Parametric models

Maximum Likelihood and Bayesian Density Estimate

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Contents

Introduction

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- 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.

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- 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.

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    - Estimate these values by maximizing the probability of obtaining the samples observed

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  - *Maximum likelihood estimation*
    - Views the parameters as quantities whose values are fixed but unknown
    - Estimate 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

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Maximum Likelihood Estimation

- Suppose we have a set $D = \{x_1, \ldots, x_n\}$ of independent and identically distributed (*i.i.d.*) samples drawn from the density $p(x|\theta)$.

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Maximum Likelihood Estimation

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- We would like to use training samples in D to estimate the unknown parameter vector θ.
- Define $L(\theta|D)$ as the *likelihood function* of θ with respect to D as

$$L(\theta|D) = p(D|\theta) = p(x_1, \ldots, x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta)$$

Maximum Likelihood Estimation

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

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

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$$\hat{\theta} = \arg\max_{\theta} L(\theta|D)$$
- It is often easier to work with the logarithm of the likelihood function (*log-likelihood function*) that gives
$$\hat{\theta} = \arg\max_{\theta} \log L(\theta|D) = \arg\max_{\theta} \sum_{i=1}^{n} \log p(x_i|\theta)$$

Maximum Likelihood Estimation

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

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

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- Then, the MLE of θ should satisfy the necessary conditions

$$\nabla_\theta \log L(\theta|D) = \sum_{i=1}^{n} \nabla_\theta \log p(x_i|\theta) = 0$$

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 $f(\hat{\theta})$.

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The Gaussian Case

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The Gaussian Case

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  - When Σ is known but μ is unknown:

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

  - When both μ and Σ are unknown:

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

The Bernoulli Case

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- The MLE of θ can be computed as

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

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Bias of Estimators

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- 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*

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

is an unbiased estimator for Σ.

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Goodness-of-fit

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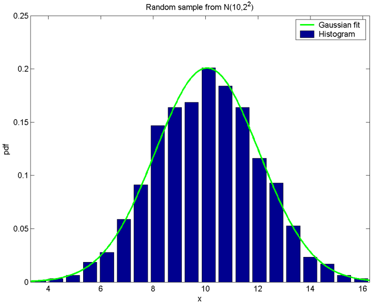
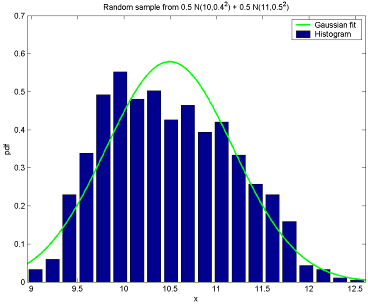
- It is defined as the maximum value of the absolute difference between the cumulative distribution function estimated from the sample and the one calculated from the fitted distribution.
- After estimating the parameters for different distributions, we can compute the Kolmogorov-Smirnov statistic for each distribution and choose the one with the smallest value as the best fit to our sample.

Maximum Likelihood Estimation Examples

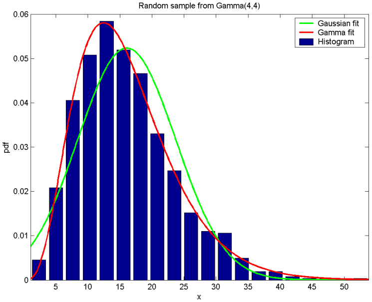


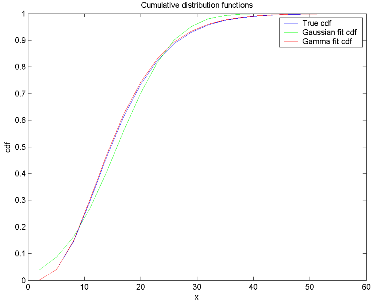
True pdf is $N(10, 4)$. Estimated pdf is $N(10.1, 3.9)$.



True pdf is $0.5N(10, 0.16)$ $+0.5N(11, 0.25)$. Estimated pdf is $N(10.5, 0.5)$.

Maximum Likelihood Estimation Examples





True pdf is Gamma$(4, 4)$. Estimated pdfs are $N(15.8, 62.1)$ and Gamma$(4.0, 3.9)$.

Cumulative distribution functions.

Contents

Bayesian Estimation

- Assume that θ is a quantity whose variation can be described by the prior probability distribution $p(\theta)$.

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- Assume that θ is a quantity whose variation can be described by the prior probability distribution $p(\theta)$.
- Suppose the set $D = \{x_1, \ldots, x_n\}$ contains the samples drawn independently from the density $p(x|\theta)$ whose form is assumed to be known but θ is not known exactly.

Bayesian Estimation

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

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

where

$$p(D) = \int p(D|\theta)\, p(\theta)\, d\theta$$

and

$$p(D|\theta) = \prod_{i=1}^{n} p(x_i|\theta)$$

Bayesian Estimation

- The posterior distribution $p(\theta|D)$ can be used to find estimates for θ (e.g., the expected value of $p(\theta|D)$ can be used as an estimate for θ).

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

$$p(x|D) = \int p(x|\theta)\, p(\theta|D)\, d\theta$$

and can be used in the Bayesian classifier.

Contents

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).

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 $p(\mu) = N(\mu_0, \sigma_0^2) \quad (\sigma^2,\ \mu_0$ 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 $D = \{x_1, \ldots, x_n\}$, we obtain

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

where

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

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

The Gaussian Case

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- 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 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 $p(\mu|D)$, the conditional density $p(x|D)$ can be computed as

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

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 $p(x|\mu) = N(\mu, \Sigma)$ where μ is the only unknown parameter with a prior distribution $p(\mu) = N(\mu_0, \Sigma_0)$ $\quad$ (Σ, μ_0 and Σ_0 are all known).

The Gaussian Case

- Consider the multivariate case $p(x|\mu) = N(\mu, \Sigma)$ where μ is the only unknown parameter with a prior distribution $p(\mu) = N(\mu_0, \Sigma_0) \quad (\Sigma,\ \mu_0$ and Σ_0 are all known).
- Given $D = \{x_1, \ldots, x_n\}$, we obtain

$$p(\mu|D) \propto \exp\left[-\frac{1}{2}\left(\mu^T\left(n\Sigma^{-1} + \Sigma_0^{-1}\right)\mu \right.\right.$$
$$\left.\left. - 2\mu^T\left(\Sigma^{-1}\sum_{i=1}^{n} x_i + \Sigma_0^{-1}\mu_0\right)\right)\right]$$

The Gaussian Case

- It follows that
$$p(\mu|D) = N(\mu_n, \Sigma_n)$$
where
$$\mu_n = \Sigma_0 \left(\Sigma_0 + \frac{1}{n}\Sigma\right)^{-1} \hat{\mu}_n + \frac{1}{n}\Sigma \left(\Sigma_0 + \frac{1}{n}\Sigma\right)^{-1} \mu_0$$
$$\Sigma_n = \frac{1}{n}\Sigma_0 \left(\Sigma_0 + \frac{1}{n}\Sigma\right)^{-1} \Sigma$$

The Gaussian Case

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

$$p(x|D) = N(\mu_n, \Sigma + \Sigma_n)$$

which can be viewed as the sum of a random vector μ with $p(\mu|D) = N(\mu_n, \Sigma_n)$ and an independent random vector y with $p(y) = N(0, \Sigma)$.

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

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

The Bernoulli Case

- The Bayes estimate of θ can be computed as the expected value of $p(\theta|D)$

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

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Conjugate Priors

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Table: Conjugate prior distributions.

pdf generating the sample	*corresponding conjugate prior*
Normal	Normal
Exponential	Gamma
Poisson	Gamma
Binomial	Beta
Multinomial	Dirichlet

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Recursive Bayes Learning

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- Given $D^n = \{x_1, \ldots, x_n\}$, for $n > 1$

$$p(D^n|\theta) = p(x_n|\theta)p(D^{n-1}|\theta)$$

and

$$p(\theta|D^n) = \frac{p(x_n|\theta)\, p(\theta|D^{n-1})}{\int p(x_n|\theta)\, p(\theta|D^{n-1})\, d\theta}$$

where

$$p(\theta|D^0) = p(\theta)$$

Recursive Bayes Learning

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where

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$\Rightarrow$ quite useful if the distributions can be represented using only a few parameters (*sufficient statistics*)