Tutorial 2: Maximum-Likelihood and Bayesian Parameter Estimation

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Outline

1. ML estimate: $\hat{\Sigma}$ of multivariate Gaussian
2. ML estimate bias: $\hat{\sigma}^2$ of univariate Gaussian
3. Bayesian estimate: Univariate Gaussian
   - brief review
   - posteriori $p(\mu|\mathcal{D})$
   - conditional probability density $p(x|w_i, \mathcal{D}_i)$

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1. ML estimate: $\hat{\Sigma}$ of multivariate Gaussian

Multivariate Gassian Case: unknown μ and Σ

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \tag{1}$$

$$\hat{\mathbf{\Sigma}} = \frac{1}{n}\sum_{k=1}^{n} (\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t \tag{2}$$

- $\hat{\mu}$ is the sample mean.
- $\hat{\mathbf{\Sigma}}$ is the arithmetic average of the n matrices $(\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t$.

1. ML estimate: $\hat{\Sigma}$ of multivariate Gaussian

Multivariate normal density

$$p(\mathbf{x} \mid \mu,\ \mathbf{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^t\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)\right] \quad (3)$$

Draw $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n$ independently from $p(\mathbf{x} \mid \mu,\ \mathbf{\Sigma})$, and the joint density (likelihood) is:

$$p(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n \mid \mu, \mathbf{\Sigma}) = \quad (4)$$

$$\frac{1}{(2\pi)^{nd/2}|\mathbf{\Sigma}|^{n/2}} \exp\left[-\frac{1}{2}\sum_{k=1}^{n}(\mathbf{x}_k-\mu)^t\mathbf{\Sigma}^{-1}(\mathbf{x}_k-\mu)\right] \quad (5)$$

Log-likelihood $l(\mu,\ \mathbf{\Sigma})$ is

$$l(\mu, \mathbf{\Sigma}) = -\frac{nd}{2}\ln(2\pi) - \frac{n}{2}\ln|\mathbf{\Sigma}| - \frac{1}{2}\sum_{k=1}^{n}(\mathbf{x}_k-\mu)^t\mathbf{\Sigma}^{-1}(\mathbf{x}_k-\mu) \quad (6)$$

1. ML estimate: $\hat{\Sigma}$ of multivariate Gaussian

Multivariate normal density

Let $A = \mathbf{\Sigma}^{-1}$

$$l(\mu, \mathbf{\Sigma}) = -\frac{nd}{2}\ln(2\pi) - \frac{n}{2}\ln|\mathbf{\Sigma}| - \frac{1}{2}\sum_{k=1}^{n}(\mathbf{x}_k - \mu)^t \mathbf{\Sigma}^{-1}(\mathbf{x}_k - \mu) \quad (7)$$

$$l(\mu, \mathbf{\Sigma}) = -\frac{nd}{2}\ln(2\pi) + \frac{n}{2}\ln \mathbf{A} - \frac{1}{2}\sum_{k=1}^{n}(\mathbf{x}_k - \mu)^t \mathbf{A}(\mathbf{x}_k - \mu) \quad (8)$$

$$\frac{\partial l(\mu, \mathbf{\Sigma})}{\partial \mathbf{A}} = \frac{n}{2}\mathbf{A}^{-1} - \frac{1}{2}\sum_{k=1}^{n}(\mathbf{x}_k - \mu)(\mathbf{x}_k - \mu)^t = 0 \quad (9)$$

Replace $\mathbf{A}$ by $\mathbf{\Sigma}^{-1}$

$$\hat{\mathbf{\Sigma}} = \frac{1}{n}\sum_{k=1}^{n}(\mathbf{x}_k - \hat{\mu})(\mathbf{x}_k - \hat{\mu})^t, \quad (\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_k) \quad (10)$$

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2. ML estimate bias: $\hat{\sigma}^2$ of univariate Gaussian

Univariate Gassian Case

ML estimator $\hat{\sigma}^2$ is biased.

$$E[\hat{\sigma}^2] = E[\frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2] = \frac{n-1}{n}\sigma^2 \tag{11}$$

An elementary unbiased estimator for σ^2 is given by $\frac{1}{n-1}\sum_{k=1}^{n}(x_k - \hat{\mu})$.

2. ML estimate bias: $\hat{\sigma}^2$ of univariate Gaussian

Univariate Gassian Case

$$E[\frac{1}{n}\sum_{k=1}^{n}(x_k-\hat{\mu})^2] = E\Big[\frac{1}{n}\sum_{k=1}^{n}(x_k-\frac{1}{n}\sum_{j=1}^{n}x_j)^2\Big] \tag{12}$$

$$= E\Big[\frac{1}{n}\sum_{k=1}^{n}(x_k^2-\frac{2}{n}x_k\sum_{j=1}^{n}x_j+\frac{1}{n^2}(\sum_{j=1}^{n}x_j)^2)\Big] \tag{13}$$

$$= E\Big[\frac{1}{n}\Big(\sum_{k=1}^{n}x_k^2-\frac{2}{n}(\sum_{k=1}^{n}x_k)^2+\frac{n}{n^2}(\sum_{k=1}^{n}x_k)^2\Big)\Big] \tag{14}$$

$$= E\Big[\frac{1}{n}\Big(\sum_{k=1}^{n}x_k^2-\frac{1}{n}(\sum_{k=1}^{n}x_k)^2\Big)\Big] \tag{15}$$

$$= \frac{1}{n}E[\sum_{k=1}^{n}x_k^2]-\frac{1}{n^2}E[(\sum_{k=1}^{n}x_k)^2] \tag{16}$$

$$= E[x^2]-\frac{1}{n^2}E\Big[\sum_{k=1}^{n}x_k^2+\sum_{i\neq j}x_ix_j\Big] \tag{17}$$

$$= E[x^2]-\frac{1}{n^2}E[\sum_{k=1}^{n}x_k^2]-\frac{1}{n^2}E[\sum_{i\neq j}x_ix_j] \tag{18}$$

$$= E[x^2]-\frac{1}{n}E[x^2]-\frac{n^2-n}{n^2}E[x_ix_j] = \frac{n-1}{n}\Big(E[x^2]-(E[x])^2\Big) \tag{19}$$

$$= \frac{n-1}{n}\sigma^2 \tag{20}$$

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3.1 Bayesian estimate: brief review

Bayesian estimate

Given sample set $\mathcal{D}$, then posteriori for estimation is

$$P(w_i|\mathbf{x},\mathcal{D}) = \frac{p(\mathbf{x}|w_i,\mathcal{D})P(w_i|\mathcal{D})}{\sum_{j=1}^{c} p(\mathbf{x}|w_i,\mathcal{D})P(w_i|\mathcal{D})} \tag{21}$$

- consider each class individually: $p(\mathbf{x}|w_i,\mathcal{D}) \rightarrow p(\mathbf{x}|\mathcal{D})$
- prior is known $P(w_i|\mathcal{D})$

Target: estimate posteriori $p(\mathbf{x}|\mathcal{D}) \rightarrow p(\mathbf{x})$

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x},\theta|\mathcal{D})d\theta \tag{22}$$

$$= \int p(\mathbf{x}|\theta,\mathcal{D})p(\theta|\mathcal{D})d\theta = \int p(\mathbf{x}|\theta)p(\theta|\mathcal{D})d\theta \tag{23}$$

3.2 Bayesian estimate of univariate Gaussian: posteriori $p(\mu|\mathcal{D})$

Bayesian estimate

$P(w_i|\mathbf{x},\mathcal{D}) \Rightarrow p(\mathbf{x}|w_i,\mathcal{D}) \Rightarrow p(\mathbf{x}|\mathcal{D}) \Rightarrow p(\mathbf{x}|\theta)\ \&\ p(\theta|\mathcal{D})$

- $p(\mathbf{x}|\theta)$ is pre-assumed in form: $p(x|\mu) \sim \mathcal{N}(\mu,\sigma^2)$
- $p(\theta|\mathcal{D})$ is the posteriori: $p(\mu|\mathcal{D})$

Posteriori $p(\mu|\mathcal{D})$ of univariate Gaussian

$$p(\mu|\mathcal{D}) = \frac{p(\mathcal{D}|\mu)p(\mu)}{\int p(\mathcal{D}|\mu)p(\mu)d\mu} \tag{24}$$

$$= \alpha \prod_{k=1}^{n} p(x_k|\mu)p(\mu) \tag{25}$$

where $p(x_k|\mu) \sim \mathcal{N}(\mu,\sigma^2)$, and $p(\mu) \sim \mathcal{N}(\mu_0,\sigma_0^2)$.

3.2 Bayesian estimate of univariate Gaussian: posteriori $p(\mu|\mathcal{D})$

Posteriori $p(\mu|\mathcal{D})$ of univariate Gaussian

$$p(\mu|\mathcal{D}) = \alpha \prod_{k=1}^{n} p(x_k|\mu)p(\mu) \tag{26}$$

$$= \alpha \prod_{k=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\Big[-\frac{1}{2}\Big(\frac{x_k-\mu}{\sigma}\Big)^2\Big] \frac{1}{\sqrt{2\pi}\sigma_0} \exp\Big[-\frac{1}{2}\Big(\frac{\mu-\mu_0}{\sigma_0}\Big)^2\Big] \tag{27}$$

$$= \alpha' \exp\Big[-\frac{1}{2}\Big(\sum_{k=1}^{n}(\frac{\mu-x_k}{\sigma})^2 + (\frac{\mu-\mu_0}{\sigma_0})^2\Big)\Big] \tag{28}$$

$$= \alpha'' \exp\Big[-\frac{1}{2}\Big[(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2})\mu^2 - 2(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2})\mu\Big]\Big] \tag{29}$$

$$\therefore \quad p(\mu|\mathcal{D}) \sim \mathcal{N}(\mu_n, \sigma_n^2),\ i.e.\ p(\mu|\mathcal{D}) = \frac{1}{\sqrt{2\pi}\sigma_n} \exp\Big[-\frac{1}{2}\Big(\frac{\mu-\mu_n}{\sigma_n}\Big)^2\Big] \tag{30}$$

$$\Longrightarrow \frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2},\ \frac{\mu_n}{\sigma_n^2} = \frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2} = \frac{n}{\sigma^2}\hat{\mu}_n + \frac{\mu_0}{\sigma_0^2} \tag{31}$$

$$\Longrightarrow \mu_n = \Big(\frac{n\sigma_0^2}{n\sigma_0^2+\sigma^2}\Big)\hat{\mu}_n + \frac{\sigma^2}{\sigma_0^2+\sigma^2}\mu_0,\ \sigma_n^2 = \frac{\sigma_0^2\sigma^2}{n\sigma_0^2+\sigma^2} \tag{32}$$

3.3 Bayesian estimate of univariate Gaussian: conditional probability density $p(x|w_i, \mathcal{D}_i)$

Conditional probability density $p(x|w_i, \mathcal{D}_i)$

$$p(x|w_i, \mathcal{D}_i) \tag{33}$$

$$\sim p(x|\mathcal{D}) \tag{34}$$

$$= \int p(x|\mu)p(\mu|\mathcal{D})d\mu \tag{35}$$

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

$$= \frac{1}{2\pi\sigma\sigma_n} \exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right] f(\sigma, \sigma_n) \tag{36}$$

$$\therefore \quad p(x|\mathcal{D}) \sim \mathcal{N}(\mu_n, \sigma^2+\sigma_n^2) \tag{37}$$

$$f(\sigma, \sigma_n) = \int \exp\left[-\frac{1}{2}\frac{\sigma^2+\sigma_n^2}{\sigma^2\sigma_n^2}\left(\mu - \frac{\sigma_n^2 x + \sigma^2\mu_n}{\sigma^2+\sigma_n^2}\right)^2\right] d\mu \tag{38}$$

3.3 Bayesian estimate of univariate Gaussian: conditional probability density $p(x|w_i, \mathcal{D}_i)$

Conditional probability density $p(x|w_i, \mathcal{D}_i)$

$$p(x|w_i, \mathcal{D}_i) \tag{39}$$
$$\sim p(x|\mathcal{D}) \tag{40}$$
$$= \int p(x|\mu)p(\mu|\mathcal{D})d\mu \tag{41}$$
$$= \int \frac{1}{\sqrt{2\pi}\sigma} \exp\Big[-\frac{1}{2}\Big(\frac{x-\mu}{\sigma}\Big)^2\Big] \frac{1}{\sqrt{2\pi}\sigma_n} \exp\Big[-\frac{1}{2}\Big(\frac{\mu-\mu_n}{\sigma_n}\Big)^2\Big] d\mu$$
$$= \frac{1}{2\pi\sigma\sigma_n} \int \exp\Big[-\frac{1}{2}\Big(\frac{x^2-2x\mu+\mu^2}{\sigma^2} + \frac{\mu^2-2\mu\mu_n+\mu_n^2}{\sigma_n^2}\Big)\Big] \tag{42}$$
$$= \frac{1}{2\pi\sigma\sigma_n} \exp\Big[-\frac{1}{2}(\frac{x^2}{\sigma^2} + \frac{\mu_n^2}{\sigma_n^2})\Big] \int \exp \tag{43}$$
$$\therefore \quad p(x|\mathcal{D}) \sim \mathcal{N}(\mu_n, \sigma^2 + \sigma_n^2) \tag{44}$$
$$f(\sigma, \sigma_n) = \int \exp\Big[-\frac{1}{2}\frac{\sigma^2+\sigma_n^2}{\sigma^2\sigma_n^2}\Big(\mu - \frac{\sigma_n^2 x + \sigma^2\mu_n}{\sigma^2+\sigma_n^2}\Big)^2\Big] d\mu \tag{45}$$