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- **Hypothesis test – to decide if estimator is 'acceptable', for the given sample size**

3. Parameter Estimation and Goodness of Fit – part one

In the frequentist approach, parameter estimation requires the definition of a lot of mathematical machinery

- **Random sample** of size M, drawn from underlying pdf

How do we decide what makes an 'acceptable' estimator?

estimate parameters of the pdf

- **Hypothesis test** – to decide if estimator is 'acceptable', for the given sample size

Example: measuring the wavelength of a spectral line

True wavelength = z_0 (fixed but unknown parameter)

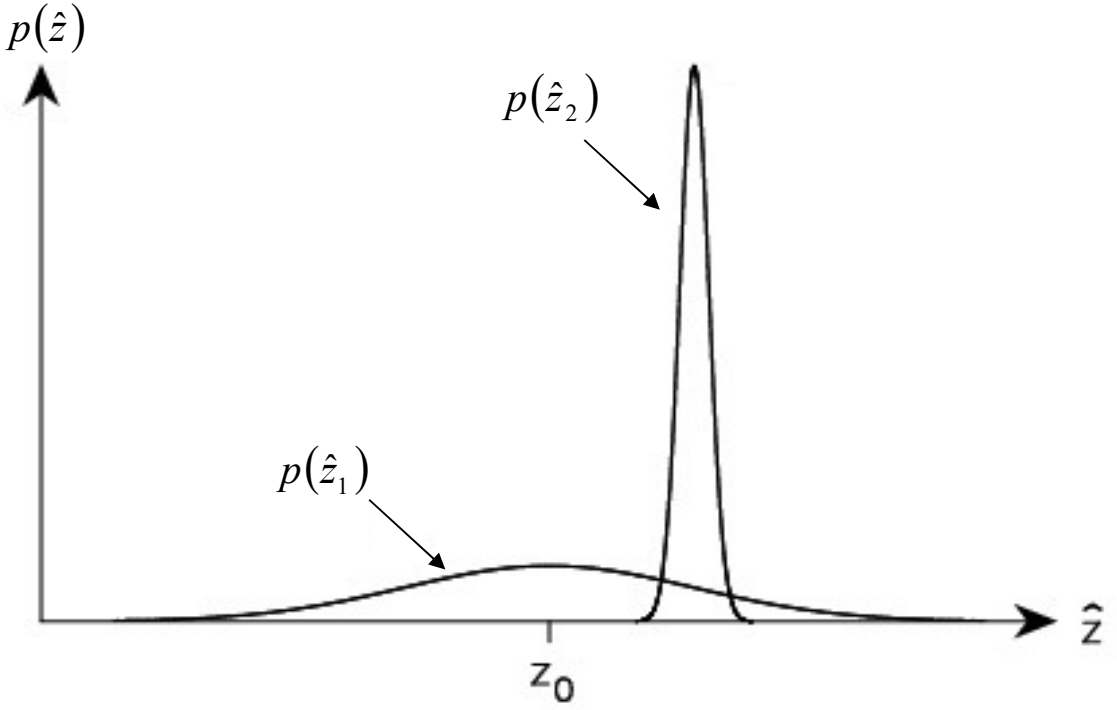
Compute sampling distribution for $\hat{z}_1$ *and* $\hat{z}_2$ *, modelling errors*

1. Low dispersion spectrometer

Unbiased:

Repeat observation a large number of times
$\Rightarrow$ average estimate is equal to z_0

$$E(\hat{z}_1) = \int \hat{z}_1 \, p(\hat{z}_1 \mid z_0) d\hat{z}_1 \quad = \quad z_0$$



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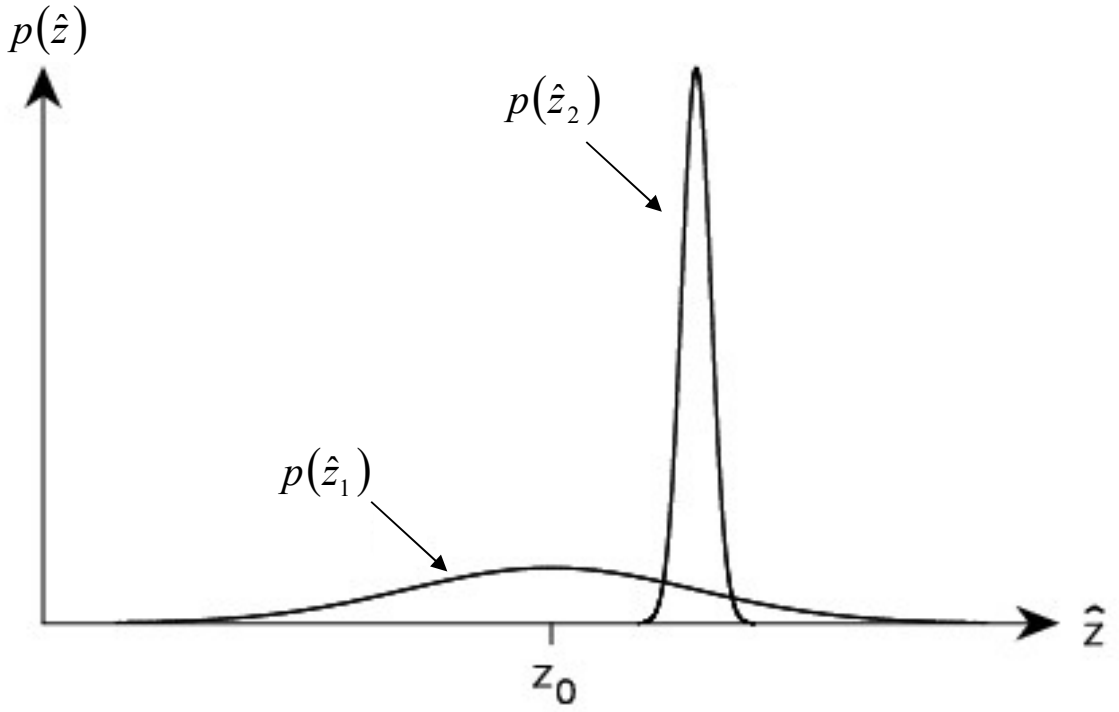

BUT $\mathrm{var}[\hat{z}_1]$ **is large**

Example: measuring the wavelength of a spectral line

True wavelength = z_0 (fixed but unknown parameter)

Compute sampling distribution for $\hat{z}_1$ *and* $\hat{z}_2$ *, modelling errors*

2. High dispersion spectrometer

   but faulty physicist!
   (e.g. wrong calibration)

   Biased:

$$E(\hat{z}_2) = \int \hat{z}_2 \, p(\hat{z}_2 \mid z_0) d\hat{z}_2 \quad \neq \quad z_0$$

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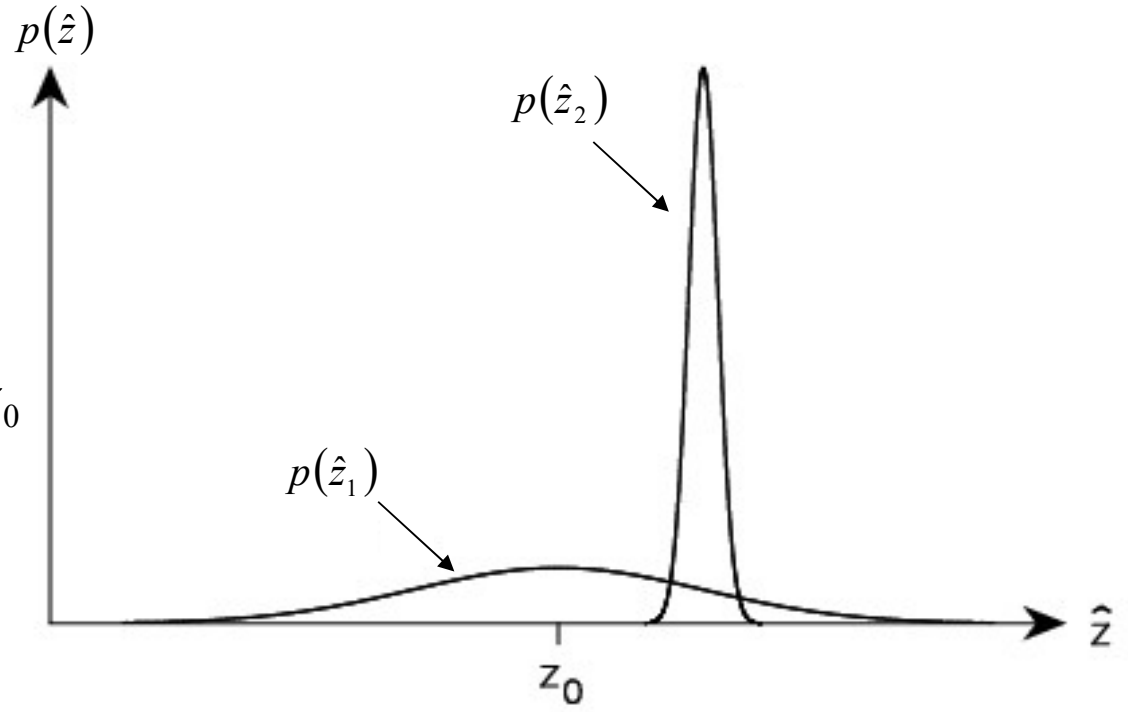

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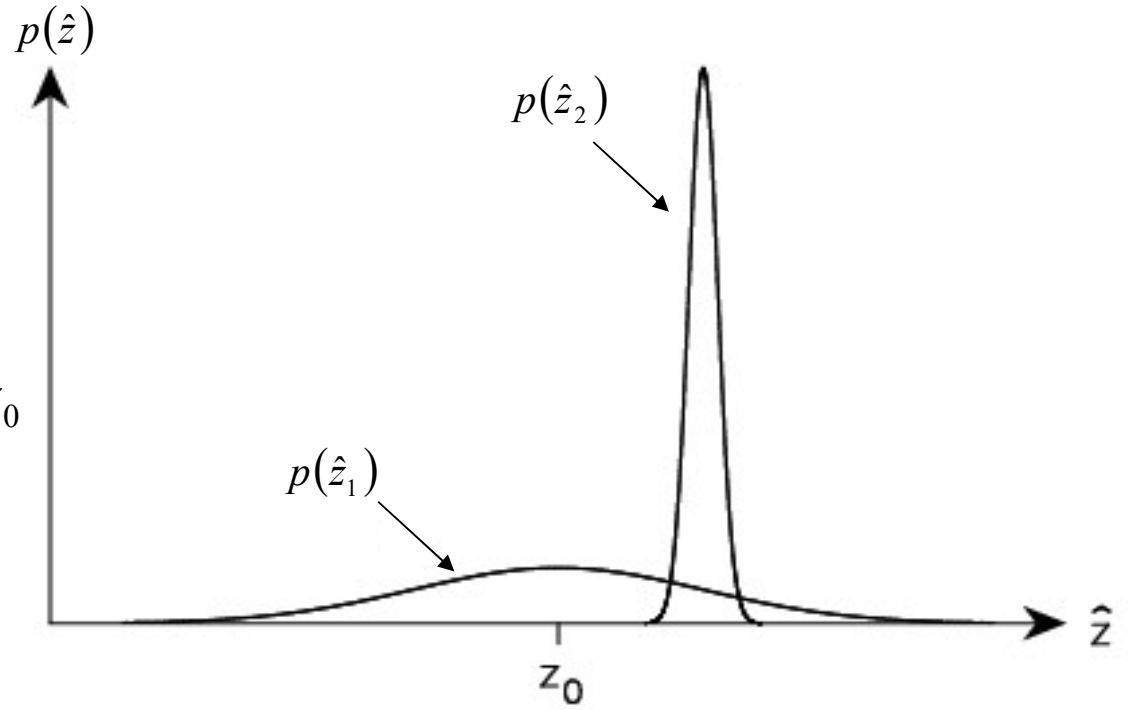

Better choice of estimator (if we can correct bias)

The Sample Mean

$\{x_1, \ldots, x_M\}$ = random sample from pdf $p(x)$ with mean μ and variance σ^2

$$\hat{\mu} = \frac{1}{M}\sum_{i=1}^{M} x_i$$ = **sample mean**

Can show that $\boxed{E(\hat{\mu}) = \mu}$ **unbiased estimator**

But bias is defined formally in terms of an infinite set of randomly chosen samples, each of size M.

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What can we say with a finite number of samples, each of finite size?

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$$\hat{\mu} = \frac{1}{M}\sum_{i=1}^{M} x_i$$ = **sample mean**

Can show that $$E(\hat{\mu}) = \mu$$ **unbiased estimator**

and $$\mathrm{var}[\hat{\mu}] = \frac{\sigma^2}{M}$$

as sample size increases, sample mean increasingly concentrated near to true mean

Linear correlation

Given sampled data $\{(x_i, y_i); i = 1, \ldots, n\}$ we can **estimate** the linear correlation between the variables as follows:

Pearson's product moment correlation coefficient

$$r = \frac{1}{n-1} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right)$$

where $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ Sample mean

$$s_x = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2}$$ Sample standard deviation

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If $p(x, y)$ is bivariate normal then r is an estimator of ρ

The bivariate normal distribution

$\mu_y + \frac{\sigma_y}{\sigma_x}\rho(x - \mu_x)$ is often referred to as the **conditional expectation** (value) of y given x, and the equation

$$y = \mu_y + \frac{\sigma_y}{\sigma_x}\rho(x - \mu_x)$$

is called the **regression line** of y on x.

Question 5: A correlation coefficient of $r = 0.8$ is calculated for a sample of paired data $\{(x, y)\}$ drawn from a bivariate normal distribution. Without being given any further information, which of the following statements can we say is correct?

A As the x values increase, the y values decrease

B The data are scattered about a line of slope 0.8

C The data are scattered about a line of unknown positive slope

D None of the above

Linear correlation

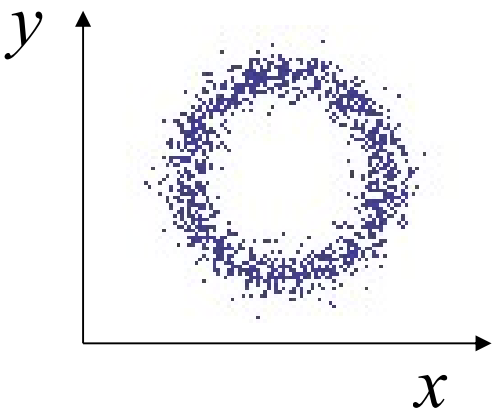
We can also rewrite the formula for r in the slightly simpler forms:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

or

$$r = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n\sum x_i^2 - \left(\sum x_i\right)^2}\sqrt{n\sum y_i^2 - \left(\sum y_i\right)^2}}$$

Question 6: Estimate r for the sample $\{(x, y)\}$ data shown in the graph below



A $r = 0$

B $r = 0.5$

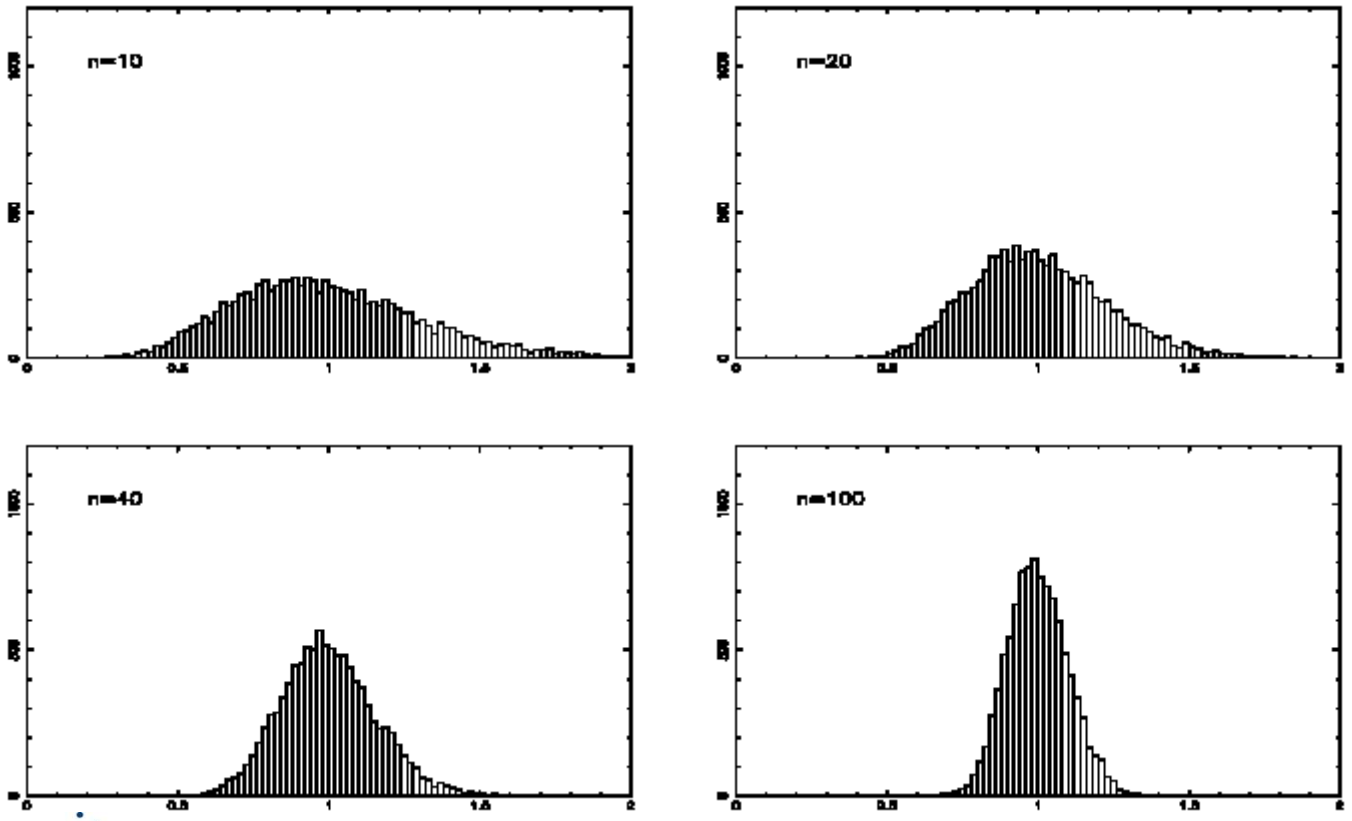
C $r = 1$

D $r = -1$

The Central Limit Theorem

For *any* pdf with finite variance σ^2, as $M \to \infty$

$\hat{\mu}$ follows a normal pdf with mean μ and variance σ^2 / M



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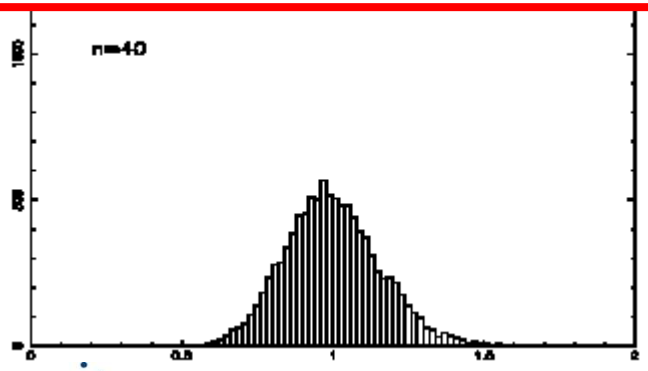
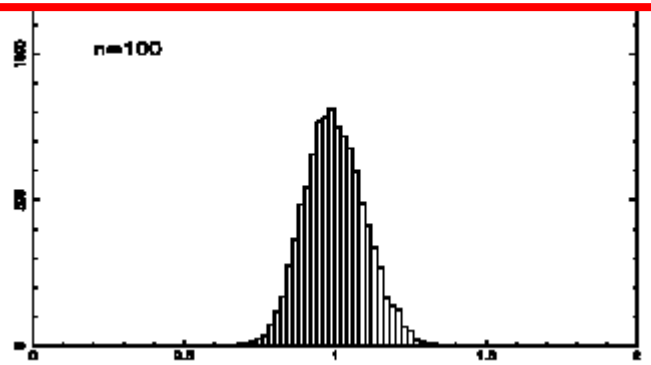
Explains importance of normal pdf in statistics.

But still based on asymptotic behaviour of an infinite ensemble of samples that we didn't actually observe!





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No 'hard and fast' rule for defining 'good' estimators. FPT invokes a number of principles – e.g. least squares, maximum likelihood

Method of Least Squares

- 'workhorse' method for fitting lines and curves to data in the physical sciences
- method often encountered (as a 'black box'?) in elementary courses
- useful demonstration of underlying statistical principles
- simple illustration of fitting straight line to (x,y) data

Ordinary Linear Least Squares

Suppose that the scatter in a plot of $\{x_i, y_i\}$ is assumed to arise from errors in only one of the two variables. This case is called **Ordinary Least Squares**. We then call x the **independent variable**, and y the **dependent variable**. Thus we suppose that we can write, for each data point:-

$$y_i = a + bx_i + \epsilon_i$$

where ϵ_i is known as the **residual** of the i^{th} data point – i.e. the difference between the observed value of y_i, and the value predicted by the best-fit straight line, characterised by parameters a and b.

Ordinary Linear Least Squares

We assume that the $\{\epsilon_i\}$ are an independently and identically distributed random sample from some underlying pdf with mean zero and variance σ^2 – i.e. the residuals are equally likely to be positive or negative and all have equal variance.

The **least squares estimators** of a and b minimise

$$S \quad = \quad \chi^2(a,b) \quad = \quad \sum_{i=1}^{n} [y_i - (a + bx_i)]^2$$

and $\hat{a}_{\rm LS}$ and $\hat{b}_{\rm LS}$ satisfy

$$\frac{\partial S}{\partial a} = 0 \quad \text{when} \quad a = \hat{a}_{\rm LS} \qquad \frac{\partial S}{\partial b} = 0 \quad \text{when} \quad b = \hat{b}_{\rm LS}$$

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Solving these equations, $\hat{a}_{\rm LS}$ and $\hat{b}_{\rm LS}$ are given by

$$\hat{a}_{\rm LS} = \frac{\sum y_i \sum x_i^2 - \sum y_i x_i \sum x_i}{n \sum x_i^2 - (\sum x_i)^2}$$

$$\hat{b}_{\rm LS} = \frac{n \sum y_i x_i - \sum y_i \sum x_i}{n \sum x_i^2 - (\sum x_i)^2}$$

where n denotes the sample size and all sums are for $i = 1, ..., n$.

We can show that $E(\hat{a}_{LS}) = a_{LS}$ i.e. LS estimators are ***unbiased***.

$$E(\hat{b}_{LS}) = b_{LS}$$

Also

$$\mathrm{var}(\hat{a}_{\mathrm{LS}}) = \frac{\sigma^2 \sum x_i^2}{n \sum x_i^2 - (\sum x_i)^2}$$

$$\mathrm{var}(\hat{b}_{\mathrm{LS}}) = \frac{\sigma^2 n}{n \sum x_i^2 - (\sum x_i)^2}$$

and

$$\mathrm{cov}(\hat{a}_{\mathrm{LS}}, \hat{b}_{\mathrm{LS}}) = \frac{-\sigma^2 \sum x_i}{n \sum x_i^2 - (\sum x_i)^2}$$

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and

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Choosing the $\{x_i\}$ so that $\sum x_i = 0$ we can make $\hat{a}_{LS}$ and $\hat{b}_{LS}$ independent.

Weighted Linear Least Squares

Suppose the i^{th} residual, $\{\epsilon_i\}$, is assumed to be drawn from some underlying pdf with mean zero and variance σ_i^2, where the variance is allowed to be different for each residual.

Define

$$S = \chi^2(a,b) = \sum_{i=1}^{n} \left[\frac{y_i - (a + bx_i)}{\sigma_i} \right]^2$$

Again we find Least Squares estimators of a and b satisfying

$$\frac{\partial S}{\partial a} = 0 \qquad \frac{\partial S}{\partial b} = 0$$

Solving, we find

$$\hat{a}_{\rm WLS} = \frac{\sum \frac{y_i}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \sum \frac{y_i x_i}{\sigma_i^2} \sum \frac{x_i}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2}$$

$$\hat{b}_{\rm WLS} = \frac{\sum \frac{1}{\sigma_i^2} \sum \frac{y_i x_i}{\sigma_i^2} - \sum \frac{y_i}{\sigma_i^2} \sum \frac{x_i}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2}$$

Also

$$\mathrm{var}(\hat{a}_{\mathrm{WLS}}) = \frac{\sum \frac{x_i^2}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2}$$

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$$\mathrm{cov}\left(\hat{a}_{\mathrm{WLS}}, \hat{b}_{\mathrm{WLS}}\right) = \frac{-\sum \frac{x_i}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2}$$

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In the case where σ_i^2 is constant, for all i, these formulae reduce to those for the unweighted case.

Extensions and Generalisations

- Errors on *both* variables?

Need to modify merit function accordingly.

$$\chi^2(a,b) = \sum_{i=1}^{N} \frac{(y_i - a - bx_i)^2}{\sigma_{y\,i}^2 + b^2\sigma_{x\,i}^2}$$

Renders equations *non-linear*; no simple analytic solution!

See e.g. Numerical Recipes 15.3

Extensions and Generalisations

- General linear models?

e.g. $$y(x) = a_1 + a_2 x + a_3 x^2 + \cdots + a_M x^{M-1}$$

We have $$\chi^2 = \sum_{i=1}^{N} \left[\frac{y_i - \sum_{k=1}^{M} a_k X_k(x_i)}{\sigma_i} \right]^2$$

Can formulate as a matrix equation and solve for parameters

See e.g. Numerical Recipes 15.4

Define $\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix}$

Vector of model parameters

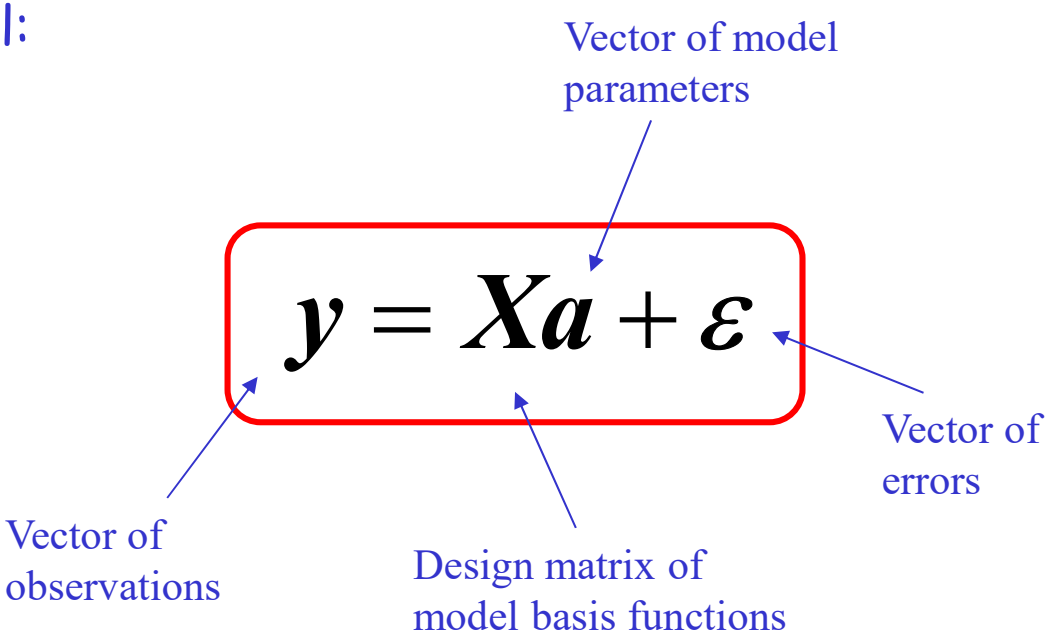
$\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$

Vector of observations

$$\boldsymbol{X} = \begin{bmatrix} X_1(x_1) \cdots X_1(x_M) \\ \vdots \qquad\qquad \vdots \\ X_N(x_1) \cdots X_N(x_M) \end{bmatrix}$$

Matrix of model basis functions

Model:



$$\varepsilon = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_N \end{bmatrix}$$

where we assume ε_i is drawn from some pdf with mean zero and variance σ^2

Weighting by errors

Define $\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix}$

Vector of model parameters

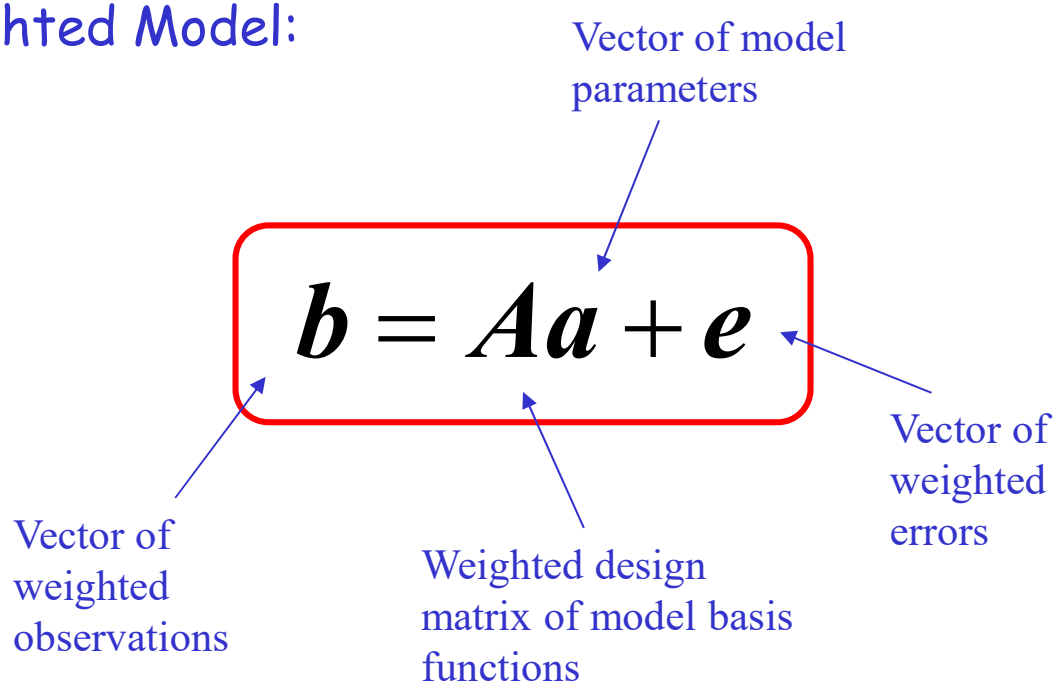
$\boldsymbol{b} = \begin{bmatrix} y_1/\sigma_1 \\ \vdots \\ y_N/\sigma_N \end{bmatrix}$

Vector of weighted observations

$$\boldsymbol{A} = \begin{bmatrix} \frac{X_1(x_1)}{\sigma_1} & \cdots & \frac{X_1(x_M)}{\sigma_1} \\ \vdots & & \vdots \\ \frac{X_N(x_1)}{\sigma_N} & \cdots & \frac{X_N(x_M)}{\sigma_N} \end{bmatrix}$$

Design matrix

Weighted Model:



$$\boldsymbol{e} = \begin{bmatrix} \varepsilon_1 / \sigma_1 \\ \vdots \\ \varepsilon_N / \sigma_N \end{bmatrix}$$

where we assume ε_i is drawn from some pdf with mean zero and variance σ_i^2

We solve for the parameter vector $\hat{\boldsymbol{a}}_{LS}$ that minimises

$$S = \boldsymbol{e}^T \cdot \boldsymbol{e} = \sum_{i=1}^{n} e_i^{\,2}$$

This has solution

$$\hat{\boldsymbol{a}}_{LS} = \left(\boldsymbol{A}^T \boldsymbol{A}\right)^{-1} \boldsymbol{A}^T \cdot \boldsymbol{b}$$

$M \times M$ *matrix*

and

$$\mathrm{cov}\left(\hat{\boldsymbol{a}}_{LS}\right) = \left(\boldsymbol{A}^T \boldsymbol{A}\right)^{-1}$$

Inverting $\left(A^T A\right)$ can be hazardous, particularly if A is a ***sparse*** matrix and/or close to singular.

Some inversion methods will break down, since they may give a formal solution, but are highly unstable to round-off error in the data.

Remedy: solution via Singular Value Decomposition.

From linear algebra theory:

> Any $N \times M$ matrix can be decomposed as the product of an $N \times M$ column-orthogonal matrix $\mathbf{U}$, an $M \times M$ diagonal matrix $\mathbf{W}$ with positive or zero elements (the *singular* values) and the transpose of an $M \times M$ orthogonal matrix $\mathbf{V}$

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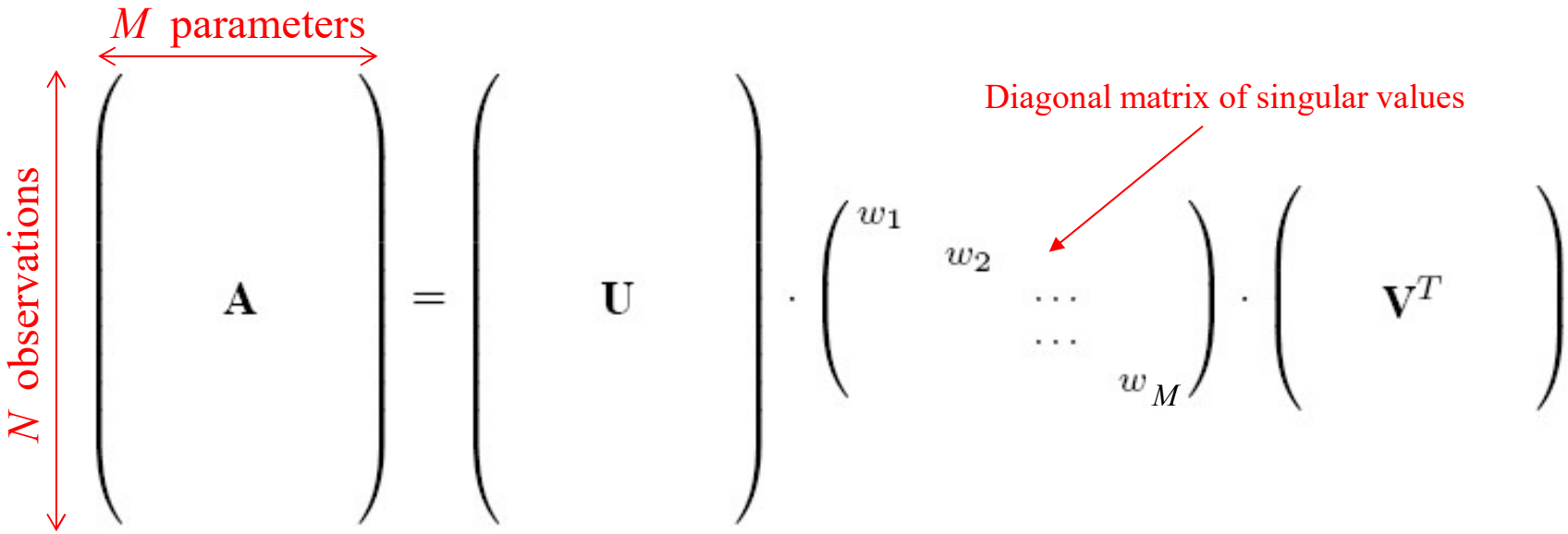

$$\sum_{i=1}^{N} U_{ik} U_{in} = \delta_{kn} \qquad \begin{matrix} 1 \le k \le M \\ 1 \le n \le M \end{matrix}$$

$$\sum_{j=1}^{M} V_{jk} V_{jn} = \delta_{kn} \qquad \begin{matrix} 1 \le k \le M \\ 1 \le n \le M \end{matrix}$$

Let the vectors $\mathbf{U}_{(i)}\ i = 1, \ldots, M$ denote the columns of $\mathbf{U}$ (each one is a vector of length N)

Let the vectors $\mathbf{V}_{(i)}; i = 1, \ldots, M$ denote the columns of $\mathbf{V}$ (each one is a vector of length M)

It can be shown that the solution to the general linear model satisfies

$$\hat{\boldsymbol{a}}_{\boldsymbol{LS}} = \sum_{i=1}^{M} \left(\frac{\mathbf{U}_{(i)} \cdot \mathbf{b}}{w_i} \right) \mathbf{V}_{(i)}$$

$$\hat{\boldsymbol{a}}_{\boldsymbol{LS}} = \sum_{i=1}^{M} \left(\frac{\mathbf{U}_{(i)} \cdot \mathbf{b}}{w_i} \right) \mathbf{V}_{(i)}$$

Very small values of w_i will amplify any round-off errors in $\mathbf{b}$

Solution:

For these very small singular values, set $\frac{1}{w_i} = 0$.

This suppresses their noisy contribution to the least-squares solution for the parameters $\hat{\boldsymbol{a}}_{\boldsymbol{LS}}$.

SVD acts as a noise filter – see also Section 7

Extensions and Generalisations

- Non-linear models? $y_i^{\rm model} \equiv y^{\rm model}(x_i; \theta_1, ..., \theta_k)$

Model parameters

Suppose $y_i^{\rm obs} = y_i^{\rm model} + \epsilon_i$

ε_i drawn from pdf with mean zero, variance σ_i^2

Then

$$S = \chi^2 = \sum_{i=1}^{n} \left[\frac{y_i^{\rm obs} - y_i^{\rm model}}{\sigma_i} \right]^2$$

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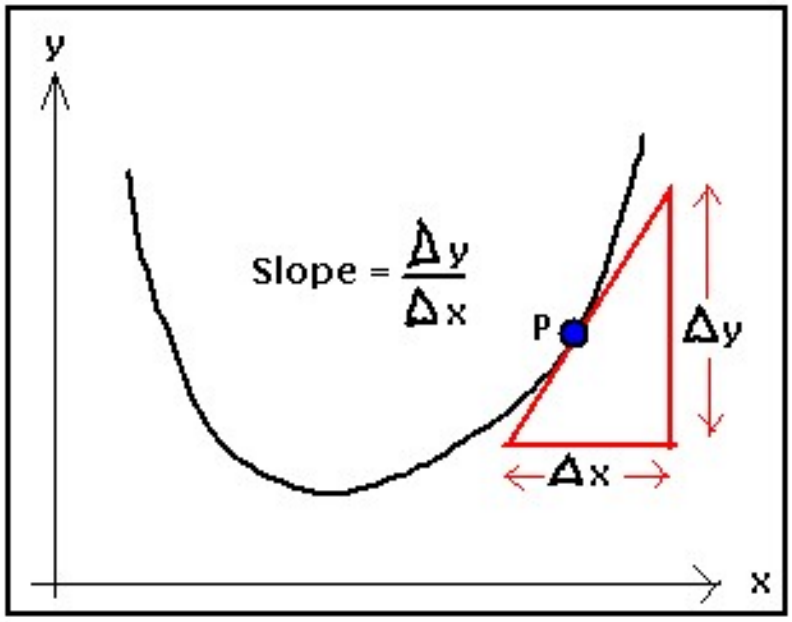
$$S = \chi^2 = \sum_{i=1}^{n} \left[\frac{y_i^{\text{obs}} - y_i^{\text{model}}}{\sigma_i} \right]^2$$

But no simple analytic method to minimise sum of squares
(e.g. no analytic solutions to $\partial S / \partial \theta_i = 0$)

Extensions and Generalisations

- Non-linear models?

Methods of solution often involve assuming *Taylor expansion* of χ^2 around minimum, and solving by gradient descent



See e.g.
Numerical Recipes 15.5
and Section 6

Extensions and Generalisations

- Correlated errors?

We need to define a **covariance matrix** $C_{ij} = \mathrm{cov}(x_i, x_j)$

$$\chi^2 = \sum_i \sum_j \left(y_i - y_i^{\mathrm{model}}\right)\left[C_{ij}\right]^{-1}\left(y_j - y_j^{\mathrm{model}}\right)$$

See e.g. Gregory, Chapter 10

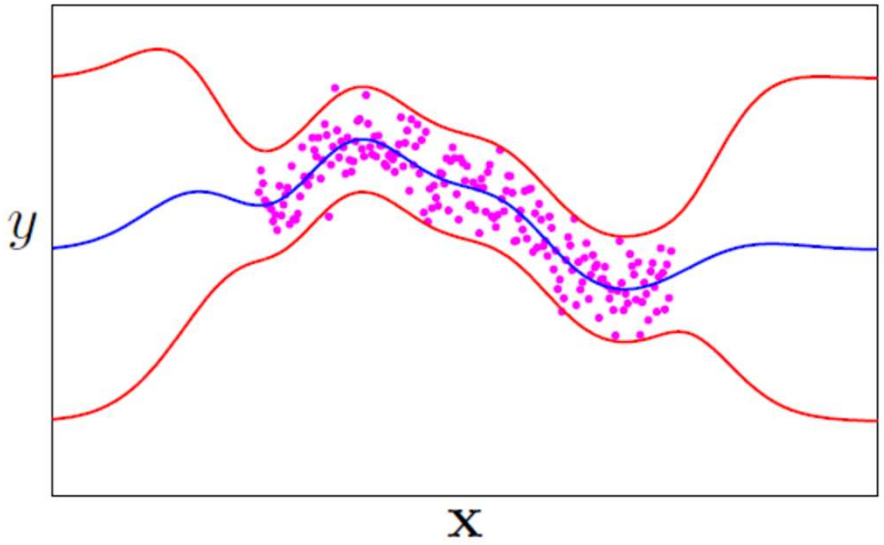
Extensions and Generalisations

[Note: not-examinable, and not included in video and audio files]

- More general non-linear approaches?

Suppose we want to derive a function $y = f(x)$ with errors from observed data $\mathcal{D}$.

We might want to use this function to interpolate or extrapolate from our data.



A **Gaussian process** (GP) defines a distribution over functions $p(f)$:

$$p(f|\mathcal{D}) = \frac{p(f)p(\mathcal{D}|f)}{p(\mathcal{D})}$$

Extensions and Generalisations

[Note: not-examinable, and not included in video and audio files]

GPs are parametrized by a **mean function** $\mu(x)$ and a kernel function $K(x, x')$

$$p(f(x), f(x')) = \mathsf{N}(\boldsymbol{\mu}, \Sigma)$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu(x) \\ \mu(x') \end{bmatrix} \quad \Sigma = \begin{bmatrix} K(x,x) & K(x,x') \\ K(x',x) & K(x',x') \end{bmatrix}$$

We can learn about these functions from the data themselves → strong connections to **machine learning** and **neural networks**

Extensions and Generalisations

[Note: not-examinable, and not included in video and audio files]

Vast, and rapidly growing, literature on GPs across the physical sciences.

Beyond the scope of ADA Course but very interesting!

See e.g. Sivia Chapter 6
for some introductory
ideas, or some nice
recent articles / lecture notes:

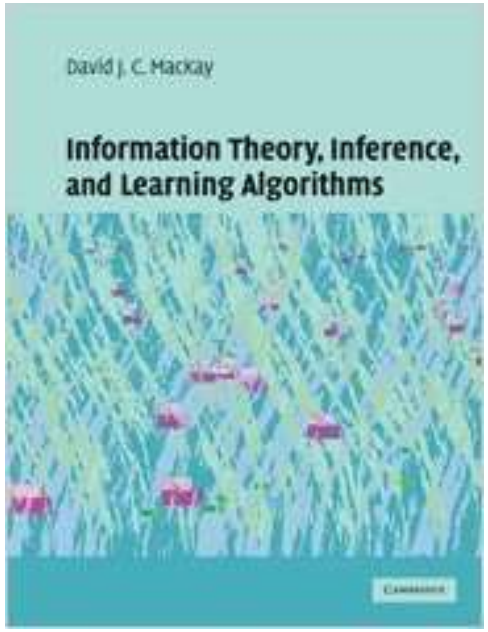
https://arxiv.org/pdf/1505.02965v2.pdf

http://www.cs.toronto.edu/~hinton/csc2515/notes/gp_slides_fall08.pdf

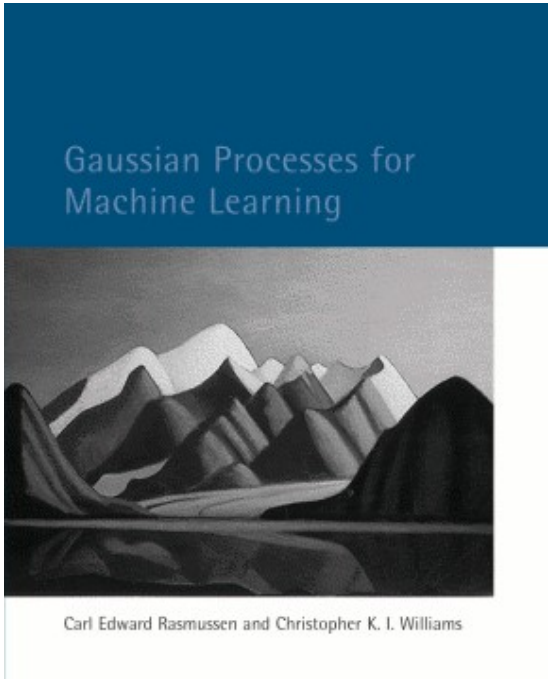
Extensions and Generalisations

[Note: not-examinable, and not included in video and audio files]

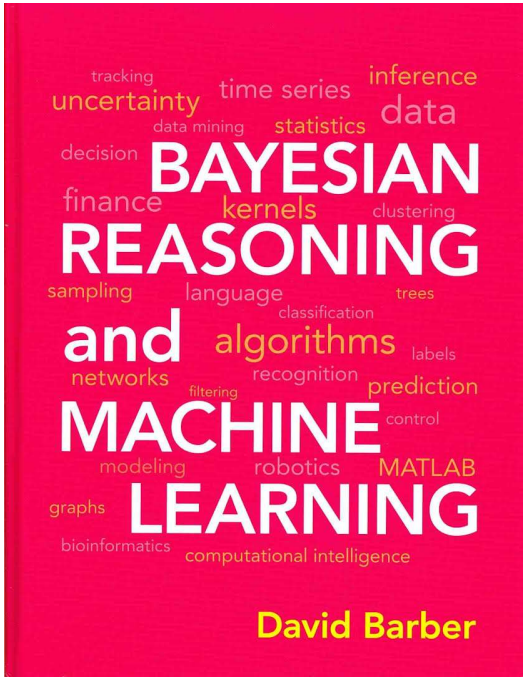
Some really excellent books available (all free, downloadable!)



http://www.inference.phy.cam.ac.uk/itprnn/book.pdf



http://www.gaussianprocess.org/gpml/



http://web4.cs.ucl.ac.uk/staff/D.Barber/textbook/090310.pdf