

5. Estimation

Statistical Signal Processing

Version 1.7

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Motivation

Based on the square footage y of a house in Paderborn, we would like to estimate its price x . Thus, we are looking for a function f such that $\hat{x} = f(y)$ is a good **estimate** of x .

- In order to build such an estimator we need to have statistical information about x and y . This allows us to model square footage and price as random variables Y and X .
- In general, f may be a **nonlinear** function. In many practical situations, however, we restrict our estimators to be **linear**, i.e., $\hat{X} = aY + b$.
- If we know the first- and second-order moments μ_X , μ_Y , σ_X^2 , σ_Y^2 , and σ_{XY} , we may build a linear estimator $\hat{X} = aY + b$ that minimizes the mean-squared error (MSE) $E\{|\hat{X} - X|^2\}$ (cf. Chapter 2).
- The required first- and second-order moments are generally unknown and need to be estimated themselves from observations of X and Y .

Frequentist vs. Bayesian estimation

There is a fundamental difference between the cases where we:

- estimate a random variable from another random variable (called **Bayesian estimation**)
- estimate an unknown, but deterministic, parameter (called **frequentist estimation**)

An example of a frequentist problem is the estimation of the mean μ_X of a random variable X from n observations x_1, \dots, x_n as

$$\hat{\mu}_X = \frac{1}{n} \sum_{i=1}^n x_i$$

The estimate $\hat{\mu}_X$ is a particular value of the **estimator**

$$\hat{M}_X = \frac{1}{n} \sum_{i=1}^n X_i$$

where we assume that the X_i are n **independent identically distributed** (i.i.d.) random variables, modeling observations of X .

5.1 Measures of performance

Bias and consistency (frequentist)

Important definitions

Let $\hat{\Theta}$ denote an estimator of a deterministic parameter θ computed from n observations X_1, X_2, \dots, X_n .

- The **bias** is $b(\theta) = E\{\hat{\Theta}|\theta\} - \theta$. If $b(\theta) = 0$, then $\hat{\Theta}$ is called **unbiased**.
- The estimator is called **consistent** if it **converges in probability**

$$\lim_{n \rightarrow \infty} P\{|\hat{\Theta} - \theta| > \epsilon\} = 0 \text{ for any } \epsilon > 0$$

- An unbiased and consistent estimator for the **mean vector**:

$$\hat{\Theta} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$$

- An unbiased and consistent estimator for the **covariance matrix**:

$$\hat{\Theta} = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \hat{\mu}_{\mathbf{x}})(\mathbf{x}_i - \hat{\mu}_{\mathbf{x}})^H$$

Mean-squared error (MSE)

By far the most common performance metric of an estimator is the mean-squared error (MSE). It can be defined for the frequentist and Bayesian approach, but the definition given here is Bayesian.

- Let $\hat{\mathbf{X}}$ be an estimator of \mathbf{X} and $\mathbf{E} = \hat{\mathbf{X}} - \mathbf{X}$ the error, then the MSE is

$$E\{\|\hat{\mathbf{X}} - \mathbf{X}\|^2\} = E\{\mathbf{E}^H \mathbf{E}\} = \text{tr } E\{\mathbf{E} \mathbf{E}^H\} = \text{tr } \mathbf{M}$$

where $\mathbf{M} = E\{\mathbf{E} \mathbf{E}^H\}$ is the **mean-squared error matrix**.

- The **Bayes bias** is $\mathbf{b} = \mu_E$ and the **error covariance matrix** is

$$\mathbf{Q} = E\{(\mathbf{E} - \mu_E)(\mathbf{E} - \mu_E)^H\} = \mathbf{M} - \mathbf{b} \mathbf{b}^H$$

Thus, $\mathbf{M} = \mathbf{Q} + \mathbf{b} \mathbf{b}^H$. Designing a minimum-MSE estimator hence requires the **right tradeoff between error covariance and bias**.

- If the estimator is **unbiased**, the error has zero mean, and then $\mathbf{Q} = \mathbf{M}$.

5.2 Frequentist approaches to estimation

Nota Bene

For the remaining sections in this chapter, we use **lower-case letters** to denote both random variables and their samples. The difference should be clear from the context.

Maximum Likelihood (ML) estimator

- Let $f_{x|\theta}(\mathbf{x}|\boldsymbol{\theta})$ be the **likelihood function**, i.e., the pdf of a random vector \mathbf{x} parametrized by the unknown deterministic parameter $\boldsymbol{\theta}$.
- Let's say we observe the value \mathbf{x}_0 . The ML estimator $\hat{\boldsymbol{\theta}}$ picks the value of $\boldsymbol{\theta}$ that maximizes the likelihood function or, equivalently, the **log-likelihood function**:

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} f_{x|\theta}(\mathbf{x}_0|\boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \log f_{x|\theta}(\mathbf{x}_0|\boldsymbol{\theta})$$

Important properties

The ML estimator is **consistent**, but it may be **biased** (even substantially so). If the data is Gaussian, then the ML estimator minimizes the variance $E\{\|\hat{\boldsymbol{\theta}} - E\{\hat{\boldsymbol{\theta}}\}\|^2\}$.

- The ML estimator requires knowledge of the pdf (often unrealistic).
- If the pdf is differentiable, the ML estimate may be computed as (one of) the root(s) of

$$\frac{\partial}{\partial \boldsymbol{\theta}} \log f_{x|\theta}(\mathbf{x}_0|\boldsymbol{\theta}) = \mathbf{0}$$

MVDR estimator

Consider the **linear model**

$$\mathbf{y} = \mathbf{H}\boldsymbol{\theta} + \mathbf{n}$$

where $\mathbf{H} \in \mathbb{C}^{m \times n}$ is known, $\boldsymbol{\theta} \in \mathbb{C}^n$ is an unknown parameter, and \mathbf{n} is an m -dim. random vector with mean zero and covariance matrix \mathbf{R}_{nn}

We are looking for a **linear minimum variance unbiased estimator** = minimum variance distortionless response (MVDR estimator) = best linear unbiased estimator (BLUE) of $\boldsymbol{\theta}$ from \mathbf{y} :

$$\hat{\boldsymbol{\theta}} = \mathbf{W}^H \mathbf{y}$$

- **Unbiasedness constraint:**

$$E\{\hat{\boldsymbol{\theta}}\} = E\{\mathbf{W}^H(\mathbf{H}\boldsymbol{\theta} + \mathbf{n})\} = \mathbf{W}^H \mathbf{H}\boldsymbol{\theta} + \mathbf{W}^H E\{\mathbf{n}\} = \boldsymbol{\theta} \Rightarrow \mathbf{W}^H \mathbf{H} = \mathbf{I}$$

- **Minimize the variance**

$$\begin{aligned} E\{\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\|^2\} &= \text{tr } E\{(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta})^H\} \\ &= \text{tr } \mathbf{R}_{\hat{\boldsymbol{\theta}}\hat{\boldsymbol{\theta}}} = \text{tr }\{\mathbf{W}^H \mathbf{R}_{yy} \mathbf{W}\} = \text{tr }\{\mathbf{W}^H \mathbf{R}_{nn} \mathbf{W}\} \end{aligned}$$

Solution to the MVDR estimation problem

MVDR optimization problem

The solution to

$$\min \text{tr} \{\mathbf{W}^H \mathbf{R}_{nn} \mathbf{W}\} \text{ under constraint } \mathbf{W}^H \mathbf{H} = \mathbf{I}$$

is

$$\mathbf{W}^H = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1}$$

which results in $\mathbf{Q} = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1}$.

- The MVDR estimator (= ML estimator for Gaussian data) is

$$\hat{\boldsymbol{\theta}} = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{y} = \boldsymbol{\theta} + (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{n}$$

(Notice that it is unbiased)

- If $\mathbf{R}_{nn} = \mathbf{I}$, then

$$\hat{\boldsymbol{\theta}} = (\mathbf{H}^H \mathbf{H})^{-1} \mathbf{H}^H \mathbf{y} = \mathbf{H}^\dagger \mathbf{y}$$

This is also the solution of the deterministic Least-Squares (LS) problem, where we minimize $\|\mathbf{y} - \mathbf{H}\boldsymbol{\theta}\|^2$ for given deterministic \mathbf{y} .

5.3 Bayesian approaches to estimation

Conditional mean estimator

- We would like to construct an estimator $\hat{\mathbf{x}}$ to estimate a random vector \mathbf{x} from another random vector \mathbf{y} .
- Its mean-squared error matrix is

$$\begin{aligned}\mathbf{Q} &= E[(\hat{\mathbf{x}} - \mathbf{x})(\hat{\mathbf{x}} - \mathbf{x})^H] \\ &= E[(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}] + E[\mathbf{x}|\mathbf{y}] - \mathbf{x})(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}] + E[\mathbf{x}|\mathbf{y}] - \mathbf{x})^H] \\ &= E[(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})^H] + E[(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}])(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})^H] \\ &\quad + E[(E[\mathbf{x}|\mathbf{y}] - \mathbf{x}) \underbrace{(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}])^H}_{g^H(\mathbf{y})} + E[(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}])(\hat{\mathbf{x}} - E[\mathbf{x}|\mathbf{y}])^H]\end{aligned}$$

- Law of total expectation:

$$E\{E[(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})g^H(\mathbf{y})|\mathbf{y}]\} = \mathbf{0}$$

makes second and third terms in \mathbf{Q} zero

The optimum estimator is the **conditional mean estimator** $\hat{\mathbf{x}} = E[\mathbf{x}|\mathbf{y}]$.

Conditional mean estimator

Consider the error vector $\mathbf{e} = \hat{\mathbf{x}} - \mathbf{x} = E[\mathbf{x}|\mathbf{y}] - \mathbf{x}$.

- $E[\mathbf{e}] = \mathbf{0}$, and thus $E[\hat{\mathbf{x}}] = E[\mathbf{x}]$. This says that $\hat{\mathbf{x}}$ is an **unbiased estimator** of \mathbf{x} .
- The covariance matrix of the error vector is

$$\mathbf{Q} = E[\mathbf{e}\mathbf{e}^H] = E[(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})^H].$$

Any competing estimator $\hat{\mathbf{x}}'$ with error covariance matrix $\mathbf{Q}' = E[(\hat{\mathbf{x}}' - \mathbf{x})(\hat{\mathbf{x}}' - \mathbf{x})^H]$ will have $\mathbf{Q}' \geq \mathbf{Q}$.

- As a consequence, the conditional mean estimator is a **minimum mean-squared error (MMSE)** estimator:

$$E\|\mathbf{e}\|^2 = \text{tr } \mathbf{Q} \leq \text{tr } \mathbf{Q}' = E\|\mathbf{e}'\|^2.$$

Orthogonality principle

The error vector \mathbf{e} is orthogonal to every measurable function of \mathbf{y} , $\mathbf{g}(\mathbf{y})$. That is, $E[\mathbf{e}\mathbf{g}^H(\mathbf{y})] = E\{(E[\mathbf{x}|\mathbf{y}] - \mathbf{x})\mathbf{g}^H(\mathbf{y})\} = \mathbf{0}$.

Linear MMSE estimation

Let's consider the n -dim. **signal** (message) \mathbf{x} and the m -dim. **observation** (measurement) \mathbf{y} , both zero mean. Their composite covariance matrix is the matrix

$$\mathbb{R}_{xy} = E \left\{ \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} [\mathbf{x}^H \quad \mathbf{y}^H] \right\} = \begin{bmatrix} \mathbf{R}_{xx} & \mathbf{R}_{xy} \\ \mathbf{R}_{xy}^H & \mathbf{R}_{yy} \end{bmatrix}.$$

The error between the signal \mathbf{x} and the linear estimator $\hat{\mathbf{x}} = \mathbf{W}\mathbf{y}$ is $\mathbf{e} = \hat{\mathbf{x}} - \mathbf{x}$ and the error covariance matrix is $\mathbf{Q} = E[(\hat{\mathbf{x}} - \mathbf{x})(\hat{\mathbf{x}} - \mathbf{x})^H]$:

$$\mathbf{Q} = E[(\mathbf{W}\mathbf{y} - \mathbf{x})(\mathbf{W}\mathbf{y} - \mathbf{x})^H] = \mathbf{W}\mathbf{R}_{yy}\mathbf{W}^H - \mathbf{R}_{xy}\mathbf{W}^H - \mathbf{W}\mathbf{R}_{xy}^H + \mathbf{R}_{xx}.$$

After completing the square, this may be written

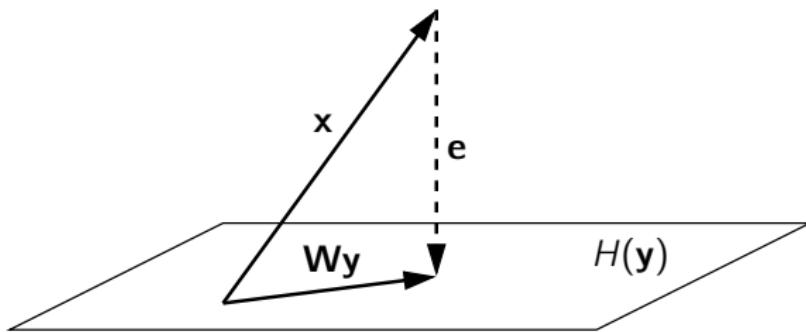
$$\mathbf{Q} = \mathbf{R}_{xx} - \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1}\mathbf{R}_{xy}^H + (\mathbf{W} - \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1})\mathbf{R}_{yy}(\mathbf{W} - \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1})^H.$$

This quadratic form in \mathbf{W} is positive semidefinite, so

$\mathbf{Q} \geq \mathbf{R}_{xx} - \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1}\mathbf{R}_{xy}^H$ with equality for

$$\mathbf{W} = \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1} \quad \text{and} \quad \mathbf{Q} = \mathbf{R}_{xx} - \mathbf{R}_{xy}\mathbf{R}_{yy}^{-1}\mathbf{R}_{xy}^H.$$

Orthogonality principle



The solution for \mathbf{W} may be written as the solution to the **normal** equations $\mathbf{W}\mathbf{R}_{yy} - \mathbf{R}_{xy} = \mathbf{0}$, or

$$E[(\mathbf{W}\mathbf{y} - \mathbf{x})\mathbf{y}^H] = \mathbf{0}.$$

The estimator error $\mathbf{e} = \mathbf{W}\mathbf{y} - \mathbf{x}$ is **orthogonal** to the measurement \mathbf{y} .

Nonzero means

- What if the signal has known mean μ_x and the measurement has known mean μ_y ?
- The centered signal and measurement $\mathbf{x} - \mu_x$ and $\mathbf{y} - \mu_y$ then share the composite covariance matrix \mathbb{R}_{xy} .
- The LMMSE estimator of $\mathbf{x} - \mu_x$ from $\mathbf{y} - \mu_y$ obeys all of the equations already derived:

$$\hat{\mathbf{x}} - \mu_x = \mathbf{W}(\mathbf{y} - \mu_y) \Leftrightarrow \hat{\mathbf{x}} = \mathbf{W}(\mathbf{y} - \mu_y) + \mu_x$$

- The **orthogonality principle** says the error between the estimator and the signal is orthogonal to the measurement:

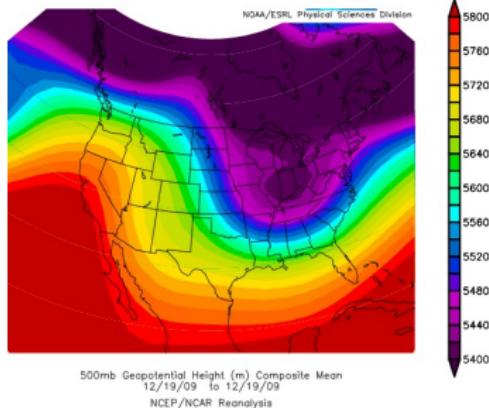
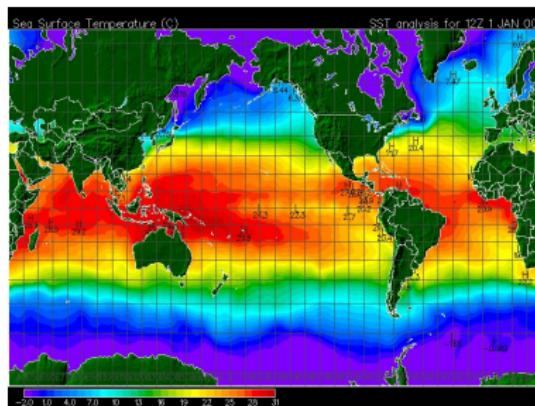
$$\begin{aligned} E[(\hat{\mathbf{x}} - \mathbf{x})\mathbf{y}^H] &= E\{[\hat{\mathbf{x}} - \mu_x - (\mathbf{x} - \mu_x)](\mathbf{y} - \mu_y)^H\} \\ &\quad + E\{[\hat{\mathbf{x}} - \mu_x - (\mathbf{x} - \mu_x)]\mu_y^H\} = \mathbf{0} \end{aligned}$$

The first term on the right is zero due to the orthogonality principle already established for zero mean LMMSE estimators.

The second term is zero because $\hat{\mathbf{x}}$ is an unbiased estimator of \mathbf{x} , i.e., $E[\hat{\mathbf{x}}] = \mu_x$.

Application of LMMSE estimation

We would like to estimate the 500 mb height (\approx air pressure) over the USA (right figure) from the sea surface temperature (left figure).



- Arrange measurements of the 500 mb height in a vector \mathbf{x} and measurements of the sea surface temperature in a vector \mathbf{y}
- We need to estimate the covariance matrices of \mathbf{x} and \mathbf{y} from sample (observation) pairs $(\mathbf{x}_i, \mathbf{y}_i)$. Which assumptions are necessary?

Tradeoff between bias and variance

Let's apply the LMMSE estimator to the linear model $\mathbf{y} = \mathbf{Hx} + \mathbf{n}$ (with \mathbf{x} and \mathbf{n} zero mean):

$$\hat{\mathbf{x}} = \mathbf{W}\mathbf{y} = \mathbf{W}(\mathbf{Hx} + \mathbf{n}) = \mathbf{WHx} + \mathbf{Wn}$$

- The LMMSE filter \mathbf{W} does not equalize \mathbf{H} to produce $\mathbf{WH} = \mathbf{I}$.
- Rather, it approximates \mathbf{I} so that the error

$$\mathbf{e} = \mathbf{W}\mathbf{y} - \mathbf{x} = (\mathbf{WH} - \mathbf{I})\mathbf{x} + \mathbf{Wn}$$

with covariance matrix

$$\mathbf{Q} = \underbrace{(\mathbf{WH} - \mathbf{I})\mathbf{R}_{xx}(\mathbf{WH} - \mathbf{I})^H}_{\text{model-bias-squared}} + \underbrace{\mathbf{WR}_{nn}\mathbf{W}^H}_{\text{filtered noise variance}}$$

provides the best tradeoff between model-bias-squared and filtered noise variance to minimize the error covariance matrix \mathbf{Q} .

Comparison with MVDR estimator

We can write the LMMSE estimator for the linear model $\mathbf{y} = \mathbf{Hx} + \mathbf{n}$ as

$$\begin{aligned}\hat{\mathbf{x}} &= \mathbf{R}_{xy} \mathbf{R}_{yy}^{-1} \mathbf{y} = \mathbf{R}_{xx} \mathbf{H}^H (\mathbf{R}_{nn} + \mathbf{H} \mathbf{R}_{xx} \mathbf{H}^H)^{-1} \mathbf{y} \\ &= (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H} + \mathbf{R}_{xx}^{-1})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{y} \\ &= (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H} + \mathbf{R}_{xx}^{-1})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{Hx} + (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H} + \mathbf{R}_{xx}^{-1})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{n}.\end{aligned}$$

Let's compare that with the MVDR estimator for the linear model $\mathbf{y} = \mathbf{H}\boldsymbol{\theta} + \mathbf{n}$ with deterministic parameter $\boldsymbol{\theta}$:

$$\hat{\boldsymbol{\theta}} = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{y} = \boldsymbol{\theta} + (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{n}$$

- The **frequentist bias** of the LMMSE estimator is $\mathbf{b}(\mathbf{x}) = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H} + \mathbf{R}_{xx}^{-1})^{-1} \mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{Hx} - \mathbf{x}$ but its **Bayes bias** is $\mathbf{b} = \mathbf{0}$. On the other hand, the MVDR estimator has zero frequentist and Bayes bias.
- The error covariances are related as

$$\mathbf{Q}_{\text{LMMSE}} = (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H} + \mathbf{R}_{xx}^{-1})^{-1} \leq (\mathbf{H}^H \mathbf{R}_{nn}^{-1} \mathbf{H})^{-1} = \mathbf{Q}_{\text{MVDR}}$$

Gaussian case

If the composite vector $[\mathbf{x}^T, \mathbf{y}^T]^T$ is multivariate Gaussian with zero mean and composite covariance matrix \mathbb{R}_{xy} , then the conditional pdf for \mathbf{x} , given \mathbf{y} , is

$$f_{x|y}(\mathbf{x}|\mathbf{y}) = \frac{f_{xy}(\mathbf{x}, \mathbf{y})}{f_y(\mathbf{y})} = \frac{\det \mathbf{R}_{yy}}{\pi^n \det \mathbb{R}_{xy}} \exp \left\{ - [\mathbf{x}^H \quad \mathbf{y}^H] \mathbb{R}_{xy}^{-1} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} + \mathbf{y}^H \mathbf{R}_{yy}^{-1} \mathbf{y} \right\}.$$

Using the identity $\det \mathbb{R}_{xy} = \det \mathbf{R}_{yy} \det \mathbf{Q}$ and one of the factorizations for \mathbb{R}_{xy}^{-1} given in Chapter 3, this pdf may be written

$$f_{x|y}(\mathbf{x}|\mathbf{y}) = \frac{1}{\pi^n \det \mathbf{Q}} \exp \left\{ - (\mathbf{x} - \mathbf{W}\mathbf{y})^H \mathbf{Q}^{-1} (\mathbf{x} - \mathbf{W}\mathbf{y}) \right\}.$$

Thus the posterior pdf for \mathbf{x} , given \mathbf{y} , is Gaussian with conditional mean $\mathbf{W}\mathbf{y}$ and conditional covariance \mathbf{Q} .

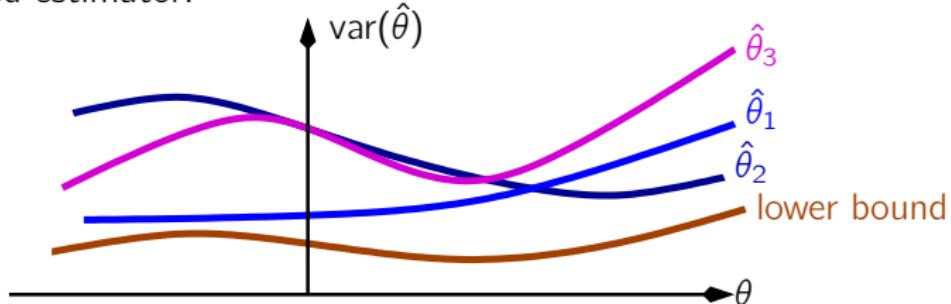
Conditional mean estimator for Gaussian data

For jointly Gaussian data, the **conditional mean estimator** $E\{\mathbf{x}|\mathbf{y}\}$ is the **linear MMSE estimator** $\mathbf{W}\mathbf{y}$.

5.4 Frequentist performance bounds for parameter estimation

Estimator accuracy considerations

- We would like to find a **lower bound** on the **error variance** of an unbiased estimator.



- There may or may not be an estimator that achieves the bound.
- The **estimation accuracy** depends directly on the likelihood function, i.e., the pdf $f_\theta(y) = f(y|\theta)$ of the measurement y conditioned on the parameter θ we would like to estimate.
- The more the likelihood function $f_\theta(y)$ is influenced by θ , the more accurately we should be able to estimate it.
 - Example:** Consider $y = \theta + n$ with $n \sim N(0, \sigma^2)$
 - If σ^2 is small, then we should be able to estimate θ more accurately.

Cramér-Rao bound for scalar parameters

A special case of the **Cramér-Rao bound** (which we will prove later) says that the variance of any unbiased estimator $\hat{\theta}$ must satisfy

$$\text{var}(\hat{\theta}) \geq \frac{1}{-E\left[\frac{\partial^2 \log f_{\theta}(y)}{\partial \theta^2}\right]}$$

- The “sharpness” of the likelihood function $f_{\theta}(y)$ should determine how accurately we can determine θ .
- This sharpness is measured by the average curvature of the log-likelihood function.

Example:

- Estimating the phase θ of a sinusoid with known amplitude A and frequency f_0 in AWGN with variance σ^2 :

$$y[n] = A \cos(2\pi f_0 n + \theta) + w[n], \quad n = 0, 1, \dots, N - 1.$$

- The Cramér-Rao bound is $\text{var}(\hat{\theta}) \geq \frac{2\sigma^2}{NA^2}$.

General quadratic frequentist bounds

Now let's talk about the general case.

Notation: From the measurement \mathbf{y} we compute the estimator $\hat{\theta}(\mathbf{y})$, which estimates the parameter $\theta \in \mathbb{R}^P$. The likelihood of the measurement is $f_\theta(\mathbf{y}) = f(\mathbf{y}|\theta)$. The estimation error is $\mathbf{e}(\mathbf{y}) = \hat{\theta}(\mathbf{y}) - \theta$ and the **centered error** is $\epsilon(\mathbf{y}) = \mathbf{e}(\mathbf{y}) - \mathbf{b}(\theta) = \hat{\theta}(\mathbf{y}) - E[\hat{\theta}(\mathbf{y})]$.

- Let's define the function $\mathbf{s}(\mathbf{y}) = [s_1(\mathbf{y}), s_2(\mathbf{y}), \dots, s_m(\mathbf{y})]^T$ to be an m -dimensional vector of **measurement scores**.
- The mean of the score is $E[\mathbf{s}(\mathbf{y})]$ and the **centered measurement score** is $\sigma(\mathbf{y}) = \mathbf{s}(\mathbf{y}) - E[\mathbf{s}(\mathbf{y})]$.
- The centered measurement score is a judiciously-chosen function of the measurement that brings information about the centered error $\epsilon(\mathbf{y})$.

We would like to approximate this centered error by using a linear function of the centered measurement score $\sigma(\mathbf{y})$. This will lead to a bound on the error covariance matrix $\mathbf{Q}(\theta) = E[\epsilon(\mathbf{y})\epsilon^H(\mathbf{y})]$.

Quadratic frequentist bound

Let's **linearly** estimate the centered error $\epsilon(\mathbf{y})$ from the centered measurement score $\sigma(\mathbf{y})$ using the LMMSE estimator

$$\hat{\epsilon}(\mathbf{y}) = \mathbf{T}^H(\theta) \mathbf{J}^{-1}(\theta) \sigma(\mathbf{y})$$

with

- the **sensitivity matrix** $\mathbf{T}(\theta) = E[\sigma(\mathbf{y})\epsilon^H(\mathbf{y})]$
- the **information matrix** $\mathbf{J}(\theta) = E[\sigma(\mathbf{y})\sigma^H(\mathbf{y})]$

This estimator has error covariance matrix $\mathbf{Q}(\theta) = \mathbf{T}^H(\theta) \mathbf{J}^{-1}(\theta) \mathbf{T}(\theta)$, which must be positive semidefinite. Hence:

Quadratic frequentist bound

The error covariance matrix is bounded by the general quadratic frequentist bound

$$\mathbf{Q}(\theta) \geq \mathbf{T}^H(\theta) \mathbf{J}^{-1}(\theta) \mathbf{T}(\theta),$$

and the mean-squared error matrix is bounded as

$$\mathbf{M}(\theta) \geq \mathbf{T}^H(\theta) \mathbf{J}^{-1}(\theta) \mathbf{T}(\theta) + \mathbf{b}(\theta) \mathbf{b}^H(\theta).$$

Fisher score

Our results for quadratic frequentist bounds so far are general. To make them applicable we need to consider a concrete score for which $\mathbf{T}(\boldsymbol{\theta})$ and $\mathbf{J}(\boldsymbol{\theta})$ can be computed. For this we choose the Fisher score:

Fisher score

The **Fisher score** is defined as

$$\mathbf{s}(\mathbf{y}) = \left[\frac{\partial}{\partial \boldsymbol{\theta}} \log f_{\boldsymbol{\theta}}(\mathbf{y}) \right]^T = \left[\frac{\partial}{\partial \theta_1} \log f_{\boldsymbol{\theta}}(\mathbf{y}), \dots, \frac{\partial}{\partial \theta_p} \log f_{\boldsymbol{\theta}}(\mathbf{y}) \right]^T,$$

where the partial derivatives are evaluated at the true value of $\boldsymbol{\theta}$.

The Fisher score has a number of important properties:

- ① We may write the partial derivative as

$$\frac{\partial}{\partial \theta_i} \log f_{\boldsymbol{\theta}}(\mathbf{y}) = \frac{1}{f_{\boldsymbol{\theta}}(\mathbf{y})} \frac{\partial}{\partial \theta_i} f_{\boldsymbol{\theta}}(\mathbf{y}),$$

which is a normalized measure of the sensitivity of the pdf $f_{\boldsymbol{\theta}}(\mathbf{y})$ to variations in the parameter θ_i . Large sensitivity is valued and this will be measured by the variance of the score.

Fisher score

- ② The Fisher score is a zero-mean random variable, hence $\sigma(\mathbf{y}) = \mathbf{s}(\mathbf{y})$.
- ③ The cross-correlation between the centered Fisher score and the centered error score is the sensitivity matrix

$$\mathbf{T}(\boldsymbol{\theta}) = \mathbf{I} + \left[\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{b}(\boldsymbol{\theta}) \right]^H.$$

The (i, j) th element of the matrix $(\partial/\partial \boldsymbol{\theta})\mathbf{b}(\boldsymbol{\theta})$ is $(\partial/\partial \theta_j)b_i(\boldsymbol{\theta})$.

When the estimator is unbiased, then $\mathbf{T} = \mathbf{I}$.

- ④ The **Fisher information matrix** is the expected Hessian of the score function (up to a minus sign):

$$\mathbf{J}_F(\boldsymbol{\theta}) = E \left\{ \left[\frac{\partial}{\partial \boldsymbol{\theta}} \log f_{\boldsymbol{\theta}}(\mathbf{y}) \right]^T \frac{\partial}{\partial \boldsymbol{\theta}} \log f_{\boldsymbol{\theta}}(\mathbf{y}) \right\} = -E \left\{ \frac{\partial}{\partial \boldsymbol{\theta}} \left[\frac{\partial}{\partial \boldsymbol{\theta}} \log f_{\boldsymbol{\theta}}(\mathbf{y}) \right]^T \right\}$$

Cramér-Rao bound

The quadratic frequentist bound for Fisher score is the **Cramér-Rao bound (CRB)**:

$$\mathbf{Q}(\theta) \geq \left[\mathbf{I} + \frac{\partial}{\partial \theta} \mathbf{b}(\theta) \right] \mathbf{J}_F^{-1}(\theta) \left[\mathbf{I} + \frac{\partial}{\partial \theta} \mathbf{b}(\theta) \right]^H$$

For an **unbiased estimator**, the Cramér-Rao bound is

$$\mathbf{Q}(\theta) \geq \mathbf{J}_F^{-1}(\theta)$$

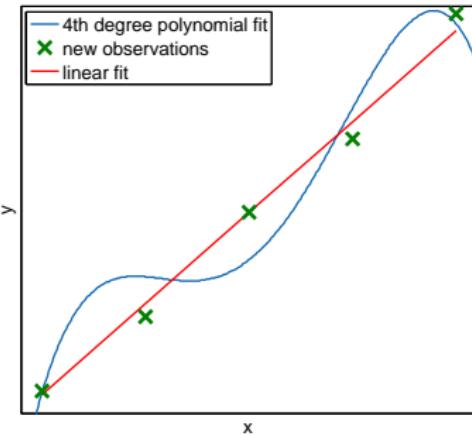
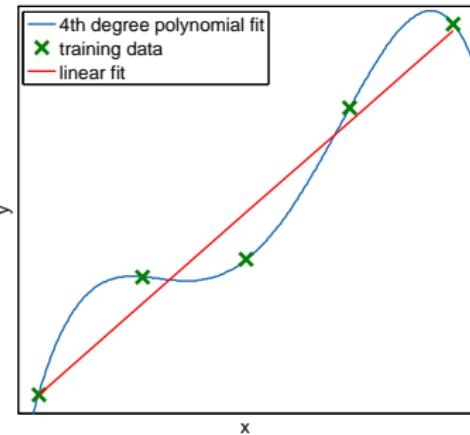
where $\mathbf{J}_F(\theta)$ is the **Fisher information matrix**.

- The CRB is only a **bound**. An estimator that achieves it (which does not always exist) is called **efficient**.
- If repeated measurements carry information about a fixed θ through the product pdf $\prod_{i=1}^N f_\theta(\mathbf{y}_i)$, then $\mathbf{T}(\theta)$ remains fixed and $\mathbf{J}_F(\theta)$ scales with N , hence the CRB decreases as N^{-1} .
- An ML estimator is **asymptotically** (for $N \rightarrow \infty$) **efficient**.

5.5 Reduced-rank estimation

Principle of parsimony

Example:

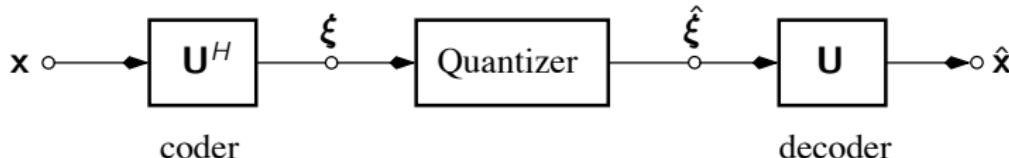


Rank reduction follows the principle of parsimony:

One should seek the **simplest possible model** to describe the phenomenon under study in order to **avoid overfitting to random noise** fluctuations. Rank reduction is a matter of finding the **right bias-variance trade-off**.

Example: Transform coder

Consider the following simplified model of a **transform coder**:



The coder and decoder are assumed to be unitary. Let's model the quantizer as an additive zero-mean white noise source: $\hat{\xi} = \xi + \mathbf{n}$, with $\mathbf{R}_{nn} = \sigma_n^2 \mathbf{I}$, uncorrelated with the data.

One can show that in order to minimize the MSE $E\{\|\hat{x} - x\|^2\}$, we

- choose the coder and decoder as the matrix of eigenvectors of \mathbf{R}_{xx} , i.e., $\mathbf{R}_{xx} = \mathbf{U}\Lambda\mathbf{U}^H$. The components of $\xi = [\xi_1, \dots, \xi_n]$ are the **principal components**.
- keep only those principal components whose variance exceeds the noise level: $\sigma_{\xi_i}^2 > \sigma_n^2$. The other components are replaced with zeros. This is a **bias-variance trade-off**.

LMMSE filtering with PCA preprocessing step

What happens in the LMMSE estimator

$$\hat{\mathbf{x}} = \mathbf{R}_{xy} \mathbf{R}_{yy}^{-1} \mathbf{y}$$

when \mathbf{R}_{yy} is singular or close to singular? This can easily happen when \mathbf{R}_{yy} is **estimated** from samples.

- We can replace \mathbf{R}_{yy}^{-1} with its pseudo-inverse \mathbf{R}_{yy}^\dagger . However, we might still run into numerical problems if \mathbf{R}_{yy} is close to singular (ill-conditioned).
- A more stable solution is to compute a rank r pseudo-inverse by considering only the largest r principal components:

$$\mathbf{R}_{yy}^{\dagger_r} = \mathbf{U}^H \boldsymbol{\Lambda}_r^{-1} \mathbf{U} \quad (\mathbf{U} : \text{eigenvectors of } \mathbf{R}_{yy})$$

where $\boldsymbol{\Lambda}_r^{-1} = \mathbf{Diag}(\lambda_1^{-1}, \lambda_2^{-1}, \dots, \lambda_r^{-1}, 0, \dots, 0)$. This is also suitable as a dimension-reduction step if the dimension of \mathbf{y} is very large.

- Problem: The components that contribute most to the variance of \mathbf{y} are not necessarily those that are most strongly correlated with \mathbf{x} .