

Parametric Models

Part I: Maximum Likelihood and Bayesian Density Estimation

Selim Aksoy

Department of Computer Engineering
Bilkent University
saksoy@cs.bilkent.edu.tr

CS 551, Fall 2012



Introduction

- ▶ Bayesian Decision Theory shows us how to design an optimal classifier if we know the prior probabilities $P(w_i)$ and the class-conditional densities $p(\mathbf{x}|w_i)$.
- ▶ Unfortunately, we rarely have complete knowledge of the probabilistic structure.
- ▶ However, we can often find design samples or *training data* that include particular representatives of the patterns we want to classify.



Introduction

- ▶ To simplify the problem, we can assume some parametric form for the conditional densities and estimate these parameters using training data.
- ▶ Then, we can use the resulting estimates as if they were the true values and perform classification using the Bayesian decision rule.
- ▶ We will consider only the supervised learning case where the true class label for each sample is known.



Introduction

- ▶ We will study two estimation procedures:
 - ▶ *Maximum likelihood estimation*
 - ▶ Views the parameters as quantities whose values are fixed but unknown.
 - ▶ Estimates these values by maximizing the probability of obtaining the samples observed.
 - ▶ *Bayesian estimation*
 - ▶ Views the parameters as random variables having some known prior distribution.
 - ▶ Observing new samples converts the prior to a posterior density.



Maximum Likelihood Estimation

- ▶ Suppose we have a set $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ of independent and identically distributed (*i.i.d.*) samples drawn from the density $p(\mathbf{x}|\boldsymbol{\theta})$.
- ▶ We would like to use training samples in \mathcal{D} to estimate the unknown parameter vector $\boldsymbol{\theta}$.
- ▶ Define $L(\boldsymbol{\theta}|\mathcal{D})$ as the *likelihood function* of $\boldsymbol{\theta}$ with respect to \mathcal{D} as

$$L(\boldsymbol{\theta}|\mathcal{D}) = p(\mathcal{D}|\boldsymbol{\theta}) = p(\mathbf{x}_1, \dots, \mathbf{x}_n|\boldsymbol{\theta}) = \prod_{i=1}^n p(\mathbf{x}_i|\boldsymbol{\theta}).$$



Maximum Likelihood Estimation

- ▶ The *maximum likelihood estimate* (MLE) of θ is, by definition, the value $\hat{\theta}$ that maximizes $L(\theta|\mathcal{D})$ and can be computed as

$$\hat{\theta} = \arg \max_{\theta} L(\theta|\mathcal{D}).$$

- ▶ It is often easier to work with the logarithm of the likelihood function (*log-likelihood function*) that gives

$$\hat{\theta} = \arg \max_{\theta} \log L(\theta|\mathcal{D}) = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta).$$



Maximum Likelihood Estimation

- ▶ If the number of parameters is p , i.e., $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)^T$, define the gradient operator

$$\nabla_{\boldsymbol{\theta}} \equiv \begin{bmatrix} \frac{\partial}{\partial \theta_1} \\ \vdots \\ \frac{\partial}{\partial \theta_p} \end{bmatrix}.$$

- ▶ Then, the MLE of $\boldsymbol{\theta}$ should satisfy the necessary conditions

$$\nabla_{\boldsymbol{\theta}} \log L(\boldsymbol{\theta}|\mathcal{D}) = \sum_{i=1}^n \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}_i|\boldsymbol{\theta}) = 0.$$



Maximum Likelihood Estimation

- ▶ Properties of MLEs:
 - ▶ The MLE is the parameter point for which the observed sample is the most likely.
 - ▶ The procedure with partial derivatives may result in several local extrema. We should check each solution individually to identify the global optimum.
 - ▶ Boundary conditions must also be checked separately for extrema.
 - ▶ Invariance property: if $\hat{\theta}$ is the MLE of θ , then for any function $f(\theta)$, the MLE of $f(\theta)$ is $f(\hat{\theta})$.



The Gaussian Case

- ▶ Suppose that $p(\mathbf{x}|\boldsymbol{\theta}) = N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
 - ▶ When $\boldsymbol{\Sigma}$ is known but $\boldsymbol{\mu}$ is unknown:

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

- ▶ When both $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are unknown:

$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \quad \text{and} \quad \hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T$$



The Bernoulli Case

- ▶ Suppose that $P(x|\theta) = \text{Bernoulli}(\theta) = \theta^x(1 - \theta)^{1-x}$ where $x = 0, 1$ and $0 \leq \theta \leq 1$.
- ▶ The MLE of θ can be computed as

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^n x_i.$$



Bias of Estimators

- ▶ *Bias* of an estimator $\hat{\theta}$ is the difference between the expected value of $\hat{\theta}$ and θ .
- ▶ The MLE of μ is an unbiased estimator for μ because $E[\hat{\mu}] = \mu$.
- ▶ The MLE of Σ is not an unbiased estimator for Σ because $E[\hat{\Sigma}] = \frac{n-1}{n}\Sigma \neq \Sigma$.
- ▶ The *sample covariance*

$$S^2 = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \hat{\mu})(\mathbf{x}_i - \hat{\mu})^T$$

is an unbiased estimator for Σ .

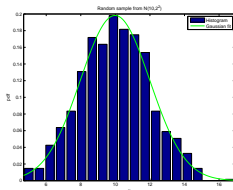


Goodness-of-fit

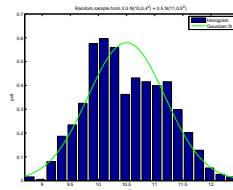
- ▶ To measure how well a fitted distribution resembles the sample data (*goodness-of-fit*), we can use the Kolmogorov-Smirnov test statistic.
- ▶ It is defined as the maximum value of the absolute difference between the cumulative distribution function estimated from the sample and the one calculated from the fitted distribution.
- ▶ After estimating the parameters for different distributions, we can compute the Kolmogorov-Smirnov statistic for each distribution and choose the one with the smallest value as the best fit to our sample.



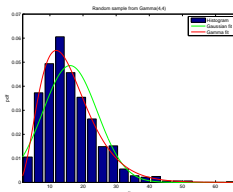
Maximum Likelihood Estimation Examples



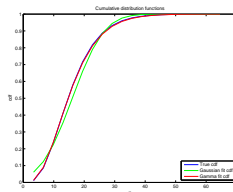
(a) True pdf is $N(10, 4)$. Estimated pdf is $N(9.98, 4.05)$.



(b) True pdf is $0.5N(10, 0.16) + 0.5N(11, 0.25)$. Estimated pdf is $N(10.50, 0.47)$.



(c) True pdf is $\text{Gamma}(4, 4)$. Estimated pdfs are $N(16.1, 67.4)$ and $\text{Gamma}(3.8, 4.2)$.



(d) Cumulative distribution functions for the example in (c).

Figure 1: Histograms of samples and estimated densities for different distributions.



Bayesian Estimation

- ▶ Suppose the set $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ contains the samples drawn independently from the density $p(\mathbf{x}|\boldsymbol{\theta})$ whose form is assumed to be known but $\boldsymbol{\theta}$ is not known exactly.
- ▶ Assume that $\boldsymbol{\theta}$ is a quantity whose variation can be described by the prior probability distribution $p(\boldsymbol{\theta})$.



Bayesian Estimation

- Given \mathcal{D} , the prior distribution can be updated to form the posterior distribution using the Bayes rule

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

where

$$p(\mathcal{D}) = \int p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

and

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^n p(\mathbf{x}_i|\boldsymbol{\theta}).$$



Bayesian Estimation

- ▶ The posterior distribution $p(\boldsymbol{\theta}|\mathcal{D})$ can be used to find estimates for $\boldsymbol{\theta}$ (e.g., the expected value of $p(\boldsymbol{\theta}|\mathcal{D})$ can be used as an estimate for $\boldsymbol{\theta}$).
- ▶ Then, the conditional density $p(\mathbf{x}|\mathcal{D})$ can be computed as

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta}$$

and can be used in the Bayesian classifier.



MLEs vs. Bayes Estimates

- ▶ Maximum likelihood estimation finds an estimate of θ based on the samples in \mathcal{D} but a different sample set would give rise to a different estimate.
- ▶ Bayes estimate takes into account the sampling variability.
- ▶ We assume that we do not know the true value of θ , and instead of taking a single estimate, we take a weighted sum of the densities $p(\mathbf{x}|\theta)$ weighted by the distribution $p(\theta|\mathcal{D})$.



The Gaussian Case

- ▶ Consider the univariate case $p(x|\mu) = N(\mu, \sigma^2)$ where μ is the only unknown parameter with a prior distribution $p(\mu) = N(\mu_0, \sigma_0^2)$ (σ^2 , μ_0 and σ_0^2 are all known).
- ▶ This corresponds to drawing a value for μ from the population with density $p(\mu)$, treating it as the true value in the density $p(x|\mu)$, and drawing samples for x from this density.



The Gaussian Case

- Given $\mathcal{D} = \{x_1, \dots, x_n\}$, we obtain

$$\begin{aligned} p(\mu|\mathcal{D}) &\propto \prod_{i=1}^n p(x_i|\mu)p(\mu) \\ &\propto \exp \left[-\frac{1}{2} \left(\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \right) \mu^2 - 2 \left(\frac{1}{\sigma^2} \sum_{i=1}^n x_i + \frac{\mu_0}{\sigma_0^2} \right) \mu \right) \right] \\ &= N(\mu_n, \sigma_n^2) \end{aligned}$$

where

$$\begin{aligned} \mu_n &= \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \hat{\mu}_n + \left(\frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \right) \mu_0 & \left(\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n x_i \right) \\ \sigma_n^2 &= \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}. \end{aligned}$$



The Gaussian Case

- ▶ μ_0 is our best prior guess and σ_0^2 is the uncertainty about this guess.
- ▶ μ_n is our best guess after observing \mathcal{D} and σ_n^2 is the uncertainty about this guess.
- ▶ μ_n always lies between $\hat{\mu}_n$ and μ_0 .
 - ▶ If $\sigma_0 = 0$, then $\mu_n = \mu_0$ (no observation can change our prior opinion).
 - ▶ If $\sigma_0 \gg \sigma$, then $\mu_n = \hat{\mu}_n$ (we are very uncertain about our prior guess).
 - ▶ Otherwise, μ_n approaches $\hat{\mu}_n$ as n approaches infinity.



The Gaussian Case

- ▶ Given the posterior density $p(\mu|\mathcal{D})$, the conditional density $p(x|\mathcal{D})$ can be computed as

$$p(x|\mathcal{D}) = N(\mu_n, \sigma^2 + \sigma_n^2)$$

where the conditional mean μ_n is treated as if it were the true mean, and the known variance is increased to account for our lack of exact knowledge of the mean μ .



The Gaussian Case

- ▶ Consider the multivariate case $p(\mathbf{x}|\boldsymbol{\mu}) = N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ where $\boldsymbol{\mu}$ is the only unknown parameter with a prior distribution $p(\boldsymbol{\mu}) = N(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ ($\boldsymbol{\Sigma}$, $\boldsymbol{\mu}_0$ and $\boldsymbol{\Sigma}_0$ are all known).
- ▶ Given $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, we obtain

$$p(\boldsymbol{\mu}|\mathcal{D}) \propto \exp \left[-\frac{1}{2} \left(\boldsymbol{\mu}^T \left(n\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}_0^{-1} \right) \boldsymbol{\mu} - 2\boldsymbol{\mu}^T \left(\boldsymbol{\Sigma}^{-1} \sum_{i=1}^n \mathbf{x}_i + \boldsymbol{\Sigma}_0^{-1} \boldsymbol{\mu}_0 \right) \right) \right].$$



The Gaussian Case

- It follows that

$$p(\boldsymbol{\mu}|\mathcal{D}) = N(\boldsymbol{\mu}_n, \boldsymbol{\Sigma}_n)$$

where

$$\begin{aligned}\boldsymbol{\mu}_n &= \boldsymbol{\Sigma}_0 \left(\boldsymbol{\Sigma}_0 + \frac{1}{n} \boldsymbol{\Sigma} \right)^{-1} \hat{\boldsymbol{\mu}}_n + \frac{1}{n} \boldsymbol{\Sigma} \left(\boldsymbol{\Sigma}_0 + \frac{1}{n} \boldsymbol{\Sigma} \right)^{-1} \boldsymbol{\mu}_0, \\ \boldsymbol{\Sigma}_n &= \frac{1}{n} \boldsymbol{\Sigma}_0 \left(\boldsymbol{\Sigma}_0 + \frac{1}{n} \boldsymbol{\Sigma} \right)^{-1} \boldsymbol{\Sigma}.\end{aligned}$$



The Gaussian Case

- ▶ Given the posterior density $p(\boldsymbol{\mu}|\mathcal{D})$, the conditional density $p(\mathbf{x}|\mathcal{D})$ can be computed as

$$p(\mathbf{x}|\mathcal{D}) = N(\boldsymbol{\mu}_n, \boldsymbol{\Sigma} + \boldsymbol{\Sigma}_n)$$

which can be viewed as the sum of a random vector $\boldsymbol{\mu}$ with $p(\boldsymbol{\mu}|\mathcal{D}) = N(\boldsymbol{\mu}_n, \boldsymbol{\Sigma}_n)$ and an independent random vector \mathbf{y} with $p(\mathbf{y}) = N(0, \boldsymbol{\Sigma})$.



The Bernoulli Case

- ▶ Consider $P(x|\theta) = \text{Bernoulli}(\theta)$ where θ is the unknown parameter with a prior distribution $p(\theta) = \text{Beta}(\alpha, \beta)$ (α and β are both known).
- ▶ Given $\mathcal{D} = \{x_1, \dots, x_n\}$, we obtain

$$p(\theta|\mathcal{D}) = \text{Beta} \left(\alpha + \sum_{i=1}^n x_i, \beta + n - \sum_{i=1}^n x_i \right).$$



The Bernoulli Case

- The Bayes estimate of θ can be computed as the expected value of $p(\theta|\mathcal{D})$, i.e.,

$$\begin{aligned}\hat{\theta} &= \frac{\alpha + \sum_{i=1}^n x_i}{\alpha + \beta + n} \\ &= \left(\frac{n}{\alpha + \beta + n} \right) \frac{1}{n} \sum_{i=1}^n x_i + \left(\frac{\alpha + \beta}{\alpha + \beta + n} \right) \frac{\alpha}{\alpha + \beta}.\end{aligned}$$



Conjugate Priors

- ▶ A *conjugate prior* is one which, when multiplied with the probability of the observation, gives a posterior probability having the same functional form as the prior.
- ▶ This relationship allows the posterior to be used as a prior in further computations.

Table 1: Conjugate prior distributions.

<i>pdf generating the sample</i>	<i>corresponding conjugate prior</i>
Gaussian	Gaussian
Exponential	Gamma
Poisson	Gamma
Binomial	Beta
Multinomial	Dirichlet



Recursive Bayes Learning

- ▶ What about the convergence of $p(\mathbf{x}|\mathcal{D})$ to $p(\mathbf{x})$?
- ▶ Given $\mathcal{D}^n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, for $n > 1$

$$p(\mathcal{D}^n|\boldsymbol{\theta}) = p(\mathbf{x}_n|\boldsymbol{\theta})p(\mathcal{D}^{n-1}|\boldsymbol{\theta})$$

and

$$p(\boldsymbol{\theta}|\mathcal{D}^n) = \frac{p(\mathbf{x}_n|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}^{n-1})}{\int p(\mathbf{x}_n|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}^{n-1}) d\boldsymbol{\theta}}$$

where

$$p(\boldsymbol{\theta}|\mathcal{D}^0) = p(\boldsymbol{\theta})$$

⇒ quite useful if the distributions can be represented using only a few parameters (*sufficient statistics*).



Recursive Bayes Learning

- Consider the Bernoulli case $P(x|\theta) = \text{Bernoulli}(\theta)$ where $p(\theta) = \text{Beta}(\alpha, \beta)$, the Bayes estimate of θ is

$$\hat{\theta} = \frac{\alpha}{\alpha + \beta}.$$

- Given the training set $\mathcal{D} = \{x_1, \dots, x_n\}$, we obtain

$$p(\theta|\mathcal{D}) = \text{Beta}(\alpha + m, \beta + n - m)$$

where $m = \sum_{i=1}^n x_i = \#\{x_i | x_i = 1, x_i \in \mathcal{D}\}$.



Recursive Bayes Learning

- ▶ The Bayes estimate of θ becomes

$$\hat{\theta} = \frac{\alpha + m}{\alpha + \beta + n}.$$

- ▶ Then, given a new training set $\mathcal{D}' = \{x_1, \dots, x_{n'}\}$, we obtain

$$p(\theta|\mathcal{D}, \mathcal{D}') = \text{Beta}(\alpha + m + m', \beta + n - m + n' - m')$$

where $m' = \sum_{i=1}^{n'} x_i = \#\{x_i | x_i = 1, x_i \in \mathcal{D}'\}$.



Recursive Bayes Learning

- The Bayes estimate of θ becomes

$$\hat{\theta} = \frac{\alpha + m + m'}{\alpha + \beta + n + n'}.$$

- Thus, recursive Bayes learning involves only keeping the counts m (related to sufficient statistics of Beta) and the number of training samples n .



MLEs vs. Bayes Estimates

Table 2: Comparison of MLEs and Bayes estimates.

	<i>MLE</i>	<i>Bayes</i>
<i>computational complexity</i>	differential calculus, gradient search	multidimensional integration
<i>interpretability</i>	point estimate	weighted average of models
<i>prior information</i>	assume the parametric model $p(\mathbf{x} \theta)$	assume the models $p(\theta)$ and $p(\mathbf{x} \theta)$ but the resulting distribution $p(\mathbf{x} \mathcal{D})$ may not have the same form as $p(\mathbf{x} \theta)$

- If there is much data (strongly peaked $p(\theta|\mathcal{D})$) and the prior $p(\theta)$ is uniform, then the Bayes estimate and MLE are equivalent.



Classification Error

- ▶ To apply these results to multiple classes, separate the training samples to c subsets $\mathcal{D}_1, \dots, \mathcal{D}_c$, with the samples in \mathcal{D}_i belonging to class w_i , and then estimate each density $p(\mathbf{x}|w_i, \mathcal{D}_i)$ separately.
- ▶ Different sources of error:
 - ▶ Bayes error: due to overlapping class-conditional densities (related to the features used).
 - ▶ Model error: due to incorrect model.
 - ▶ Estimation error: due to estimation from a finite sample (can be reduced by increasing the amount of training data).

