Analytic Estimation

Modern Theory of Detection and Estimation. Block-1: Estimation

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Estimation problem definition

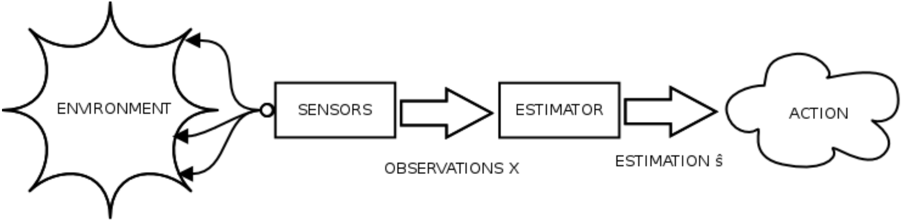
Goal in a estimation problem

You receive a scalar observation (x) or **a vector observation** ($\mathbf{x}$), and your task is to find out (**estimate**) the value of a real number s. The variable you want to find out can be either deterministic or random.

Examples:

- Estimate the number of stocks of a certain instrument that will be traded tomorrow.
- Estimate the daily energy consumption in a building as a function of the weather, season of year, day of week.
- Estimate the price of a house given the surface, number of rooms, size of the yard, distance to the centre of the town, etc.
- Guess the foot length of people based on their height.

Estimation problem setup



- Sensors sample information about the environment and construct observations $\mathbf{x}^k$, $k = 1, \ldots, l$.
- Estimator constructs estimated variable $\hat{s}$ as a function of the observations. There **must be** a statistical relationship between the observations and the variable we want to estimate, s.
- Then we use the estimation $\hat{s}$ instead of s to take actions. Remember we **never** have access to s (that's why we need to estimate it!!)

Notation

- $\mathbf{X}$: **observations**. Random in the analytical case setup. Could be scalars or vectors.
- S: **desired output**. This is the variable we want to estimate. It can be random (S) or deterministic (s). It can be a vector or an scalar, most of the time this course it will be an scalar.
- $\hat{S}$: **estimator**. $\hat{S} = f(\mathbf{X})$ is our approximation to the value of S given the observation. In the analytic estimation case $\hat{S}$ is random since it is a deterministic function ($f()$) of a random variable ($\mathbf{X}$), therefore its pdf can be obtained applying random variable transformation to the pdf of the observations.
- $p_{X,S}(\mathbf{x}, s)$: **statistical relationship between observations and estimated variable**. We can estimate S using $\mathbf{X}$ as input because they are related. We express this relationship as a joint pdf.

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Random variable vs. Deterministic parameter

The variable we want to estimate can be either random S, or deterministic s. Examples:

- Deterministic: I've thought the mean of a Gaussian distribution m. I draw K samples from the distribution and ask you to estimate m. Note that m is unknown but does not follow any prior distribution $p(m)$; m is a fixed [unknown] constant.
- Random: I pick at random one student from the class, I tell you his/her foot length ($X = x$) and you have to guess his/her height ($S = s$). S is random because I can pick any student in the class.

Analytic estimation vs. machine estimation

- **Machine estimation or regression**: the problem is defined in terms of a set of examples, $\{\mathbf{x}^k, s^k\}_{k=1}^l$. We use the examples to fit an estimation model, for example a linear regressor:

  $$\hat{s} = f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$$

  we learn $\mathbf{w}$ and w_0 with the training set $\{\mathbf{x}^k, s^k\}_{k=1}^l$.
  Notice in the machine estimation setting the training observations $\{\mathbf{x}^k, s^k\}_{k=1}^l$ are not random (we do know them). The test observations can be considered random.
- **Analytic estimation**: the problem is defined in terms of a complete statistical characterisation: there exists a joint pdf $p_{\mathbf{X},S}(\mathbf{x}, s)$ and we know how to calculate it for any pair $(\mathbf{x}, s)$. In this setting $\mathbf{X}$ is random.
- **Semi-analytic estimation**: The problem is defined in terms of a data set, as in the regression case. We do not use this data to fit a regression model but to **learn the statistics**, i.e., estimate $p_{\mathbf{X},S}(\mathbf{x}, s)$. Once we have an estimation of the joint pdf (or any other useful pdf) we can apply analytic estimation.

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Likelihood

We rely on different pdfs that capture the relationship between $\mathbf{x}$ and s.

Likelihood

$$p_{\mathbf{X}|S}(\mathbf{x}|s)$$

It's the key pdf. You will have a likelihood in both random and deterministic variable estimation cases.

The likelihood models the generation of observations for every possible value of the target variable S. If S changes, we get different statistics in the observations. That is why we can guess the value of S.

If s is deterministic there is no point in conditioning in the value of s since it is always the same. Anyway we use $p_{\mathbf{X}|s}(\mathbf{x}|s)$ to unify notations.

S is random

If S is a random variable we have three other pdfs:

- **Prior** or marginal of S: $p_S(s)$ gives information about how are the values of S distributed without access to the observations.
- **Joint distribution** of S and $\mathbf{X}$: $p_{\mathbf{X},S}(\mathbf{x}, s)$
- **Posterior** of S given the observation $\mathbf{X} = \mathbf{x}$: $p_{S|\mathbf{X}}(s|\mathbf{x})$ gives the values of S that concentrate a higher probability density for each particular observed value of $\mathbf{X}$. It is a key pdf in the design of estimators since to know $\mathbf{X} = \mathbf{x}$ **narrows** the uncertainty about S expressed in the prior (I mean $p_{S|\mathbf{X}}(s|\mathbf{x})$ as a function of s is “narrower” than $P_S(s)$).

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Cost Functions

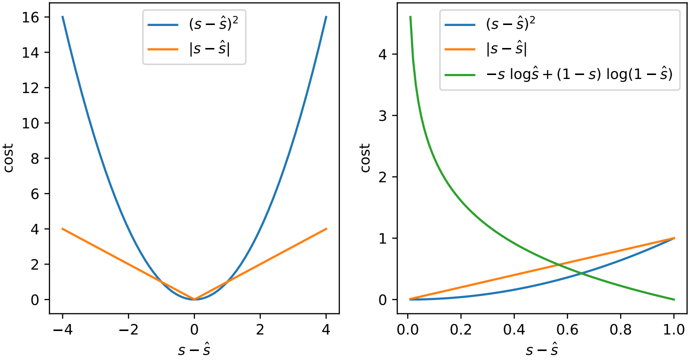
- An estimator is a function of the observations: $\hat{s} = f(\mathbf{x})$.
- The of design an estimator involves an optimisation to pick the best estimation function $f^*()$ from within a family or set of candidates.
- We need a criterion to select this best estimation function from the set of potential candidates. This criterion is the **cost function**.

Cost function

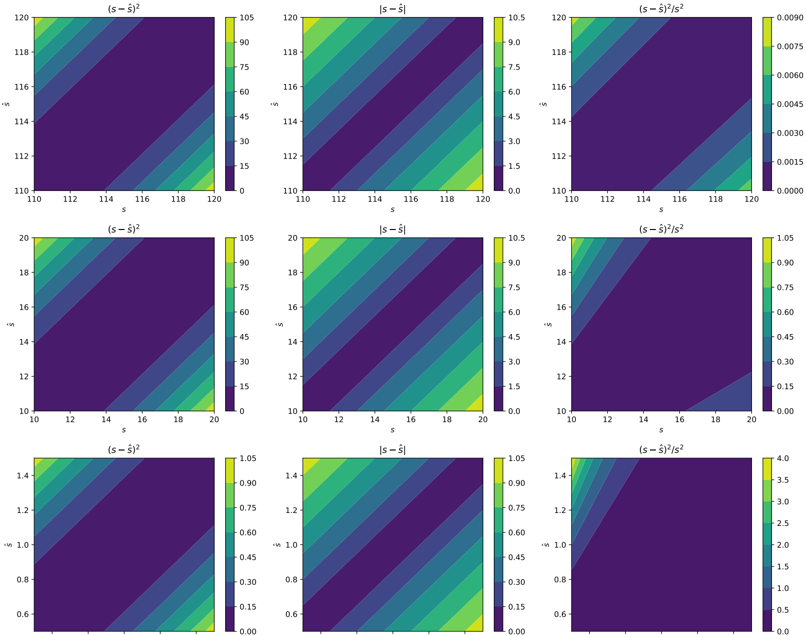
Function of the estimator and of the estimated variable: $C(S, \hat{S})$. It compares both quantities and determines the penalty in which we incur if we approximate $S = s$ with $\hat{S} = \hat{s}$. In most cases exact estimations ($\hat{s} = s$) yield zero cost: $C(s, \hat{s} = s) = 0$. The cost is always positive $C(S, \hat{S}) \geq 0$.

Examples of cost function

- Quadratic Cost: $c(e) = e^2$.
- Absolute Value of the error: $c(e) = |e|$.
- Relative Square Error: $c(s, \hat{s}) = \frac{(s-\hat{s})^2}{s^2}$
- Log loss: $c(s, \hat{s}) = -s \ln \hat{s} - (1-s)\ln(1-\hat{s})$, for $s \in \{0, 1\}$, and $\hat{s} \in [0, 1]$



Examples of cost function



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Expected Cost

Since we plan to use the estimator a large number of times, we are more interested in the expected cost, that takes into account all the possible values of S and $\hat{S}$.

Expected cost

$$\mathbb{E}\{c(S,\hat{S})\} = \int_{\mathbf{x}}\int_{s} c(s,\hat{s}(\mathbf{x}))\mathbf{p}_{\mathbf{S},\mathbf{X}}(\mathbf{s},\mathbf{x})\mathbf{dsdx}$$

Notice that $\hat{S} = \hat{S}(\mathbf{X})$ is a deterministic function of $\mathbf{X}$, therefore the statistics of $\hat{S}$ can be univocally defined in terms of the statistics of $\mathbf{X}$ (transformation of random variable).

Example

Let X be a noisy observation of S, such that

$$X = S + R$$

with S a random variable with mean 0 and variance 1, and R a Gaussian random variable, independent of S, with mean 0 and variance v. Consider the estimator $\hat{S} = X$, the expected quadratic cost is

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$$\mathbb{E}\{(S - \hat{S})^2\} = \mathbb{E}\{(S - X)^2\} = \mathbb{E}\{R^2\} = v$$

The expected absolute cost is

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The expected absolute cost is

$$\begin{aligned} \mathbb{E}\{|S - \hat{S}|\} = \mathbb{E}\{|R|\} &= \int_{-\infty}^{\infty} |r| \frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{r^2}{2v}\right) dr \\ &= 2\int_0^{\infty} r \frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{r^2}{2v}\right) dr = \sqrt{\frac{2v}{\pi}} \end{aligned}$$

Example: Calculation of Expected Quadratic Cost

Two random variables S and X follow a joint pdf

$$p_{S,X}(s,x) = \begin{cases} \frac{1}{x}, & 0 < s < x, \quad 0 < x < 1 \\ 0, & \text{otherwise} \end{cases}$$

Consider two estimators $\hat{S}_1 = \frac{1}{2}X$ and $\hat{S}_2 = X$. Which is the best estimator from the point of view of minimising the quadratic cost?

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For a general w,

$$\begin{aligned} \mathbb{E}\{(S - wX)^2\} &= \int_0^1 \int_0^x (s - wx)^2 p_{S,X}(s,x) ds dx \\ &= \int_0^1 \int_0^x (s - wx)^2 \frac{1}{x} ds dx \\ &= \int_0^1 \left(\frac{1}{3} - w + w^2 \right) x^2 dx \\ &= \frac{1}{3} \left(\frac{1}{3} - w + w^2 \right) \end{aligned}$$

Example: Calculation of Expected Quadratic Cost (ctd)

If $w = 1/2$

$$\mathbb{E}\{(S - \hat{S}_1)^2\} = \mathbb{E}\{(S - \frac{1}{2}X)^2\} = \frac{1}{3}\left(\frac{1}{3} - \frac{1}{2} + \frac{1}{4}\right) = \frac{1}{36} \quad (1)$$

Alternatively, if $w = 1$

$$\mathbb{E}\{(S - \hat{S}_2)^2\} = \mathbb{E}\{(S - X)^2\} = \frac{1}{3}\left(\frac{1}{3} - 1 + 1\right) = \frac{1}{9} \quad (2)$$

Therefore, from the point of view of the mean square error, $\hat{S}_1$ is better estimator than $\hat{S}_2$.

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Bayesian estimation

Given a cost function and a statistical relationship (joint distribution) between observations and estimated variable, the Bayesian Estimator is the one that minimizes the expected cost.

$$\hat{S}_{\text{Bayes}} = \arg\min_{\hat{S}} \mathbb{E}\{c(S, \hat{S})\} = \arg\min_{\hat{S}} \int_{\mathbf{x}} \int_{s} c(s, \hat{s}) p_{S,\mathbf{X}}(s, \mathbf{x}) ds d\mathbf{x}$$

$$= \arg\min_{\hat{S}} \int_{\mathbf{x}} \int_{s} c(s, \hat{s}) p_{S|\mathbf{X}}(s|\mathbf{x}) ds \; p_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} =$$

$$\arg\min_{\hat{S}} \int_{\mathbf{x}} \mathbb{E}\{c(S, \hat{S})|\mathbf{X}\} p_{\mathbf{X}}(\mathbf{x}) d\mathbf{x}$$

Bayesian estimation

If we look carefully into the last integral, we see that $\mathbb{E}\{c(S,\hat{S})|\mathbf{X}\}$ is multiplied by a positive function $(p_{\mathbf{X}}(\mathbf{x}))$. Therefore, to minimize the expected global cost is to minimise the integral and it is achieved minimising $\mathbb{E}\{c(S,\hat{S})|\mathbf{X}\}$. Thus a first result is

$$\hat{S}_{\text{Bayes}} = \arg\min_{\hat{S}} \mathbb{E}\{c(S,\hat{S})|\mathbf{X}\}$$

In summary, to compute a Bayesian Estimator we need to take two steps:

1. Select a cost function $c(S,\hat{S})$.
2. Minimise $\mathbb{E}\{c(S,\hat{S})|\mathbf{X}\}$

Example: Find Bayesian estimation with Quadratic Cost

Two random variables S and X follow a joint pdf

$$p_{S,X}(s,x) = \begin{cases} \frac{1}{x}, & 0 < s < x, \quad 0 < x < 1 \\ 0, & \text{otherwise} \end{cases}$$

Find the Bayesian estimator that minimizes the quadratic cost

Example: Find Bayesian estimation with Quadratic Cost

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Find the Bayesian estimator that minimizes the quadratic cost

First, find the posterior

$$p_{S|X}(s|x) = \frac{p_{S,X}(s,x)}{p_X(x)}$$

$$p_{S|X}(s|x) = \begin{cases} \frac{1}{x}, & 0 < s < x, \quad 0 < x < 1 \\ 0, & \text{otherwise} \end{cases}$$

Where you should apply that

$$p_X(x) = \int_{(s)} p_{S,X}(s,x)ds = \int_0^x \frac{1}{x} ds = 1$$

Example: Find Bayesian estimation with Quadratic Cost

The expected cost given x:

Example: Find Bayesian estimation with Quadratic Cost

The expected cost given x:

$$\begin{aligned}
\mathbb{E}\{c(S,\hat{S})|\mathbf{X}=\mathbf{x}\} &= \mathbb{E}\{(S-\widehat{s})^2)|\mathbf{X}=\mathbf{x}\} \\
&= \int_{(s)} (s-\widehat{s})^2 p_{S|X}(s|x)ds \\
&= \frac{1}{x}\int_0^x (s-\widehat{s})^2 ds \\
&= \frac{1}{x}\left(\frac{(x-\widehat{s})^3}{3}+\frac{\widehat{s}^3}{3}\right) \\
&= \frac{1}{3}x^2-\widehat{s}x+\widehat{s}^2
\end{aligned}$$

The expected cost given x, as a function of $\widehat{s}$, is a 2nd degree polynomial. We can minimize it by equating its derivative to 0.

Example: Find Bayesian estimation with Quadratic Cost

The expected cost given x:

$$\begin{aligned}\mathbb{E}\{c(S,\hat{S})|\mathbf{X}=\mathbf{x}\} &= \mathbb{E}\{(S-\widehat{s})^2)|\mathbf{X}=\mathbf{x}\} \\ &= \frac{1}{3}x^2 - \widehat{s}x + \widehat{s}^2\end{aligned}$$

The expected cost given x, as a function of $\widehat{s}$, is a 2nd degree polynomial. We can minimize it by equating its derivative to 0.

$$\frac{d}{d\widehat{s}}\mathbb{E}\{c(S,\hat{S})|\mathbf{X}=\mathbf{x}\} = -x + 2\widehat{s} = 0$$

And the solution is:

$$\widehat{s}_{\text{Bayes}} = \frac{1}{2}x$$

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Minimum Mean Square Error (MMSE) Estimator

This is the Bayesian Estimator when the cost function is the quadratic error: $c(s, \hat{s}) = e^2 = (s - \hat{s})^2$. Therefore the estimator is the solution to the optimisation problem given by

$$\hat{s}_{\text{MMSE}} = \arg\min \hat{s}\mathbb{E}\{c(S, \hat{s})|\mathbf{X} = \mathbf{x}\} = \arg\min \hat{s} \int_s (s - \hat{s})^2 p_{S|\mathbf{X}}(s|\mathbf{x})ds$$

Minimum Mean Square Error (MMSE) Estimator

To minimise, we take the derivative with respect to $\hat{s}$ and make it equal to zero.

$$\frac{\mathrm{d}}{\mathrm{d}\hat{s}} \int_s (s-\hat{s})^2 p_{S|\mathbf{X}}(s|\mathbf{x}) ds = \int_s \frac{\partial}{\partial \hat{s}} (s-\hat{s})^2 p_{S|\mathbf{X}}(s|\mathbf{x}) ds$$

$$= \int_{-\infty}^{\infty} -2(s-\hat{s}) p_{S|\mathbf{X}}(s|\mathbf{x}) ds$$

In the optimum the above integral is equal to zero:

$$\int_{-\infty}^{\infty} -2(s-\hat{s}_{\text{Bayes}}) p_{S|\mathbf{X}}(s|\mathbf{x}) ds = 0 \Rightarrow$$

$$\hat{s}_{\text{Bayes}} = \mathbb{E}\{s|\mathbf{X}\}$$

The intuition behind this result is that the knowledge of $\mathbf{X}$ determines as optimum estimator the one corresponding to choosing the expected value of S for that particular observed value of $\mathbf{X}$.

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Expected absolute cost

The minimum absolute error estimator corresponds to the cost function $c(e) = |e| = |s - \widehat{s}|$. Therefore:

$$\begin{aligned}\widehat{s}_{\mathrm{MAD}} &= \arg\min_{\widehat{s}} \mathbb{E}\{c(S,\widehat{s})|\mathbf{X}=\mathbf{x}\} \\ &= \arg\min_{\widehat{s}} \int_s |s-\widehat{s}| p_{S|\mathbf{X}}(s|\mathbf{x}) ds\end{aligned}$$

$$\begin{aligned}\mathbb{E}\{|S-\widehat{s})|\mathbf{X}=\mathbf{x}\} &= \int_{-\infty}^{\widehat{s}} (\widehat{s}-s) p_{S|\mathbf{X}}(s|\mathbf{x}) ds + \int_{\widehat{s}}^{\infty} (s-\widehat{s}) p_{S|\mathbf{X}}(s|\mathbf{x}) ds \\ &= \widehat{s}\left[\int_{-\infty}^{\widehat{s}} p_{S|\mathbf{X}}(s|\mathbf{x}) ds - \int_{\widehat{s}}^{\infty} p_{S|\mathbf{X}}(s|\mathbf{x}) ds\right] + \\ &+ \int_{\widehat{s}}^{\infty} s\, p_{S|\mathbf{X}}(s|\mathbf{x}) ds - \int_{-\infty}^{\widehat{s}} s\, p_{S|\mathbf{X}}(s|\mathbf{x}) ds\end{aligned}$$

Minimization of the average cost a posteriori

The Fundamental Theorem of Calculus enables to get the derivative of the average cost a posteriori as:

$$\frac{d\mathbb{E}\{|S-\widehat{s}||\mathbf{X}=\mathbf{x}\}}{d\widehat{s}} =$$

$$\frac{d}{d\widehat{s}}\left(\widehat{s}\left[\int_{-\infty}^{\widehat{s}} p_{S|\mathbf{X}}(s|\mathbf{x})ds - \int_{\widehat{s}}^{\infty} p_{S|\mathbf{X}}(s|\mathbf{x})ds\right] + \right.$$

$$\left.\int_{\widehat{s}}^{\infty} s\, p_{S|\mathbf{X}}(s|\mathbf{x})ds - \int_{-\infty}^{\widehat{s}} s\, p_{S|\mathbf{X}}(s|\mathbf{x})ds\right)$$

and then make

$$\frac{d\mathbb{E}\{|S-\widehat{s}||\mathbf{X}=\mathbf{x}\}}{d\widehat{s}} = 0$$

MAD estimator

MAD estimator

$$\widehat{s}_{\text{MAD}}(\mathbf{x}) = \text{median}\{S|\mathbf{X} = \mathbf{x}\}$$

Note: It is usually computed with the following expression:

$$\int_{-\infty}^{\widehat{s}_{\text{MAD}}} p_{S|\mathbf{X}}(s|\mathbf{x})ds = \int_{\widehat{s}_{\text{MAD}}}^{\infty} p_{S|\mathbf{X}}(s|\mathbf{x})ds = \frac{1}{2}$$

Example: Find Bayesian estimation with Absolute Error Cost

Two random variables S and X follow a joint pdf

$$p_{S,X}(s,x) = \begin{cases} \frac{1}{x}, & 0 < s < x, \quad 0 < x < 1 \\ 0, & \text{otherwise} \end{cases}$$

Find the Bayesian estimator that minimizes the absolute error cost
From previous example retrieve the posterior

$$p_{S|X}(s|x) = \begin{cases} \frac{1}{x}, & 0 < s < x, \quad 0 < x < 1 \\ 0, & \text{otherwise} \end{cases}$$

Example: Find Bayesian estimation with Absolute Error Cost

$$\widehat{s}_{\mathrm{MAD}} \Rightarrow \int_0^{\widehat{s}_{\mathrm{MAD}}} p_{S|\mathbf{x}}(s|\mathbf{x})ds = \frac{1}{2} = \int_{\widehat{s}_{\mathrm{MAD}}}^{x} p_{S|\mathbf{x}}(s|\mathbf{x})ds$$

$$\int_0^{\widehat{s}_{\mathrm{MAD}}} \frac{1}{x}ds = \frac{1}{2} \quad \Rightarrow \quad \widehat{s}_{\mathrm{MAD}}(x) = \frac{x}{2}$$

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MAP estimator

MAP Estimator

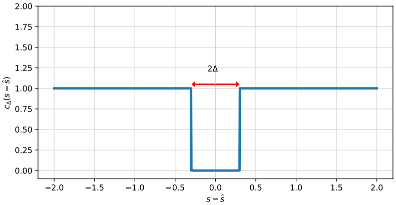
$$\begin{aligned}\widehat{s}_{\mathrm{MAP}}(\mathbf{x}) &= \arg\max_{s} p_{S|\mathbf{X}}(s|\mathbf{x}) \\ &= \arg\max_{s} \ln\left[p_{S|\mathbf{X}}(s|\mathbf{x})\right]\end{aligned}$$

When the distribution a posteiori presents several global maxima, the MAP estimator is not unique!

MAP estimator from a Bayesian point of view

Strictly speaking, the MAP estimator is not Bayesian because it is not minimizing any expected cost. However, if we consider the following cost function:

$$c_\Delta(s - \widehat{s}) = \begin{cases} 1, & \text{if } |s - \widehat{s}| > \Delta \\ 0, & \text{if } |s - \widehat{s}| < \Delta \end{cases}$$



and $\widehat{s}_\Delta$ as the bayesian estimator corresponding to c_Δ:

$$\widehat{s}_{\text{MAP}} = \lim_{\Delta \to 0} \widehat{s}_\Delta$$

Therefore the MAP estimator can be considered a limit case in a family of bayesian estimators.

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Maximum Likelihood (ML) Estimator

ML estimator

$$\hat{s}_{ML} = \arg\max_{s} p_{\mathbf{x}|s}(\mathbf{x}|s) = \arg\max_{s} \ln(p_{\mathbf{x}|s}(\mathbf{x}|s))$$

- No associated cost function, therefore **in general the ML is not a Bayesian estimator**. It could happen that the $\hat{s}_{ML}$ coincides with a Bayesian estimator, but by definition the $\hat{s}_{ML}$ does not optimise a cost function
- $\hat{s}_{ML}$ does not take into account the prior distribution $p_S(s)$. Therefore it can be used when s is a **deterministic parameter**.

Relationship between the MAP estimator and the ML estimator

$$\hat{s}_{MAP} = \arg\max_s p_{S|\mathbf{X}}(s|\mathbf{x}) = \arg\max_s \frac{p_{\mathbf{X}|S}(\mathbf{x}|s)p_S(s)}{p_{\mathbf{X}}(\mathbf{x})}$$

If we don't know $p_S(s)$, we can assume it is **uniform** (no preference for any particular value of s). Therefore

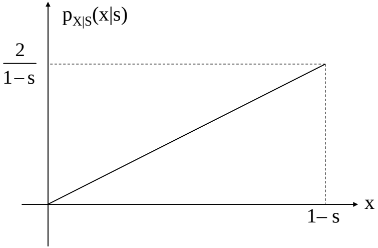
$$\arg\max_s \frac{p_{\mathbf{X}|S}(\mathbf{x}|s)p_S(s)}{p_{\mathbf{X}}(\mathbf{x})} \sim \arg\max_s p_{\mathbf{X}|S}(\mathbf{x}|s) = \hat{s}_{ML}$$

Example: ML estimation of a random variable

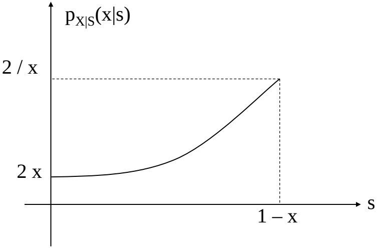
One wishes to estimate the value of a random variable S from the observed value of another variable X, statistically related to S through:

$$p_{X|S}(x|s) = \frac{2x}{(1-s)^2}, \;\; 0 < x < 1-s, \;\; 0 < s < 1$$

We need to maximise $p_{X|S}(x|s)$ with respect to s, (not to x)



$p_{X|S}(x|s)$ as a function of x



$p_{X|S}(x|s)$ as a function of s

Solution: $\hat{s}_{ML} = 1 - X$

Example: Estimation of the parameters of a Gaussian

We have access to a collection of l data samples $\{X^{(k)}\}_{k=1}^{l}$ drawn **independently** from a Gaussian pdf. Construct estimators for the mean m and the variance v of the Gaussian.

- The likelihood of each observation given m and v is

$$p_X(x) = p_{X|m,v}(x|m,v) = \frac{1}{\sqrt{2\pi v}} \exp\left[-\frac{(x-m)^2}{2v}\right]$$

- Since we observe l samples, the **joint** pdf will be the product of the individual pdfs.

$$p_{\{X^{(k)}\}|m,v}(\{x^{(k)}\}|m,v) = \prod_{k=1}^{l} p_{X|m,v}(x^{(k)}|m,v)$$

$$= \frac{1}{(2\pi v)^{l/2}} \prod_{k=1}^{l} \exp\left[-\frac{(x^{(k)}-m)^2}{2v}\right]$$

Example: Estimation of the parameters of a Gaussian

- Taking logs and optimising

$$\hat{m}_{\mathrm{ML}} = \frac{1}{l}\sum_{k=1}^{l} x^{(k)}$$

- Using $\hat{m}_{\mathrm{ML}}$ in the expression for the estimator of the variance

$$\hat{v}_{\mathrm{ML}} = \frac{1}{l}\sum_{k=1}^{l} (x^{(k)} - \hat{m}_{\mathrm{ML}})^2$$

Gaussian case. Linear Mean Squared Error Estimation. Quality of estimators.

Modern Theory of Detection and Estimation. Block-1: Estimation

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Estimation with Gaussian pdfs

- Estimation of **random variables** when the joint distribution of all the involved variables is a multivariate Gaussian.
- This is a very frequent case in real world problems.
- It is straightforward to proof that in this case all the marginals and all the conditionals will be Gaussian.
- Particularly, $p_{S|\mathbf{X}}(s|\mathbf{x})$ being Gaussian implies that the mean, the median and the mode of the posterior distribution coincide. Therefore $\hat{S}_{\mathrm{MMSE}} = \hat{S}_{\mathrm{MAD}} = \hat{S}_{\mathrm{MAP}}$. We focus on $\hat{S}_{\mathrm{MMSE}}$.

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Review of a Gaussian joint pdf for 1D variables

Assume $\mathbb{E}\{X\} = 0$ and $\mathbb{E}\{S\} = 0$. Then

$$p_{S,X}(s,x) \sim G\left(\left[\begin{array}{c} 0 \\ 0 \end{array} \right], \left[\begin{array}{cc} v_S & \rho \\ \rho & v_X \end{array} \right] \right)$$

where v_S is the variance of S, v_X is the variance of X and $\rho = \mathbb{E}\{SX\} - \mathbb{E}\{S\}\mathbb{E}\{X\}$ is their covariance.
Then the posterior is given by

$$p_{S|X}(s|x) = \frac{p_{S,X}(s,x)}{p_X(x)}$$

$$= \frac{\frac{1}{2\pi\sqrt{v_X v_S - \rho^2}} \exp\left[-\frac{1}{2(v_X v_S - \rho^2)} \left[\begin{array}{cc} s & x \end{array} \right] \left[\begin{array}{cc} v_X & -\rho \\ -\rho & v_S \end{array} \right] \left[\begin{array}{c} s \\ x \end{array} \right] \right]}{\frac{1}{\sqrt{2\pi v_X}} \exp\left[-\frac{x^2}{2v_X} \right]}$$

MMSE in 1D

We need the mean of $p_{S|X}(s|x)$. We exploit that $p_{S|X}(s|x)$ is Gaussian:

$$p_{S|X}(s|x) \sim G\left(m_{S|X}, v_{S|X}\right) = \frac{1}{\sqrt{2\pi v_{S|X}}} \exp\left[-\frac{(s - m_{S|X})^2}{2v_{S|X}}\right]$$

After developing both expressions for the same Gaussian and making term identification:

$$\frac{m_{S|X}^2}{v_{S|X}} = \frac{v_S x^2}{v_X v_S - \rho^2} - \frac{x^2}{v_X}$$

$$\frac{s\ m_{S|X}}{v_{S|X}} = \frac{\rho x s}{v_X v_S - \rho^2}$$

$$\frac{s^2}{v_{S|X}} = \frac{v_X s^2}{v_X v_S - \rho^2}$$

Therefore $\hat{s}_{\mathrm{MMSE}} = m_{S|X} = \frac{\rho}{v_X} x$. Notice it is a **linear function** of x.

Example: Estimation of a Gaussian signal with additive Gaussian noise

$X = S + N$, S is a Gaussian signal with zero mean and variance v_S. N is a Gaussian noise with zero mean and variance v_N independent of S.

We need to construct an estimator for S given X.

Example: Estimation of a Gaussian signal with additive Gaussian noise

$X = S + N$, S is a Gaussian signal with zero mean and variance v_S. N is a Gaussian noise with zero mean and variance v_N independent of S.

We need to construct an estimator for S given X.

According to the previous result $\hat{S} = \rho X / v_X$

$$\rho = \mathbb{E}\{(X - m_X)(S - m_S)\} = \mathbb{E}\{X\ S\} = \mathbb{E}\{(S+N)S\} = \mathbb{E}\{S^2\} + \mathbb{E}\{S\ N\} = v_S$$

$$v_X = v_S + v_N \text{ since they are independent}$$

Therefore $\hat{S} = \frac{v_S X}{v_S + v_N}$.

Physical interpretation when $v_S \gg v_N$ or $v_N \gg v_S$

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Joint multivariate Gaussian pdf

In a general multivariate case $\mathbf{S}$ and $\mathbf{X}$ are random vectors of dimensions N and M, respectively. Their joint pdf is

$$p_{\mathbf{S},\mathbf{X}}(\mathbf{s},\mathbf{x}) \sim G\left(\begin{bmatrix} \mathbf{m_S} \\ \mathbf{m_X} \end{bmatrix}, \begin{bmatrix} \mathbf{V_S} & \mathbf{V_{SX}} \\ \mathbf{V_{SX}^T} & \mathbf{V_X} \end{bmatrix} \right)$$

where $\mathbf{m_S}$ and $\mathbf{m_X}$ are the mean vectors and the covariances are

$$\mathbf{V_S} = \mathbb{E}\{(\mathbf{S}-\mathbf{m_S})(\mathbf{S}-\mathbf{m_S})^T\}$$
$$\mathbf{V_X} = \mathbb{E}\{(\mathbf{X}-\mathbf{m_X})(\mathbf{X}-\mathbf{m_X})^T\}$$
$$\mathbf{V_{SX}} = \mathbb{E}\{(\mathbf{S}-\mathbf{m_S})(\mathbf{X}-\mathbf{m_X})^T\}$$

Posterior distribution, multivariate case

The posterior $p_{\mathbf{S}|\mathbf{X}}(\mathbf{S}|\mathbf{X})$ is also a multivariate Gaussian with parameters

- mean:
$$\mathbf{m}_{\mathbf{S}|\mathbf{X}} = \mathbf{m}_{\mathbf{S}} + \mathbf{V}_{\mathbf{SX}}\mathbf{V}_{\mathbf{X}}{}^{-1}(\mathbf{x} - \mathbf{m}_{\mathbf{X}})$$
- and covariance:
$$\mathbf{V}_{\mathbf{S}|\mathbf{X}} = \mathbf{V}_{\mathbf{S}} - \mathbf{V}_{\mathbf{SX}}\mathbf{V}_{\mathbf{X}}{}^{-1}\mathbf{V}_{\mathbf{SX}}^{T}$$

Therefore the MMSE estimator is given by

$$\hat{\mathbf{s}}_{\mathrm{MMSE}} = \mathbb{E}\{\mathbf{s}|\mathbf{x}\} = \mathbf{m}_{\mathbf{S}} + \mathbf{V}_{\mathbf{SX}}\mathbf{V}_{\mathbf{X}}{}^{-1}(\mathbf{x} - \mathbf{m}_{\mathbf{X}})$$

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Estimator with a fixed shape

- Sometimes you need to add a priori information about the estimation problem in the design of the estimator.
- Most of the times it means to fix a parametric shape for the estimation function $f_{\mathbf{w}}(\mathbf{X})$, with $\mathbf{w}$ a vector of parameters.
- Example: Observations in 2D and fix a shape for the estimator $\hat{S} = w_0 + w_1 X_1^2 + w_2 X_2^2$ (non-linear terms). The design task involves finding appropriate values for w_0, w_1 and w_2
- Minimize expected cost, but introducing the shape of the estimator as a constraint in the optimization

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \; \mathbb{E}\{c(S, \hat{S})\} = \arg\min_{\mathbf{w}} \; \mathbb{E}\{c(S, f_{\mathbf{w}}(\mathbf{X}))\}$$

$$= \arg\min_{\mathbf{w}} \int_{\mathbf{x}} \int_{s} c(s, f_{\mathbf{w}}(\mathbf{x})) p_{S,\mathbf{X}}(s, \mathbf{x}) ds d\mathbf{x}$$

Example: Estimation with constraints

Two random variables S and X follow a joint pdf

$$p_{S,X}(s,x) = \left[\begin{array}{ll} \frac{1}{x}, & 0 < s < x < 1 \\ 0, & \text{otherwise} \end{array} \right.$$

Find the estimator of the form $\hat{s} = wx^2$ that minimizes the quadratic cost.

Example: Estimation with constraints

Two random variables S and X follow a joint pdf

$$p_{S,X}(s,x) = \left[\begin{array}{ll} \frac{1}{x}, & 0 < s < x < 1 \\ 0, & \text{otherwise} \end{array} \right.$$

Find the estimator of the form $\hat{s} = wx^2$ that minimizes the quadratic cost.

$$\hat{s} = \arg\min_{w} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (s - wx^2)^2 p_{S,X}(s,x) ds dx$$

Taking derivatives and making them equal to zero

$$\hat{s} = \frac{5}{8} x^2$$

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LMMSE Estimator motivation

- Bayesian estimation: minimize expected cost. Leads to
  - MSE: $\mathbb{E}\{s|\mathbf{X}\}$. You need $p_{S|\mathbf{X}}(s|\mathbf{x})$ and compute an integral
  - MAP: $\arg\max_s p_{S|\mathbf{X}}(s|\mathbf{x})$. You need also $p_{S|\mathbf{X}}(s|\mathbf{x})$ and maximize.
- Under Gaussian joint pdfs MAP and MSE estimators coincide and they are **linear**
- What if we can't access the complete $p_{S|\mathbf{X}}(s|\mathbf{x})$?

LMMSE essence

- Assume linearity $\hat{s} = \mathbf{w}^T\mathbf{x} + w_0$
- Minimize MSE

LMMSE properties

- Depends only on first and second order statistics
- Easy to evaluate
- In general LMMSE is suboptimal
- ... but optimal in the ubiquitous Gaussian case

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1D case

1. MMSE:
$$\hat{s} = \arg\min_{\hat{s}} \mathbb{E}\{(s - \hat{s})^2\}$$
2. Linearity
$$\hat{s} = w_0 + w_1 x \rightarrow \hat{s} = \arg\min_{w_0, w_1} \mathbb{E}\{(s - w_0 - w_1 x)^2\}$$
3. Optimizing
   - $\frac{\partial}{\partial w_0}\mathbb{E}\{(s - w_0 - w_1 x)^2\} = 0 \rightarrow \mathbb{E}\{(s - w_0 - w_1 x)\} = \mathbb{E}\{e\} = 0$: **Error with zero mean**
   - $\frac{\partial}{\partial w_1}\mathbb{E}\{(s - w_0 - w_1 x)^2\} = 0 \rightarrow \mathbb{E}\{(xe)\} = 0$ **Error orthogonal to observations**
4. Solution
$$w_1 = \frac{\text{Covariance}(x, s)}{\text{Variance}(x)}, \qquad w_0 = \mathbb{E}\{s\} - \frac{\text{Covariance}(x, s)}{\text{Variance}(x)}\mathbb{E}\{x\}$$
   Notice $w_0 = 0$ if x and s are zero mean.
5. MSE: $\mathbb{E}\{e^2\} = \mathbb{E}\{s^2\} - w_0\mathbb{E}\{s\} - w_1\mathbb{E}\{sx\}$

Multivariate case

1. $\hat{s} = w_0 + \sum_{j=1}^{d} w_j x_j = w_0 + \mathbf{w}^T \mathbf{x}$
2. $\hat{s} = \arg\min_{w_0,\mathbf{w}} \mathbb{E}\{(s - w_0 - \mathbf{w}^T \mathbf{x})^2\}$
3. Optimization
   - $\frac{\partial}{\partial w_0} \mathbb{E}\{(s - w_0 - \mathbf{w}^T \mathbf{x})^2\} = 0 \rightarrow \mathbb{E}\{e\} = 0$: **Error with zero mean** $w_0 = \mathbb{E}\{s\} - \mathbf{w}^T \mathbb{E}\{\mathbf{x}\}$
   - $\nabla_w \mathbb{E}\{(s - w_0 - \mathbf{w}^T \mathbf{x})^2\} = \mathbf{0} \rightarrow \mathbb{E}\{(\mathbf{x}e)\} = \mathbf{0}$ **Error orthogonal to each of the observed variables**
   - Consequently: **Error orthogonal to the estimator** $\mathbb{E}\{\hat{s}e\} = 0$
4. **Normal Equations** We develop the principle of orthogonality for the ith variable x_i:

$$\mathbb{E}\{(x_i e)\} = 0 \Rightarrow \mathbb{E}\{x_i s\} - w_0 \mathbb{E}\{x_i\} - \sum_j w_j \mathbb{E}\{x_i x_j\} = 0$$

Substituting w_0

$$\mathbb{E}\{x_i s\} - \mathbb{E}\{s\}\mathbb{E}\{x_i\} + \sum_j w_j \mathbb{E}\{x_j\}\mathbb{E}\{x_i\} - \sum_j w_j \mathbb{E}\{x_i x_j\} = 0$$

Multivariate case

Remember

$$\mathrm{cov}(s, x_i) = \mathbb{E}\{x_i s\} - \mathbb{E}\{x_i\}\mathbb{E}\{s\}; \quad \mathrm{cov}(x_i, x_j) = \mathbb{E}\{x_i x_j\} - \mathbb{E}\{x_i\}\mathbb{E}\{x_j\}$$

Substituting covariances yields

$$\mathrm{cov}(s, x_i) - \sum_j w_j \mathrm{cov}(x_i, x_j) = 0, \quad \forall i = 1, \ldots, d$$

Stack the d equations (one for each x_i) and write in matrix form:

$$\mathbf{c}_{\mathbf{x},s} = C_{\mathbf{x},\mathbf{x}}\mathbf{w}$$

5. Solution:

$$\mathbf{w} = C_{\mathbf{x},\mathbf{x}}^{-1}\mathbf{c}_{\mathbf{x},s}$$

$$w_0 = w_0 = \mathbb{E}\{s\} - \mathbf{c}_{\mathbf{x},s}^T C_{\mathbf{x},\mathbf{x}}^{-1}\mathbb{E}\{\mathbf{x}\}$$

6. MSE: $\mathbb{E}\{e^2\} = \mathrm{var}(s) - \mathbf{c}_{\mathbf{x},s}^T C_{\mathbf{x},\mathbf{x}}^{-1}\mathbf{c}_{\mathbf{x},s}$

Example

The statistical relationship between S and the observed variables X_1 and X_2 is given by:

$$\begin{array}{lll}
\mathbb{E}\{S\} = 1/2 & \mathbb{E}\{X_1\} = 1 & \mathbb{E}\{X_2\} = 0 \\
\mathbb{E}\{S^2\} = 4 & \mathbb{E}\{X_1^2\} = 3/2 & \mathbb{E}\{X_2^2\} = 2 \\
\mathbb{E}\{SX_1\} = 1 & \mathbb{E}\{SX_2\} = 2 & \mathbb{E}\{X_1 X_2\} = 1/2
\end{array}$$

Determine the LMMSE estimator of S given the observations.

Example

The statistical relationship between S and the observed variables X_1 and X_2 is given by:

$$\begin{array}{lll} \mathbb{E}\{S\} = 1/2 & \mathbb{E}\{X_1\} = 1 & \mathbb{E}\{X_2\} = 0 \\ \mathbb{E}\{S^2\} = 4 & \mathbb{E}\{X_1^2\} = 3/2 & \mathbb{E}\{X_2^2\} = 2 \\ \mathbb{E}\{SX_1\} = 1 & \mathbb{E}\{SX_2\} = 2 & \mathbb{E}\{X_1X_2\} = 1/2 \end{array}$$

Determine the LMMSE estimator of S given the observations.

$$\hat{s} = \mathbf{c}_{S,\mathbf{X}}^T C_{\mathbf{x},\mathbf{x}}^{-1}\mathbf{x} + \mathbb{E}\{s\} - \mathbf{c}_{\mathbf{x},s}^T C_{\mathbf{x},\mathbf{x}}^{-1}\mathbb{E}\{\mathbf{x}\}$$

$$\hat{s} = \begin{bmatrix} .5 & 2 \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 2 \end{bmatrix}^{-1} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + 0.5 - \begin{bmatrix} .5 & 2 \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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Assessing the quality of an estimator

- One can design different estimators to work in a same scenario (problem).
- Fix **criteria** that enable a **fair comparison** between estimators.
- **Expected cost** for a determined cost function leads to always choose the Bayesian estimator as optimum.
- **Other measures** that can be of interest in different scenarios you may come accross.
  - **Bias** ($\sim$ systematic error)
  - **Variance** (concentration of the estimations around their expected value)

  Important! Bias and variance depend on if the variable to be estimated is random or deterministic.

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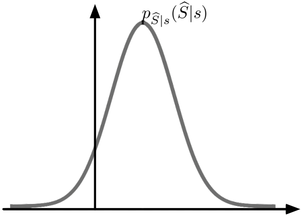
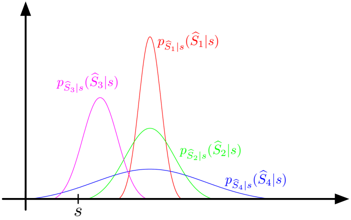
Probability density of the estimator

- $p_{\widehat{S}|s}(\widehat{s}|s)$ provides a complete characterization of the behaviour of the estimator.
  (Since $\widehat{S}$ is a function of the observations, $\widehat{S} = f(\mathbf{X})$, $p_{\widehat{S}|s}(\widehat{s}|s)$ can be obtained from $p_{\mathbf{X}|s}(\mathbf{X}|s)$ with a transformation of random variable.



Motivation

Imagine a case of estimation of a parameter s with 4 different estimators ($\widehat{S}_1 = f_1(\mathbf{X})$, $\widehat{S}_2 = f_2(\mathbf{X})$, $\widehat{S}_3 = f_3(\mathbf{X})$ and $\widehat{S}_4 = f_4(\mathbf{X})$) Examining their pdfs, which estimator seems more appropriate?



Perhaps $\widehat{S}_3$ as the probability of getting estimations close to the true s is significantly larger.

Bias and variance when s is deterministic

- **Bias**:
  - Expresses how far is the mean of $p_{\widehat{S}|s}(\widehat{s}|s)$ from the true value of s

$$\mathrm{Bias}\left\{\widehat{S}|s\right\} = \mathbb{E}\left\{s - \widehat{S}|s\right\} = \mathbb{E}\{s|s\} - \mathbb{E}\left\{\widehat{S}|s\right\} = s - \mathbb{E}\left\{\widehat{S}|s\right\}$$

- **Variance**:

$$\mathrm{Variance}\left\{\widehat{S}|s\right\} = \mathbb{E}\left\{\left(\widehat{S} - \mathbb{E}\left\{\widehat{S}\right\}\right)^2\Big|s\right\} = \mathbb{E}\left\{\widehat{S}^2|s\right\} - \mathbb{E}^2\left\{\widehat{S}|s\right\}$$

  If s is a deterministic parameter, the variance of the estimator coincides with the estimation error.

$$\mathrm{Variance}\left\{\widehat{S} - s\Big|s\right\} = \mathrm{Variance}\left\{\widehat{S}|s\right\} - \mathrm{Variance}\{s|s\} = \mathrm{Variance}\left\{\widehat{S}|s\right\}$$

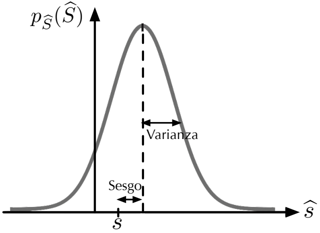
Important! The bias and the variance of the estimators of a deterministic parameter are a function of its true value (s).

Properties

Bias and variance of the estimador of a deterministic paramter

$\text{Bias}\{\widehat{S}|s\} = s - \mathbb{E}\{\widehat{S}|s\}$

$\text{Variance}\left\{\widehat{S}|s\right\} = \mathbb{E}\{\widehat{S}^2|s\} - \mathbb{E}^2\{\widehat{S}|s\}$



- The estimators with **zero bias** are known as **unbiased estimators**.
- If the estimator operates on a number K of observations of a random variable and $\text{Variance}(\widehat{S}) \to 0$ if $K \to \infty$, the estimator is **consistent in variance**.

Mean squared error

Mean squared error of the estimator of a deterministic parameter

$$\begin{aligned}\mathbb{E}\Big\{(s-\widehat{S})^2\big|s\Big\} &= \text{Variance}\Big\{\widehat{S}-s\big|s\Big\}+\mathbb{E}^2\{s-\widehat{S}|s\}\\ &= \text{Variance}\{\widehat{S}|s\}+\Big[\text{Bias}(\widehat{S}|s)\Big]^2\end{aligned}$$

Example

Calculate the bias and variance of the sample estimation of the mean of a random variable.

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General vision

- As in the deterministic case, one could directly use $p_{\widehat{S}|S}(\widehat{s}|s)$ to study the performance of an estimador.
- However, when S is a random variable, the true value $(S = s)$ changes every time we repeat the experiment of drawing the observations and running the estimator.

Bias and variance

Bias and variance of the estimator of a random variable

$$\text{Bias}\{\widehat{S}\} = \mathbb{E}\{S - \widehat{S}\} = \mathbb{E}\{S\} - \mathbb{E}\{\widehat{S}\}$$
$$\text{Variance}\left\{\widehat{S}\right\} = \mathbb{E}\left\{\left(\widehat{S} - \mathbb{E}\{\widehat{S}\}\right)^2\right\} = \mathbb{E}\{\widehat{S}^2\} - \mathbb{E}^2\{\widehat{S}\}$$

The calculation of these expectations uses the joint pdf of S and $\mathbf{X}$.

Important! The bias and variance of the estimators of a random variable **are not** a **function** of the true value of S (s).

Mean squared error

The mean squared error of the estimator of a deterministic parameter was deterministic

$$\mathbb{E}\left\{(S-\widehat{S})^2\right\} = \text{Variance}\left\{\widehat{S}-S\right\} + \mathbb{E}^2\{S-\widehat{S}\}$$
$$= \text{Variance}\{\widehat{E}\} + \left[\text{Bias}(\widehat{S})\right]^2$$

If $(\widehat{S})$ is random, the variance of the error in general will not be equal to the variance of the estimator.

Properties

- The **unconstrained minimum mean square error estimator is unbiased**:

$$
\begin{aligned}
\text{Bias}\{\widehat{S}_{\text{MMSE}}\} &= \mathbb{E}\left\{S - \widehat{S}_{\text{MMSE}}\right\} = \mathbb{E}\{S\} - \mathbb{E}\left\{\widehat{S}_{\text{MMSE}}\right\} \\
&= \mathbb{E}\{S\} - \int \mathbb{E}\ \{S|\mathbf{X} = \mathbf{x}\} p_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} \\
&= \mathbb{E}\{S\} - \mathbb{E}\{S\} \\
&= 0
\end{aligned}
$$

- The **linear MMSE** is **unbiased**.
  $(\mathbb{E}(E^*) = 0)$