f(d,\vartheta)\,|\,d=x\,]$$

and thus:

$$E\,[\,f(d,\vartheta)\,|\,d=x\,]$$
$$= E\,[\,\vartheta^2\,|\,d=x\,] - 2\,E\,[\,\vartheta\,h(d)\,|\,d=x\,] + E\,[\,h(d)^2\,|\,d=x\,]$$

Bayes Estimation (cont.)

- Setting $d = x$ implies that $h(d)$ becomes a deterministic quantity and hence

$$E\,[\,f(d,\vartheta)\,|\,d=x\,] = E\,[\,\vartheta^2\,|\,d=x\,] - 2\,h(x)\,E\,[\,\vartheta\,|\,d=x\,] + h(x)^2$$

- Adding and subtracting $\{E\,[\,\vartheta\,|\,d=x\,]\}^2$ one gets (completing the squares)

$$\begin{aligned}E\,[\,f(d,\vartheta)\,|\,d=x\,] &= \{E\,[\,\vartheta\,|\,d=x\,]\}^2 - 2\,h(x)\,E\,[\,\vartheta\,|\,d=x\,] + h(x)^2 \\ &\quad + E\,[\,\vartheta^2\,|\,d=x\,] - \{E\,[\,\vartheta\,|\,d=x\,]\}^2 \\ &= \|E\,[\,\vartheta\,|\,d=x\,] - h(x)\|^2 + E\,[\,\vartheta^2\,|\,d=x\,] - \{E\,[\,\vartheta\,|\,d=x\,]\}^2\end{aligned}$$

Bayes Estimation (cont.)

- Therefore:

$$E\left[\|\vartheta - h(d)\|^2\right] = \int_x \left[\int_y f(x,y)\, p(y\,|x)\, dy\right] p(x)\, dx$$
$$= \int_x \left[\|E\,[\,\vartheta\,|\,d = x\,] - h(x)\|^2 + E\,[\,\vartheta^2\,|\,d = x\,] - \{E\,[\,\vartheta\,|\,d = x\,]\}^2\right] p(x)dx$$
$$= \int_x \left[\underbrace{\|E\,[\,\vartheta\,|\,d = x\,] - h(x)\|^2}_{\geq 0} + \underbrace{\mathrm{var}\,[\,\vartheta\,|\,d = x\,]}_{\geq 0}\right] p(x)dx$$

- Hence, one concludes that:

$$h^\circ(x) = E\,(\vartheta\,|\,d = x)$$

Bayes Estimation (cont.)

Optimal Bayes Estimator

The optimal Bayes estimator is the expected value conditioned to the actual observed data:

$$\hat{\vartheta} = h^{\circ}(\delta) = E\left(\vartheta \,|\, d = \delta\right)$$

where δ is the specific value taken on by d as outcome of the random experiment

Remark. The generalisation to the vector case is trivial

The Optimal Bayes Estimator

Optimal Bayes Estimation in the Gaussian Case

Bayes Estimation in the Gaussian Case

Assume that d and ϑ are marginally and jointly Gaussian random variables:

$$\begin{bmatrix} d \\ \vartheta \end{bmatrix} \sim G\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \lambda_{dd} & \lambda_{d\vartheta} \\ \lambda_{\vartheta d} & \lambda_{\vartheta\vartheta} \end{bmatrix}\right)$$

and

$$p(d,\vartheta) = C \exp\left(-\frac{1}{2}\,[d \quad \vartheta] \begin{bmatrix} \lambda_{dd} & \lambda_{d\vartheta} \\ \lambda_{\vartheta d} & \lambda_{\vartheta\vartheta} \end{bmatrix}^{-1} \begin{bmatrix} d \\ \vartheta \end{bmatrix}\right)$$

Letting $\lambda^2 = \lambda_{\vartheta\vartheta} - \lambda_{\vartheta d}^2/\lambda_{dd}$ and recalling that $\lambda_{d\vartheta} = \lambda_{\vartheta d}$ one gets:

$$\begin{aligned} \begin{bmatrix} \lambda_{dd} & \lambda_{\vartheta d} \\ \lambda_{\vartheta d} & \lambda_{\vartheta\vartheta} \end{bmatrix}^{-1} &= \frac{1}{\lambda_{dd}(\lambda_{\vartheta\vartheta} - \lambda_{\vartheta d}^2/\lambda_{dd})} \begin{bmatrix} \lambda_{\vartheta\vartheta} & -\lambda_{\vartheta d} \\ -\lambda_{\vartheta d} & \lambda_{dd} \end{bmatrix} \\ &= \frac{1}{\lambda^2} \begin{bmatrix} \lambda_{\vartheta\vartheta}/\lambda_{dd} & -\lambda_{\vartheta d}/\lambda_{dd} \\ -\lambda_{\vartheta d}/\lambda_{dd} & 1 \end{bmatrix} \end{aligned}$$

Bayes Estimation in the Gaussian Case (cont.)

Therefore:

$$\frac{1}{2}\begin{bmatrix} d & \vartheta \end{bmatrix} \begin{bmatrix} \lambda_{dd} & \lambda_{\vartheta d} \\ \lambda_{\vartheta d} & \lambda_{\vartheta\vartheta} \end{bmatrix}^{-1} \begin{bmatrix} d \\ \vartheta \end{bmatrix} = \cdots = \frac{1}{2\lambda^2}\left(\frac{\lambda_{\vartheta\vartheta}}{\lambda_{dd}} d^2 - 2\frac{\lambda_{\vartheta d}}{\lambda_{dd}} d\vartheta + \vartheta^2\right)$$

Moreover, by assumption: $p(d) = C' \exp\left(-\frac{1}{2\lambda_{dd}}\, d^2\right)$. Hence:

$$\begin{aligned} p(\vartheta \,|\, d) = \frac{p(d,\vartheta)}{p(d)} &= \frac{C}{C'} \exp\left[-\frac{1}{2\lambda^2}\left(\frac{\lambda_{\vartheta\vartheta}}{\lambda_{dd}} d^2 - 2\frac{\lambda_{\vartheta d}}{\lambda_{dd}} d\vartheta + \vartheta^2 - \frac{\lambda^2 d^2}{\lambda_{dd}}\right)\right] \\ &= \frac{C}{C'} \exp\left\{-\frac{1}{2\lambda^2}\left[\frac{d^2}{\lambda_{dd}}\left(\lambda_{\vartheta\vartheta} - \lambda^2\right) - 2\frac{\lambda_{\vartheta d}}{\lambda_{dd}} d\vartheta + \vartheta^2\right]\right\} \\ &= \frac{C}{C'} \exp\left[-\frac{1}{2\lambda^2}\left(\frac{\lambda_{\vartheta d}^2}{\lambda_{dd}^2}\, d^2 - 2\frac{\lambda_{\vartheta d}}{\lambda_{dd}} d\vartheta + \vartheta^2\right)\right] \\ &= \frac{C}{C'} \exp\left[-\frac{1}{2\lambda^2}\left(\vartheta - \frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d\right)^2\right] \end{aligned}$$

Bayes Estimation in the Gaussian Case (cont.)

Optimal Bayes Estimator in the Gaussian Case

$$p(\vartheta \mid d) = \frac{C}{C'} \exp\left[-\frac{1}{2\lambda^2}\left(\vartheta - \frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d\right)^2\right]$$

$p(\vartheta \mid d)$ is Gaussian with:

- Expected value: $\frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d$
- Variance: $\lambda^2 = \lambda_{\vartheta\vartheta} - \frac{\lambda_{\vartheta d}^2}{\lambda_{dd}}$

Thus, the Optimal Bayes Estimator is given by:

$$\hat{\vartheta} = h^\circ(x) = E\left(\vartheta \mid d = x\right) = \frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d$$

and

$$\mathrm{var}\left(\vartheta - \hat{\vartheta}\right) = E\left[\left(\vartheta - \hat{\vartheta}\right)^2\right] = \lambda_{\vartheta\vartheta} - \frac{\lambda_{\vartheta d}^2}{\lambda_{dd}} = \lambda^2$$

The Optimal Bayes Estimator

Optimal Linear Estimator

Optimal Linear Estimator

- Let us remove the assumption that d and ϑ are marginally and jointly Gaussian random variables
- Let again $E(d^2) = \lambda_{dd}$, $E(\vartheta^2) = \lambda_{\vartheta\vartheta}$, $E(\vartheta d) = \lambda_{\vartheta d}$
- Impose that the estimator takes on a linear structure:

$$\hat{\vartheta} = \alpha d + \beta$$

  where α and β are suitable parameters to be determined.
- Introduce the cost function:

$$J = E\left[\left(\vartheta - \hat{\vartheta}\right)^2\right] = E\left[(\vartheta - \alpha\, d - \beta)^2\right]$$

Optimal Linear Estimator (cont.)

Thus, one gets:

$$\begin{aligned} J &= E\left(\vartheta^2 + \alpha^2 d^2 + \beta^2 - 2\alpha\vartheta d - 2\beta\vartheta + 2\alpha\beta d\right) \\ &= \lambda_{\vartheta\vartheta} + \alpha^2\lambda_{dd} + \beta^2 - 2\alpha\lambda_{\vartheta d} - 2\beta E(\vartheta) + 2\alpha\beta E(d) \end{aligned}$$

Hence:

$$\begin{cases} \dfrac{\partial J}{\partial \alpha} = 2\alpha\lambda_{dd} - 2\lambda_{\vartheta d} \quad \Longrightarrow \quad \alpha = \dfrac{\lambda_{\vartheta d}}{\lambda_{dd}} \\ \dfrac{\partial J}{\partial \beta} = 2\beta \quad \Longrightarrow \quad \beta = 0 \end{cases}$$

thus getting the Optimal Linear Estimator:

$$\hat{\vartheta} = \frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d$$

Its variance is given by:

$$\mathrm{var}\,(\vartheta - \hat{\vartheta}) = E\left[(\vartheta - \hat{\vartheta})^2\right] = \lambda_{\vartheta\vartheta} + \alpha^2\lambda_{dd} + \beta^2 - 2\alpha\lambda_{\vartheta d} = \cdots = \lambda^2$$

Optimal Linear Estimator (cont.)

Remarks:

- The optimal linear estimator is formally equal to the Bayes one.
- If the Gaussian assumption on the random variables holds, then the optimal linear estimator actually is the best possible in the minimum variance sense
- If the Gaussian assumption on the random variables does not hold, then the linear estimator is sub-optimal, but still it is the best estimator constrained to take on a linear structure in the case in which no further assumptions are introduced on the probabilistic characteristics of the random variables

Generalisation, Interpretations and Remarks

Bayes Estimation: Generalisations

- If $E(d) = d_m$, $E(\vartheta) = \vartheta_m$, then:

$$\begin{cases} \hat{\vartheta} = \vartheta_m + \dfrac{\lambda_{\vartheta d}}{\lambda_{dd}} (d - d_m) \\ \mathrm{var}\,(\vartheta - \hat{\vartheta}) = \lambda_{\vartheta\vartheta} - \dfrac{\lambda_{\vartheta d}^2}{\lambda_{dd}} \end{cases}$$

- If d and ϑ are vectors with $E(d) = d_m$, $E(\vartheta) = \vartheta_m$ and

$$\mathrm{var}\left(\begin{bmatrix} d \\ \vartheta \end{bmatrix} \right) = \begin{bmatrix} \Lambda_{dd} & \Lambda_{d\vartheta} \\ \Lambda_{\vartheta d} & \Lambda_{\vartheta\vartheta} \end{bmatrix} \qquad \Lambda_{d\vartheta} = \Lambda_{\vartheta d}^{\top}$$

Then:

$$\begin{cases} \hat{\vartheta} = \vartheta_m + \Lambda_{\vartheta d}\, \Lambda_{dd}{}^{-1} (d - d_m) \\ \mathrm{var}\,(\vartheta - \hat{\vartheta}) = \Lambda_{\vartheta\vartheta} - \Lambda_{\vartheta d}\, \Lambda_{dd}{}^{-1} \Lambda_{d\vartheta} \end{cases}$$

Bayes Estimation: Interpretations and Remarks

- Consider for simplicity the Bayes estimator in the case:

$$\hat{\vartheta} = \vartheta_m + \frac{\lambda_{\vartheta d}}{\lambda_{dd}} \left(d - d_m\right)$$

Then:

  - $\vartheta_m = E(\vartheta)$ is the a priori estimate: in case of no availability of observations , it is the “more reasonable” estimate. In this case, we have:

$$\mathrm{var}\left(\vartheta - \hat{\vartheta}\right) = \lambda_{\vartheta\vartheta} = \mathrm{var}\left(\vartheta\right)$$

  - Instead, when observations are available, we have:

$$\hat{\vartheta} = \underbrace{\vartheta_m}_{\text{a-priori estimate}} + \underbrace{\frac{\lambda_{\vartheta d}}{\lambda_{dd}} \left(d - d_m\right)}_{\text{correction due to the observation}}$$

Bayes Estimation: Interpretations and Remarks (cont.)

- Clearly:
  - If $\lambda_{\vartheta d} = 0$ then $\hat{\vartheta} = \vartheta_m$ and this is correct: it means that the data observation d is uncorrelated with ϑ and hence it does not convey useful information for the estimate: the a-posteriori estimate coincides with the a-priori one.
  - If $\lambda_{\vartheta d} \neq 0$ then the estimate is corrected on the basis of the observed data:
    - If $\lambda_{\vartheta d} > 0$ then $\hat{\vartheta} - \vartheta_m$ and $d - d_m$ in the average keep the same sign and the correction is more likely to keep the same sign as well
    - If $\lambda_{\vartheta d} < 0$ then $\hat{\vartheta} - \vartheta_m$ and $d - d_m$ in the average have a different sign and the correction is more likely to change the same sign as well

Bayes Estimation: Interpretations and Remarks (cont.)

- It also very important to enhance the role played by the variance λ_{dd} that "quantifies" the degree of uncertainty of the observed data:

$$\hat{\vartheta} = \vartheta_m + \frac{\lambda_{\vartheta d}}{\lambda_{dd}} (d - d_m)$$

  Hence: the larger λ_{dd}, the smaller the applied correction, that is, the update is "more cautious"

- Moreover:

$$\mathrm{var}\,(\vartheta - \hat{\vartheta}) = \lambda_{\vartheta\vartheta} - \frac{\lambda_{\vartheta d}^2}{\lambda_{dd}} = \lambda_{\vartheta\vartheta} \left(1 - \frac{\lambda_{\vartheta d}^2}{\lambda_{\vartheta\vartheta}\lambda_{dd}}\right)$$

  and thus $\mathrm{var}\,(\vartheta - \hat{\vartheta}) \leq \mathrm{var}\,(\vartheta)$ and

$$\mathrm{var}\,(\vartheta - \hat{\vartheta}) < \mathrm{var}\,(\vartheta) \text{ if } \lambda_{\vartheta d} \neq 0$$

  The estimate cannot but improve whenever the observed data convey useful information

Geometric Interpretation

Bayes Estimation: Geometric Interpretation

- Assume that d and ϑ are marginally and jointly Gaussian random variables:

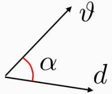
$$\begin{bmatrix} d \\ \vartheta \end{bmatrix} \sim G\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \lambda_{dd} & \lambda_{d\vartheta} \\ \lambda_{\vartheta d} & \lambda_{\vartheta\vartheta} \end{bmatrix} \right)$$

  Hence d and ϑ can be interpreted as vectors in a vector space
- Define the scalar product $(\vartheta, d) = E(\vartheta \cdot d)$
- The usual properties of vector spaces equipped with scalar product hold true. In particular:

$$\|\vartheta\| = \sqrt{(\vartheta, \vartheta)}$$

$$\|d\| = \sqrt{(d, d)}$$

$$(\vartheta, d) = \|\vartheta\| \, \|d\| \, \cos\alpha$$



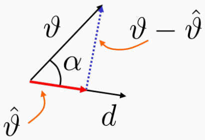
- Uncorrelated random variables: orthogonal vectors

Bayes Estimation: Geometric Interpretation (cont.)

- Now:

$$\hat{\vartheta} = \frac{\lambda_{\vartheta d}}{\lambda_{dd}}\, d = \frac{E(\vartheta \cdot d)}{E(d \cdot d)}\, d = \frac{(\vartheta, d)}{\|d\|^2}\, d = \frac{(\vartheta, d)}{\|d\|^2}\, \frac{\|\vartheta\|}{\|\vartheta\|}\, d$$
$$= \frac{(\vartheta, d)}{\|\vartheta\|\|d\|}\, \|\vartheta\|\, \frac{d}{\|d\|} = \|\vartheta\|\, \cos\alpha\, \frac{d}{\|d\|}$$

The optimal estimate $\hat{\vartheta}$ is the projection of ϑ on the data vector d



- Consider the vector $\vartheta - \hat{\vartheta}$. It follows that:

$$\|\vartheta - \hat{\vartheta}\|^2 = \|\vartheta\|^2 - \|\hat{\vartheta}\|^2 = \|\vartheta\|^2 - \|\vartheta\|^2\, (\cos\alpha)^2$$
$$= \lambda_{\vartheta\vartheta} - \lambda_{\vartheta\vartheta}\, \frac{\lambda_{\vartheta d}^2}{\lambda_{dd}\lambda_{\vartheta\vartheta}} = \lambda_{\vartheta\vartheta} - \frac{\lambda_{\vartheta d}^2}{\lambda_{dd}}$$

The square of the length of vector $\vartheta - \hat{\vartheta}$ is the variance of the estimation error and is minimal.

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Lecture 9
Bayes Estimation

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