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M L D M Chapter 3 Parameter Estimation

Contents

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- Introduction
- Maximum-Likelihood Estimation
- Bayesian Estimation

Bayesian Theorem

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$$P(\omega_i \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \omega_i) P(\omega_i)}{p(\mathbf{x})}$$
$$p(\mathbf{x}) = \sum_{j=1}^{c} p(\mathbf{x} \mid \omega_j) P(\omega_j)$$

To compute posterior probability $P(\omega_i | \mathbf{x})$, we need to know:

 $p(\mathbf{x} \mid \omega_i) \qquad P(\omega_i)$

How can we get these values?

Samples

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$$\mathcal{D} = \{\mathcal{D}_1, \mathcal{D}_2, \mathbf{K}, \mathcal{D}_c\}$$

The samples in D_j are drawn independently according to the probability law $p(\mathbf{x}|\omega_j)$. That is, examples in D_j are i.i.d. random variables, i.e., independent and identically distributed.

It is easy to compute the prior probability:



Samples

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For class-conditional pdf:

• Case I: $p(\mathbf{x}|\omega_j)$ has certain parametric form

□e.g.

$$p(\mathbf{x} \mid \boldsymbol{\omega}_j) \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$

$$\boldsymbol{\theta}_j \qquad \boldsymbol{\theta}_j = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \mathbf{K}, \boldsymbol{\theta}_m)^T$$

 $\Box \operatorname{If} X \in \mathbb{R}^d \ \theta_j$ contains "d + d(d+1)/2" free parameters.

■ Case II: p(x|ω_j) doesn't have parametric form
□ Next chapter.

Goal

$$\mathcal{D} = \{\mathcal{D}_1, \mathcal{D}_2, \mathbf{K}, \mathcal{D}_c\}$$

$$p(\mathbf{x} \,|\, \boldsymbol{\omega}_j) \equiv p(\mathbf{x} \,|\, \boldsymbol{\theta}_j)$$

Use \mathcal{D}_{j} to estimate the unknown parameter vector θ_{j}

$$\boldsymbol{\theta}_{j} = (\theta_{1}, \theta_{2}, \mathbf{K}, \theta_{m})^{T}$$

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 θ_2

 $\dot{\mathbf{\theta}}_3$

H

 $\hat{\mathbf{\theta}}$

 θ_1

Estimation Under Parametric Form

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Maximum-Likelihood Estimation

View parameters as quantities whose values are fixed but unknown



Estimate parameter values by maximizing the likelihood (probability) of observing the actual examples.

Bayesian Estimation

View parameters as random variables having some known prior distribution Observation of the actual training examples transforms parameters' prior into posterior distribution. (via Bayes rule)

Maximum-Likelihood Estimation

- Because each class is considered individually, the subscript used before will be dropped.
- Now the problem becomes:

Given a sample set D, whose elements are drawn independently from a population possessing a known parameter form, say $p(x | \theta)$, we want to choose a $\hat{\theta}$ that will make D to occur most likely.



Maximum-Likelihood Estimation (Cont.)

Criterion of ML

 $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{K}, \mathbf{x}_n\}$

By the independence assumption, we have

$$p(\mathcal{D} | \boldsymbol{\theta}) = p(\mathbf{x}_1 | \boldsymbol{\theta}) p(\mathbf{x}_2 | \boldsymbol{\theta}) \Lambda \ p(\mathbf{x}_n | \boldsymbol{\theta}) = \prod_{k=1}^n p(\mathbf{x}_k | \boldsymbol{\theta})$$

The Likelihood Function

$$L(\boldsymbol{\theta} \mid \mathcal{D}) = p(\mathcal{D} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_{k} \mid \boldsymbol{\theta})$$

The maximum-likelihood estimation:

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} L(\boldsymbol{\theta} \mid \boldsymbol{D})$$

Maximum-Likelihood Estimation (Cont.)

Often, we resort to maximize the log-likelihood function

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} l(\boldsymbol{\theta} \mid \mathcal{D})$$

Maximum-Likelihood Estimation (Cont.)

- Find the extreme values using the method in differential calculus.
- Gradient Operator
 - Let $f(\theta)$ be a continuous function, where $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$.

Gradient
Operator
$$\nabla_{\boldsymbol{\theta}} = \left(\frac{\partial}{\partial \theta_1}, \frac{\partial}{\partial \theta_2}, \Lambda, \frac{\partial}{\partial \theta_n}\right)^T$$

Find the extreme values by solving

$$\nabla_{\theta} f = 0$$

Case I: unknown μ , and \sum is known

$$p(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2}} \exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right]$$
$$L(\boldsymbol{\mu} | \mathcal{D}) = p(\mathcal{D} | \boldsymbol{\mu}) = \prod_{k=1}^n p(\mathbf{x}_k | \boldsymbol{\theta})$$
$$= \frac{1}{(2\pi)^{nd/2}} \prod_{k=1}^n \exp\left[-\frac{1}{2}(\mathbf{x}_k - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu})\right]$$
$$l(\boldsymbol{\mu} | \mathcal{D}) = \ln L(\boldsymbol{\mu} | \mathcal{D})$$
$$= -\ln(2\pi)^{nd/2} | \boldsymbol{\Sigma} |^{n/2} - \frac{1}{2} \sum_{k=1}^n (\mathbf{x}_k - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu})$$

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 $l(\boldsymbol{\mu} \mid \mathcal{D}) = \ln L(\boldsymbol{\mu} \mid \mathcal{D})$

Intuitive Result: Maximum estimate for the unknown μ is just the arithmetic average of training samples---sample mean.



- Case II: both μ and \sum are unknown
- Consider univariate case

$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \qquad \boldsymbol{\theta} = (\theta_1, \theta_2)^T = (\mu, \sigma^2)^T$$

$$L(\boldsymbol{\theta} \mid \mathcal{D}) = p(\mathcal{D} \mid \boldsymbol{\theta}) = \prod_{k=1}^{n} p(x_k \mid \boldsymbol{\theta}) = \frac{1}{(2\pi)^{n/2}} \sigma^n \prod_{k=1}^{n} \exp\left[-\frac{(x_k - \mu)^2}{2\sigma^2}\right]$$

$$l(\mathbf{\theta} \mid \mathcal{D}) = \ln L(\mathbf{\theta} \mid \mathcal{D}) = -\ln(2\pi)^{n/2} \sigma^n - \frac{1}{2\sigma^2} \sum_{k=1}^n (x_k - \mu)^2$$
$$= -\ln(2\pi)^{n/2} \theta_2^{n/2} - \frac{1}{2\theta_2} \sum_{k=1}^n (x_k - \theta_1)^2$$

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$$l(\boldsymbol{\theta} \mid \mathcal{D}) = -\ln(2\pi)^{n/2} \theta_2^{n/2} - \frac{1}{2\theta_2} \sum_{k=1}^n (x_k - \theta_1)^2$$

$$\nabla_{\boldsymbol{\theta}} l(\boldsymbol{\theta} \mid \mathcal{D}) = \begin{bmatrix} \frac{1}{\theta_2} \sum_{k=1}^n (x_k - \theta_1) \\ -\frac{n}{2\theta_2} + \sum_{k=1}^n \frac{(x_k - \theta_1)^2}{2\theta_2^2} \end{bmatrix} = \boldsymbol{0} \quad \begin{array}{l} \textbf{Unbiased Estimator:} \\ E[\hat{\boldsymbol{\theta}}] = \boldsymbol{\theta} \\ \textbf{Consistent Estimator:} \\ \lim_{n \to \infty} E[\hat{\boldsymbol{\theta}}] = \boldsymbol{\theta} \\ \textbf{unbiased} \\ \hline \boldsymbol{1} \quad \boldsymbol{n} \end{bmatrix}$$

 $\hat{\mu} = \hat{\theta}_1 = \frac{1}{n} \sum_{k=1}^n x_k$ Arithmetic average of *n* vectors $\hat{\sigma}^2 = \hat{\theta}_2 = \frac{1}{n} \sum_{k=1}^n (x_k - \hat{\mu})^2$ Arithmetic average of *n* matrices $(\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^T$

hiased

$$(\mathbf{x}_k - \hat{\boldsymbol{\mu}})(\mathbf{x}_k - \hat{\boldsymbol{\mu}})^T$$

MLE for Normal Population

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$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{k=1}^{n} \mathbf{x}_{k}$$

Sample Mean $E[\hat{\mu}] = \mu$

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{k=1}^{n} (\mathbf{x}_{k} - \hat{\boldsymbol{\mu}}) (\mathbf{x}_{k} - \hat{\boldsymbol{\mu}})^{T}$$

 $E[\hat{\Sigma}] = \frac{n-1}{n} \Sigma \neq \Sigma$

$$\mathbf{C} = \frac{1}{n-1} \sum_{k=1}^{n} (\mathbf{x}_{k} - \hat{\boldsymbol{\mu}}) (\mathbf{x}_{k} - \hat{\boldsymbol{\mu}})^{T}$$

Sample Covariance Matrix $E[\mathbf{C}] = \mathbf{\Sigma}$

$$E(\sigma_{ML}^{2}) = E(\frac{1}{N}\sum_{n=1}^{N}(x_{n} - \mu_{ML})^{2}) = E[\frac{1}{N}\sum_{n=1}^{N}(x_{n}^{2} - 2x_{n}\mu_{ML} + \mu_{ML}^{2})]$$

$$= E[\frac{1}{N}\sum_{n=1}^{N}(x_{n}^{2}) - 2\mu_{ML} \cdot \frac{1}{N}\sum_{n=1}^{N}x_{n} + \mu_{ML}^{2}] = E[\frac{1}{N}\sum_{n=1}^{N}(x_{n}^{2}) - 2\mu_{ML} \cdot \mu_{ML} + \mu_{ML}^{2}]$$

$$= E[\frac{1}{N}\sum_{n=1}^{N}(x_{n}^{2}) - \mu_{ML}^{2}] = \frac{1}{N}\sum_{n=1}^{N}E(x_{n}^{2}) - E(\mu_{ML}^{2})$$

$$E(x_{n}^{2}) = \sigma^{2} + \mu^{2}$$

$$E(\mu_{ML}^2) = D(\mu_{ML}) + [E(\mu_{ML})]^2 = D(\frac{1}{N}\sum_{n=1}^N x_n) + [E(\mu_{ML})]^2 = \frac{1}{N^2}\sum_{n=1}^N D(x_n) + \mu^2$$

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Bayesian Estimation

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- Settings
 - The parametric form of the likelihood function for each category is known
 - However, θ_j is considered to be random variables instead of being fixed (but unknown) values.



Posterior Probabilities from sample

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 $\mathcal{D} = \{\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_c\}$

$$P(\omega_i \mid \mathbf{x}, \mathcal{D}) = \frac{P(\omega_i, \mathbf{x}, \mathcal{D})}{P(\mathbf{x}, \mathcal{D})} = \frac{P(\omega_i, \mathbf{x}, \mathcal{D})}{\sum_{j=1}^{c} P(\omega_j, \mathbf{x}, \mathcal{D})}$$

 $P(\omega_i, \mathbf{x}, \mathcal{D}) = P(D) \cdot P(\omega_i, \mathbf{x} \mid \mathcal{D}) = P(D) \cdot P(\omega_i \mid \mathcal{D}) \cdot P(\mathbf{u}_i \mid \mathcal{D}) \cdot P(\mathbf{u}_i \mid \mathcal{D})$

Assumptions:



Problem Formulation



$$P(\omega_i \mid \mathbf{x}, \mathcal{D}) = \frac{P(\mathbf{x} \mid \omega_i, \mathcal{D}_i) P(\omega_i)}{\sum_{j=1}^{c} P(\mathbf{x} \mid \omega_j, \mathcal{D}_j) P(\omega_j)}$$

The key problem is to determine, $P(\mathbf{x} | \omega_i, \mathcal{D}_i)$, treat each class independently, the problem becomes $P(\mathbf{x} | \mathcal{D})$

This is always the central problem of Bayesian Learning.

Class-Conditional Density Estimation

Assume p(x) is unknown but knowing it has a fixed form with parameter vector θ .





Bayesian Estimation: General Procedure

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Phase III:

$$P(\omega_i \mid \mathbf{x}, \mathcal{D}) = \frac{P(\mathbf{x} \mid \omega_i, \mathcal{D}_i) P(\omega_i)}{\sum_{j=1}^{c} P(\mathbf{x} \mid \omega_j, \mathcal{D}_j) P(\omega_j)}$$

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The univariate Gaussian: unknown μ $p(\boldsymbol{\theta} \mid \mathcal{D}) = \alpha \prod p(\mathbf{x}_k \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})$ Phase I: $p(\mu) + p(x \mid \mu) + D$ $p(\mu \mid D)$ $p(x \mid \mu) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$ $p(\mu) = \frac{1}{\sqrt{2\pi\sigma_0}} \exp \left| -\frac{1}{2} \left(\frac{\mu - \mu_0}{\sigma_0} \right)^2 \right|$ Other form of prior pdf could be assumed as well

The Gaussian Case

$$p(\mu) = \frac{1}{\sqrt{2\pi\sigma_0}} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right] \quad p(x|\mu) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

$$p(\theta|\mathcal{D}) = \alpha \prod_{k=1}^n p(\mathbf{x}_k|\theta)p(\theta)$$

$$p(\mu|\mathcal{D}) = \alpha \prod_{k=1}^n \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x_k-\mu}{\sigma}\right)^2\right] \cdot \frac{1}{\sqrt{2\pi\sigma_0}} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right]$$

$$= \alpha' \exp\left[-\frac{1}{2}\left(\sum_{k=1}^n \left(\frac{x_k-\mu}{\sigma}\right)^2 + \left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right)\right]$$

$$= \alpha'' \exp\left[-\frac{1}{2}\left[\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^n x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right]\right]$$

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 $p(\mu | D)$ is an exponential function of a quadratic function of μ ; thus $p(\mu | D)$ is also a normal.

$$p(\mu \mid D) \sim N(\mu_n, \sigma_n^2)$$

$$p(\mu \mid D) = \frac{1}{\sqrt{2\pi}\sigma_n} \exp\left[-\frac{1}{2}\left(\frac{\mu - \mu_n}{\sigma_n}\right)^2\right]$$

$$= \frac{1}{\sqrt{2\pi}\sigma_n} \exp\left[-\frac{1}{2\sigma_n^2}\left(\mu^2 - 2\mu_n\mu + \mu_n^2\right)\right]$$

$$p(\mu \mid D) = \alpha'' \exp\left[-\frac{1}{2}\left[\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^n x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right]\right]$$

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Equating the coefficients in both form; then, we have

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2}\right)\hat{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2}\mu_0 \qquad \hat{\mu}_n = \frac{1}{n}\sum_{k=1}^n x_k$$

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n \sigma_0^2 + \sigma^2}$$

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



The Gaussian Case

$$p(\mathbf{x} \mid \mathcal{D}) = \int p(\mathbf{x} \mid u) p(u \mid \mathcal{D}) d\theta \qquad p(x \mid \mu) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

$$p(\mu \mid \mathcal{D}) \sim N(\mu_n, \sigma_n^2)$$

$$p(x \mid \mathcal{D}) = \frac{1}{2\pi\sigma\sigma_n} \int \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_n}{\sigma_n}\right)^2\right] d\mu$$

$$= \frac{1}{2\pi\sigma\sigma_n} \exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right] \int \exp\left[-\frac{1}{2}\frac{\sigma^2+\sigma_n^2}{\sigma^2\sigma_n^2}\left(\mu-\frac{\sigma_n^2x+\sigma^2\mu_n}{\sigma^2+\sigma_n^2}\right)^2\right] d\mu$$

$$p(x \mid \mathcal{D}) \text{ is an exponential function of a quadratic function of x; thus, it is also a normal pdf.} =?$$

The Gaussian Case

$$p(\mathbf{x} \mid \mathcal{D}) = \int p(\mathbf{x} \mid u) p(u \mid \mathcal{D}) d\theta \qquad p(x \mid \mu) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \\ p(\mu \mid \mathcal{D}) \sim N(\mu_n, \sigma_n^2) \\ p(x \mid \mathcal{D}) \sim N(\mu_n, \sigma^2 + \sigma_n^2) \\ = \frac{1}{2\pi\sigma\sigma_n} \exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2 + \sigma_n^2}\right] \exp\left[-\frac{1}{2}\frac{\sigma^2 + \sigma_n^2}{\sigma^2\sigma_n^2}\left(\mu - \frac{\sigma_n^2 x + \sigma^2 \mu_n}{\sigma^2 + \sigma_n^2}\right)^2\right] d\mu \\ p(x \mid \mathcal{D}) \text{ is an exponential function of a quadratic function of x thus, it is also a normal pdf.}$$

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Phase III:

$$P(\omega_i \mid \mathbf{x}, \mathcal{D}) = \frac{P(\mathbf{x} \mid \omega_i, \mathcal{D}_i) P(\omega_i)}{\sum_{j=1}^{c} P(\mathbf{x} \mid \omega_j, \mathcal{D}_j) P(\omega_j)}$$

Summary

Key issue

- Estimate prior and class-conditional pdf from training set
- Basic assumption on training examples: i.i.d.
- Two strategies to key issue
 - Parametric form for class-conditional pdf
 - Maximum likelihood estimation
 - □ Bayesian estimation
 - No parametric form for class-conditional pdf

Summary

- Maximum likelihood estimation
 - Settings: parameters as fixed but unknown values
 - The objective function: log-likelihood function
 - The gradient for the objective function should be zero
 - Gaussian
- Bayesian estimation
 - Settings: parameters as random variables
 - General procedure: I, II, III
 - Gaussian case
 - Project 3.2

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Thank You!

Any Question?

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