COEN281 -- Introduction to Pattern Recognition and Data Mining

Lecture 4: Parameter Estimation

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Syllabus

Week 1	Introduction; R (Ch.1)
Week 2	Bayesian Decision Theory (Ch.2; DHS: 2.1-2.6, 2.9) **Parameter Estimation** (DHS: 3.1-3.4)
Week 3	Linear Discriminant Functions (Ch.3&4; DHS: 3.8.2, 5.1-5.8) Regularization (Ch.6; SE: Ch.3)
Week 4	Neural Networks (DHS: 6.1-6.6, 6.8); Deep Learning
Week 5	Support Vector Machines (Ch.9)
Week 6	Decision Trees (Ch. 8.1; DHS: 8.3; Ch 2 SE)
Week 7	Ensemble Methods (Ch. 8.2; SE: Ch 4, 5)
Week 8	Clustering (Ch. 10; DHS: 10.6, 10.7) Clustering (DHS: 10.9); How many clusters are there? (DHS: 10.10)
Week 9	Non-metric: Association Rules Collaborative Filtering
Week 10	Text Retrieval; Other topics

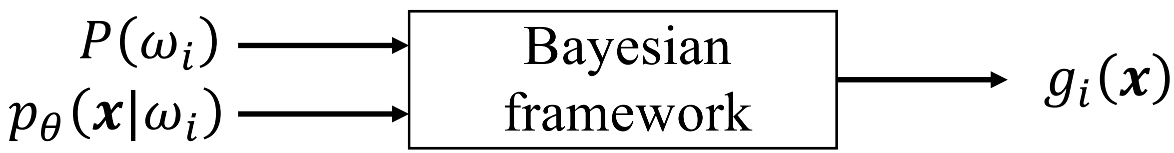
Overview

- Introduction
  - Statistical inference
  - Estimator's bias and variance
- Maximum Likelihood (ML) estimation
  - Binomial distribution
  - Normal distribution
  - Simple linear regression
- *Bayesian estimation*

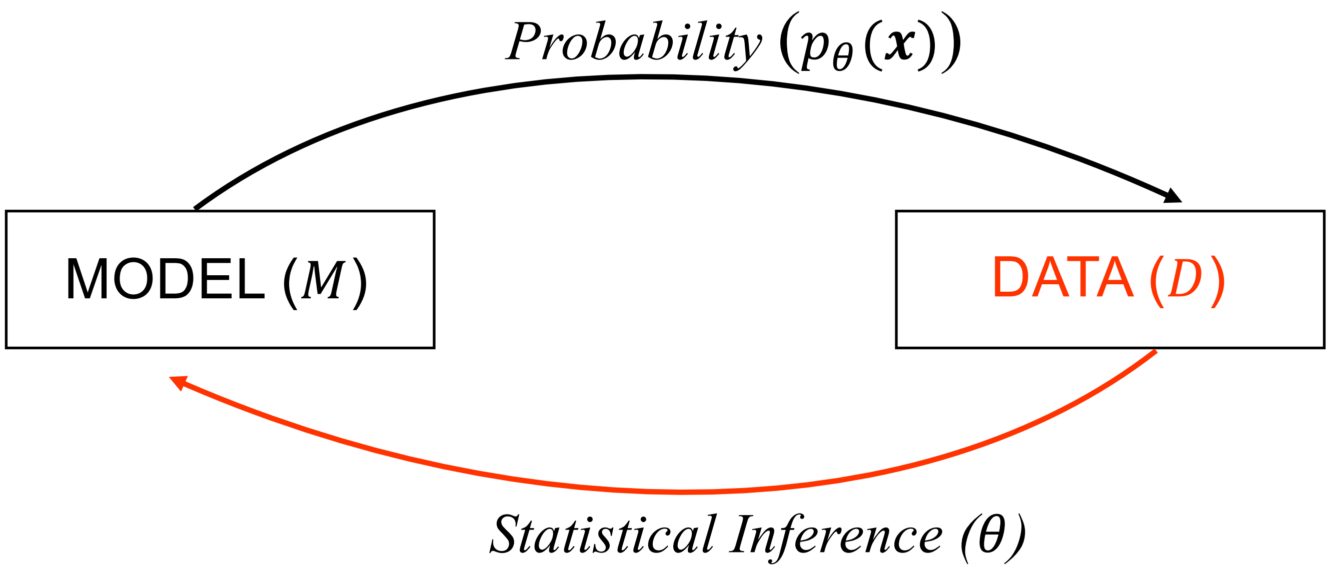
Introduction

Statistical Inference

- Bayesian classifier



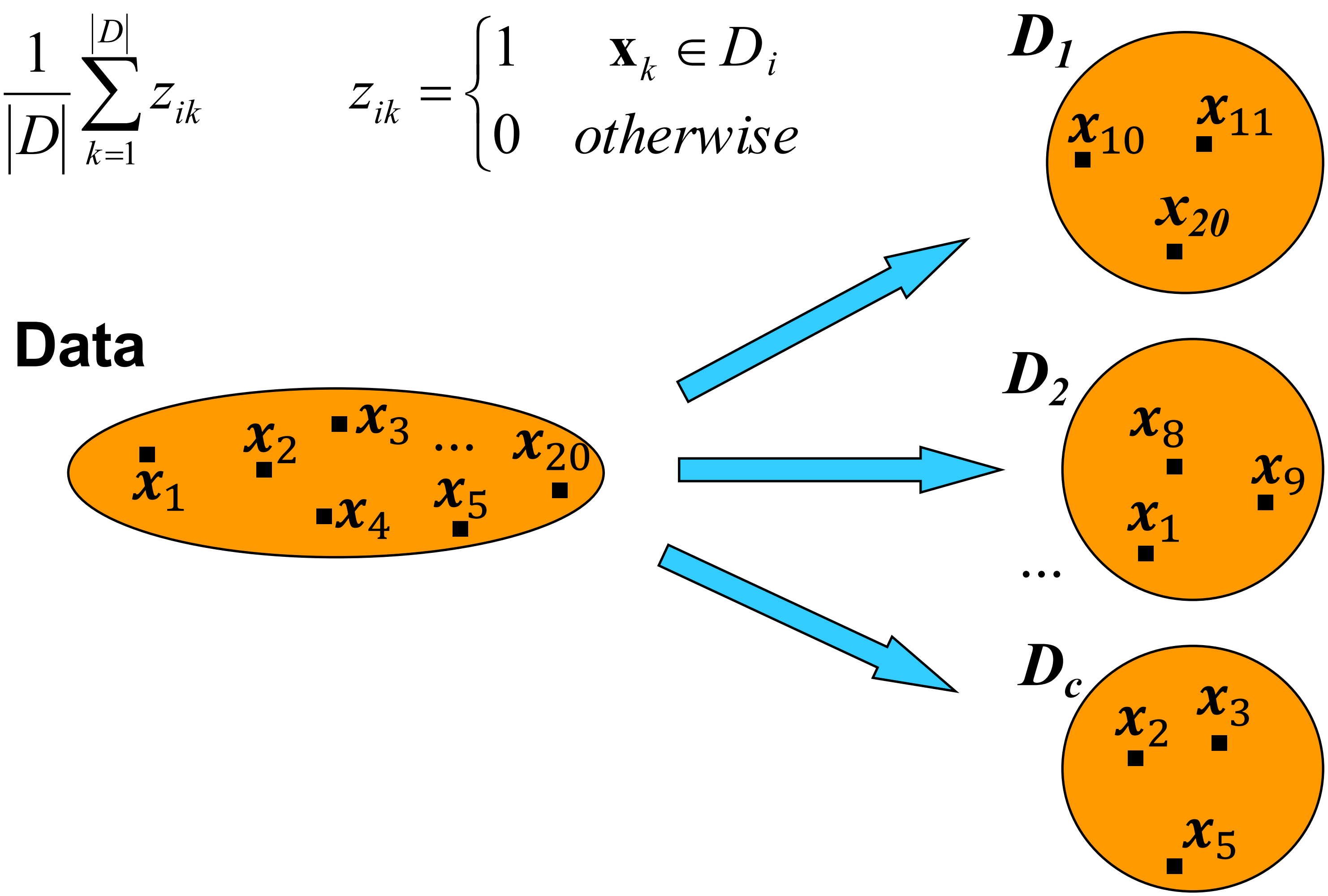
- Dual role of probability and statistical inference



Introduction
Statistical Inference (2)

- Estimation of priors is simple

$$\hat{P}(\omega_i) = \frac{1}{|D|}\sum_{k=1}^{|D|} z_{ik} \qquad z_{ik} = \begin{cases} 1 & \mathbf{x}_k \in D_i \\ 0 & otherwise \end{cases}$$



Introduction
Statistical Inference (3)

- Suppose D contains n samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$
  - Assume C separate problems
- Premise 1 – *i.i.d.*
  - Samples have been drawn at random according to $p_\theta(\boldsymbol{x})$ – the model
  - Samples are independent
- Premise 2 – known parametric form
  - $p_\theta(\boldsymbol{x})$ is determined uniquely by a parameter vector θ

∓sometimes we write $p_\theta(\boldsymbol{x})$ as $p(\boldsymbol{x}|\theta, M)$

Introduction
Statistical Inference (4)

- Probability of observed data arising under an implicitly assumed model M

$$p(D \mid \theta, M) = \prod_{i=1}^{n} p(\mathbf{x}_i \mid \theta, M)$$

  - θ are the parameters of the model
  - when regarded as a function of θ, it is called the likelihood $L(\theta \mid D)$

- We use $p(D \mid \theta, M)$ to decide how realistic the assumed model is
  - Reject/change model if the likelihood is low

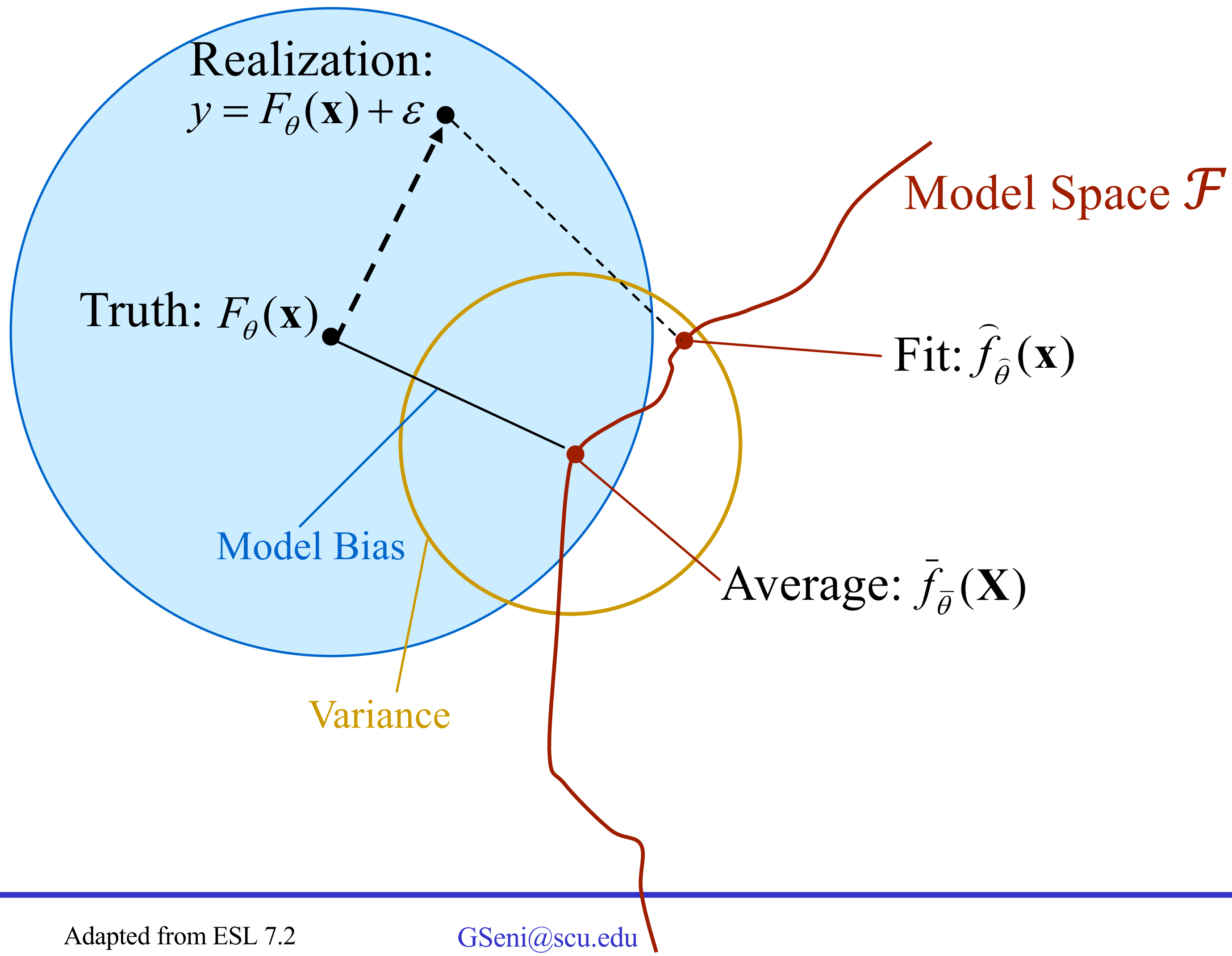
Introduction
Statistical Inference (5)

- Let $\widehat{\theta}$ be an estimator of a θ
  - $\widehat{\theta}$ is a random variable, with different values arising as different samples are drawn (e.g., by repeatedly subsampling original data set)

- Measures of quality
  - $Bias(\widehat{\theta}) = \varepsilon(\widehat{\theta}) - \theta$:
    - reflects any systematic error in our prediction
  - $Var(\widehat{\theta}) = \varepsilon(\widehat{\theta} - \varepsilon(\widehat{\theta}))^2$:
    - measures how much our estimates will vary across different data sets (sensitivity to particular training data set)

Introduction
Statistical Inference (6)

- Bias-Variance schematic:



Maximum-Likelihood Estimate θ_{ML}

- $\hat{\theta}$ that maximizes $L(\theta|D)$
  - value of θ that best agrees with or supports the observed training samples
- Often more convenient to work in log domain $l(\theta|D)$
- Assuming a well-behaved, differentiable function

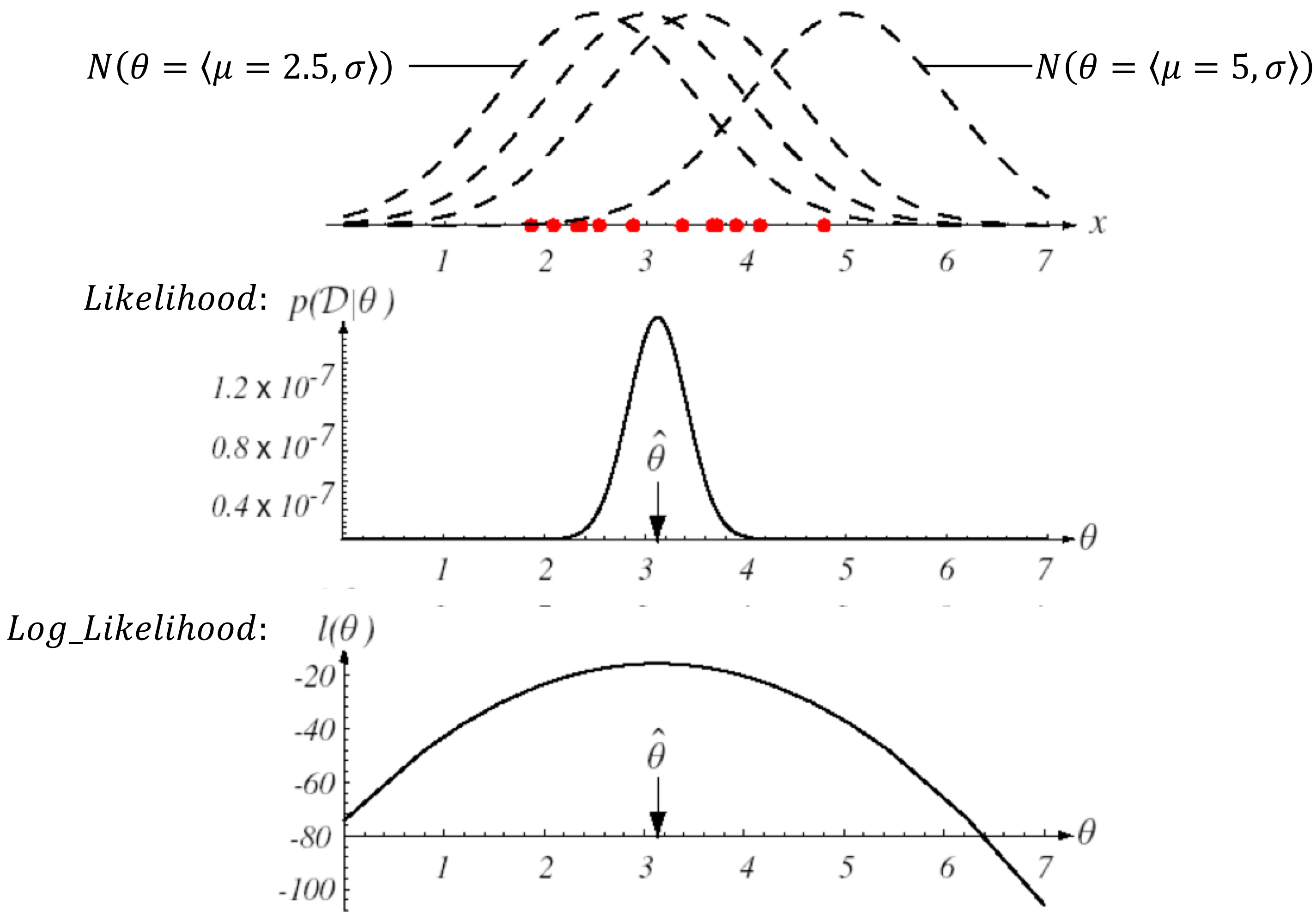
$$\boxed{\hat{\theta} = \arg\max_{\theta} l(\theta | D)} \qquad l(\theta) = \sum_{i=1}^{n} \ln p(x_i | \theta)$$

Solve $\boxed{\nabla_{\theta} l = 0}$

$$\nabla_{\theta} l = \sum_{i=1}^{n} \nabla_{\theta} \ln p(x_i | \theta)$$

Maximum-Likelihood Estimate
Example

- Assumed model: $p(\boldsymbol{x}|\theta) \sim N(\theta = \langle \mu, \sigma \rangle)$ – i.e., M is Gaussian



Maximum-Likelihood Estimate

Binomial Distribution

- Assumed model: $P(x \mid \theta) = \theta^{x}(1-\theta)^{1-x} \qquad x \in \{0,1\}$
- Scenario: customers at a supermarket either purchase or don't purchase milk; θ is the probability that milk is purchased by a random customer

$$L(\theta \mid x_1,\ldots,x_n) = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} = \theta^{r}(1-\theta)^{n-r}$$

where r is number among *n* sample customers who bought milk

$$l(\theta) = r\ln\theta + (n-r)\ln(1-\theta)$$

$$\frac{\partial}{\partial\theta} l(\theta) = \frac{r}{\theta} - \left(\frac{n-r}{1-\theta}\right) = 0 \;\Rightarrow\; \hat{\theta}_{ML} = \frac{r}{n}$$

Maximum-Likelihood Estimate
Normal Density – Unknown μ

- Consider a single point $\boldsymbol{x}_i$

$$p(x_i \mid \theta) = \frac{1}{(2\pi)^{d/2} \mid \Sigma \mid^{1/2}} e^{-\frac{1}{2}(x_i - \theta)^t \Sigma^{-1} (x_i - \theta)}$$

$$\ln p(x_i \mid \theta) = -\tfrac{1}{2} \ln[(2\pi)^d \mid \Sigma \mid] - \tfrac{1}{2}(x_i - \theta)^t \Sigma^{-1} (x_i - \theta)$$

$$\nabla_\theta \ln p(x_i \mid \theta) = \Sigma^{-1}(x_i - \theta)$$

For the full log-likelihood:

$$\nabla_\theta l = \sum_{i=1}^{n} \Sigma^{-1}(x_i - \theta) = 0$$

$$\boxed{\hat{\mu}_{ML} = \hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} x_i}$$

the sample mean!

Maximum-Likelihood Estimate

Normal Density – Unknown μ and Σ

- Univariate case $p(x_i \mid \boldsymbol{\theta}) = \dfrac{1}{\sqrt{2\pi\theta_2}} e^{-\frac{1}{2\theta_2}(x_i-\theta_1)^2}$

$$\ln p(x_i \mid \boldsymbol{\theta}) = -\tfrac{1}{2}\ln 2\pi\theta_2 - \tfrac{1}{2\theta_2}(x_i-\theta_1)^2$$

$$\nabla_{\boldsymbol{\theta}} \ln p(x_i \mid \boldsymbol{\theta}) = \begin{bmatrix} \frac{1}{\theta_2}(x_i-\theta_1) \\ -\frac{1}{2\theta_2} + \frac{(x_i-\theta_1)^2}{2\theta_2^2} \end{bmatrix}$$

For the full log-likelihood:

$$\frac{\partial l}{\partial \theta_1} = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} \frac{1}{\theta_2}(x_i-\theta_1) = 0 \quad \Rightarrow \quad \hat{\theta}_1 = \hat{\mu}_{ML}$$

$$\frac{\partial l}{\partial \theta_2} = 0 \quad \Rightarrow \quad -\sum_{\mathrm{i}=1}^{\mathrm{n}} \frac{1}{\theta_2} + \sum_{i=1}^{n} \frac{(x_i-\theta_1)^2}{\theta_2^2} = 0 \quad \Rightarrow \quad \boxed{\hat{\theta}_2 = \hat{\sigma}^2_{ML} = \frac{1}{n}\sum_{i=1}^{n}(x_i-\hat{\theta}_1)^2}$$

Maximum-Likelihood Estimate

Normal Density – Unknown μ and Σ (2)

- Multivariate case…

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})(x_i - \hat{\mu})^t$$

- $\hat{\mu}_{ML}$ is unbiased

$$\mathcal{E}(\hat{\mu}) = \mathcal{E}\left[\frac{1}{n}(x_1 + x_2 + \ldots + x_n)\right] = \frac{1}{n}\mathcal{E}(x_1 + x_2 + \ldots + x_n)$$

$$= \frac{1}{n}(\mathcal{E}(x_1) + \mathcal{E}(x_2) + \ldots + \mathcal{E}(x_n)) = \frac{1}{n}(\mu + \mu + \ldots + \mu)$$

$$= \mu$$

Maximum-Likelihood Estimate

Normal Density – Unknown μ and Σ (3)

- $\hat{\sigma}_{ML}$ is biased

$$\mathcal{E}(\hat{\sigma}) = \mathcal{E}\left[\frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2\right]$$

$$= \mathcal{E}\left[\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2\right] - \mathcal{E}\left[\frac{1}{n}\sum_{i=1}^{n}(\hat{\mu} - \mu)^2\right]$$

$$= \sigma^2 - \frac{\sigma^2}{n} = \frac{n-1}{n}\sigma^2 \neq \sigma^2$$

$\Rightarrow$ but asymptotically unbiased!

Maximum-Likelihood Estimate

Normal Density – Example

- Consider the following data sets:

$$D_1 = \{\langle 3,4\rangle, \langle 4,6\rangle, \langle 2,6\rangle, \langle 3,8\rangle\} \qquad D_2 = \{\langle 3,0\rangle, \langle 1,-2\rangle, \langle 5,-2\rangle, \langle 3,-4\rangle\}$$

- Compute ML estimates for μ_1, μ_2 and Σ_1, Σ_2:

$$\hat{\boldsymbol{\mu}}_1 = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i = \frac{1}{4}\begin{pmatrix} 3+4+2+3 \\ 4+6+6+8 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \end{pmatrix} \qquad \hat{\boldsymbol{\mu}}_2 = \frac{1}{4}\begin{pmatrix} 3+1+5+3 \\ 0-2-2-4 \end{pmatrix} = \begin{pmatrix} 3 \\ -2 \end{pmatrix}$$

$$\hat{\boldsymbol{\Sigma}}_1 = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^t = \frac{1}{4}\left[\begin{pmatrix} 3-3 \\ 4-6 \end{pmatrix}\begin{pmatrix} 3-3 & 4-6 \end{pmatrix} + \begin{pmatrix} 4-3 \\ 6-6 \end{pmatrix}\begin{pmatrix} 4-3 & 6-6 \end{pmatrix}\right.$$

$$\left. + \begin{pmatrix} 2-3 \\ 6-6 \end{pmatrix}\begin{pmatrix} 2-3 & 6-6 \end{pmatrix} + \begin{pmatrix} 3-3 \\ 8-6 \end{pmatrix}\begin{pmatrix} 3-3 & 8-6 \end{pmatrix}\right]$$

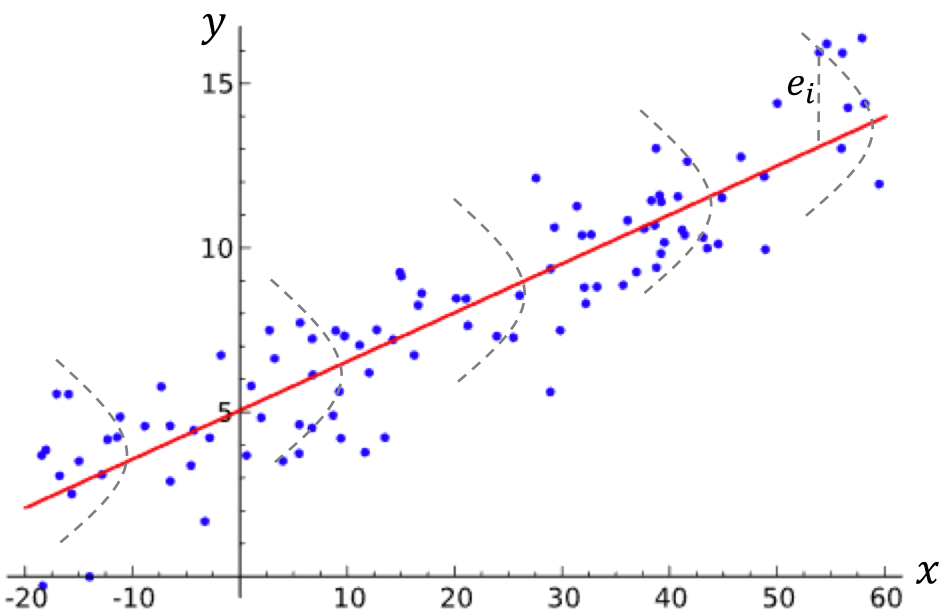
$$= \frac{1}{4}\left[\begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 4 \end{pmatrix}\right] = \begin{bmatrix} 1/2 & 0 \\ 0 & 2 \end{bmatrix}$$

$$\widehat{\Sigma}_2 = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

Maximum-Likelihood Estimate

Simple Linear Regression

- Assumed model: $Y = a + bX + e$
- Data: $\{\langle x_1, y_1\rangle, \langle x_2, y_2\rangle, \ldots, \langle x_n, y_n\rangle\}$



- e error term; random variable assumed to be $\sim N(\theta = \langle 0, \sigma\rangle)$; we can write $e = Y - (a + bX)$

Maximum-Likelihood Estimate

Simple Linear Regression (2)

- Distribution of error term:

$$p(e_i \mid \theta) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y_i - (a + bx_i)}{\sigma}\right)^2}$$

- Likelihood

$$L(a, b | D, \theta) = \prod_{i=1}^{n} p(e_i \mid \theta) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - (a + bx_i))^2}$$

Maximum-Likelihood Estimate

Simple Linear Regression (3)

- Log-likelihood:

$$l(a,b\,|\,\theta) = -\frac{n}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\underbrace{\sum_{i=1}^{n}(y_i-(a+bx_i))^2}$$

- To maximize *l(a,b|D)* we need to minimize the sum of squared differences

  ⇒ Least Squares (LS) Method!

- LS method arises naturally from the choice of a Normal distribution for the error term in the model

Bayesian Estimation
Overview

- *Frequentist* view of probability:
  - Probability is an objective property of the outside world
  - Probability of an event as a "limiting proportion"
    - Tossing a coin
    - Customer buying milk
    - Not one-off events
  - Intrinsic variability lies in the data D
  - θ is fixed but unknown
- Subjective (Bayesian) probability
  - Probability is an individual belief that event will occur
  - Subjective component given as a prior – initial belief event will happen

Bayesian Estimation

Overview (2)

- Subjective (Bayesian) probability
  - θ is a random variable having a distribution of possible values
  - i.e., Known prior density $p(\theta)$
    - Broad and flat if we aren't' very sure
  - Information in D leads to a modification of this distribution to a posterior density $p(\theta|D)$
    - Which, we hope, is sharply peaked about the true value of θ
  - Maximum a posteriori method (MAP)
    - Pick the mode of the distribution
    - ML estimator is MAP estimator for a uniform $p(\theta)$

Bayesian Estimation
General Theory

- To obtain $p(x|D) = p(x|\omega_j, D_j)$ (to build our classifier)

- Compute $\boxed{p(x \mid D) = \int p(x|\theta)\, p(\theta \mid D)\, d\theta}$

where form of $p(x|\theta)$ is assumed known (as before)

and $p(\theta|D) \propto \underbrace{p(D|\theta)}_{\text{likelihood}} \times \underbrace{p(\theta)}_{\text{parameter prior}}$

Bayesian Estimation

Normal Density – Unknown μ

- Assumed model: $p(x|\theta) \sim N(\theta_\mu, \sigma^2)$
- Assumed prior: $p(\theta_\mu) \sim N(\mu_0, \sigma_0^2)$

$$\Rightarrow \quad p(\theta_\mu|D) = \alpha \prod_{i=1}^{n} p(x_i \mid \theta_\mu) p(\theta_\mu)$$

- Easily shown that $p(\theta_\mu|D) \sim N(\mu_n, \sigma_n^2)$ where

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \hat{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0 \quad ; \text{ where } \hat{\mu}_n \text{ is sample mean}$$

i.e., μ_n represents our best guess for θ_μ after observing n samples

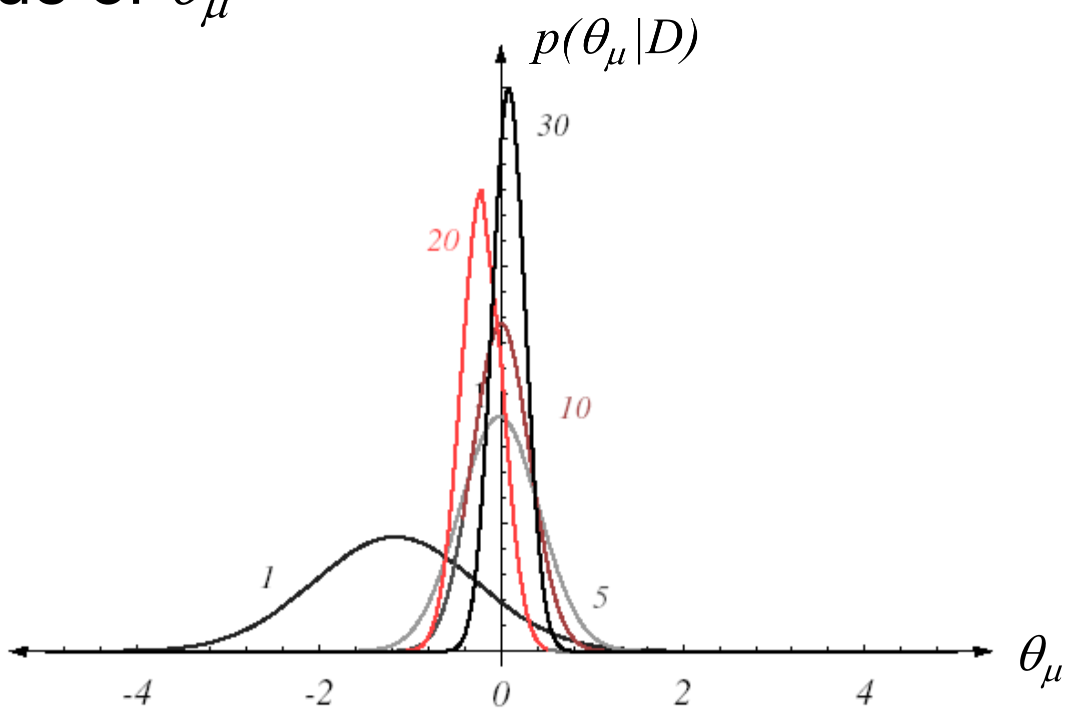
Consider $n \to \infty$, $\sigma_0 \approx 0$, and $\sigma_0 >> \sigma$

Bayesian Estimation
Normal Density – Unknown μ (2)

and

$$\sigma_n^2 = \frac{\sigma_0^2\sigma^2}{n\sigma_0^2 + \sigma^2} \qquad \Rightarrow \qquad \lim_{n\to\infty} \sigma_n^2 = \frac{\sigma^2}{2}$$

- i.e., each additional observation decreases our uncertainty about the true value of θ_μ



Bayesian Estimation
Normal Density – Unknown μ (3)

- We now can compute the class-conditional density

$$p(x \mid D) = \int p(x \mid \theta_\mu) p(\theta_\mu \mid D) d\theta_\mu$$
$$= \int N(\theta_\mu, \sigma^2) N(\mu_n, \sigma_n^2) d\theta_\mu$$
$$\sim N(\mu_n, \sigma^2 + \sigma_n^2)$$

- i.e., in $p(x|\theta) \sim N(\theta_\mu, \sigma^2)$ we set $\theta_\mu = \mu_n$ and replace σ^2 with $\sigma^2 + \sigma_n^2$
  - Treat $\mu_n = \alpha \cdot \hat{\mu}_n + \beta \cdot \mu_0$ as if it were the true mean
  - Increase the known variance σ^2 to account for the additional uncertainty resulting from our lack of exact knowledge of the mean

Parameter Estimation

When ML and Bayesian Methods Differ?

- Equivalent in the asymptotic limit of infinite training data or with a "flat" or uniform prior
- Computational complexity
  - ML uses Differential Calculus or gradient search for $\hat{\theta}$
  - B requires complex multidimensional integration
- Interpretability
  - ML returns a single best model/parameter
  - B gives a weighted average
- Confidence in prior information
  - ML solution is of assumed parametric form… not necessarily so in B approach