University of California San Diego

ECE 271 Notes

Instructor: Prof. Nuno Vasconcelos

Organized by Ray Tsai

Bayes Decision Rule

$$\begin{split} g^*(x) &= \mathop{\arg\min}_{g(x)} \ \sum_i P_{Y|X}(i|x) L[g(x),i] \\ &= \mathop{\arg\max}_i P_{Y|X}(i|x) \qquad \qquad \text{(for 0-1 loss function)} \\ &= \mathop{\arg\max}_i P_{X|Y}(x|i) P_Y(i) \qquad \qquad \text{(for 0-1 loss function)} \\ &= \mathop{\arg\max}_i \log P_{X|Y}(x|i) + \log P_Y(i). \qquad \qquad \text{(for 0-1 loss function)} \end{split}$$

For binary classification, the likelihood ratio form is: pick 0 if $\frac{P_{X|Y}(x|0)}{P_{X|Y}(x|1)} > T^* = \frac{P_Y(1)}{P_X(0)}$.

Associated Risk

$$R^* = \int P_X(x) \sum_{i \neq g^*(x)} P_{Y|X}(i|x) dx = \int P_{Y,X}(y \neq g^*(x), x) dx \quad \text{(For 0-1 loss function)}$$

Gaussian Classifier

For single variable, we assume $\sigma_i = \sigma$ and pick 0 if

$$x < \frac{\mu_1 + \mu_0}{2} + \frac{1}{\frac{\mu_1 - \mu_0}{\sigma^2}} \log \frac{P_Y(0)}{P_Y(1)}.$$

Generalizing it to multiple variables, we assume $\Sigma_i = \Sigma$, then the BDR becomes

$$i^*(x) = \arg\min_{i} [d(x, \mu_i) + \alpha_i],$$

where
$$d(x,y) = (x-y)^T \Sigma^{-1} (x-y)$$
 and $\alpha_i = \log \left[(2\pi)^d |\Sigma| \right] - 2 \log P_Y(i)$.

Alternatively,

$$i^*(x) = \arg\max_{i} g_i(x),$$

where $g_i(x) = w_i^T x + w_{i0}$, $w_i = \Sigma^{-1} \mu_i$, and $w_{i0} = -\frac{1}{2} \mu_i^T \Sigma^{-1} \mu_i + \log P_Y(i)$.

Geometric Interpretation

Thus, the hyperplane between class 0 and 1 is

$$g_0(x) - g_1(x) = w^T x + b = 0,$$

where
$$w = \Sigma^{-1}(\mu_0 - \mu_1)$$
 and $b = -\frac{(\mu_0 + \mu_1)^T \Sigma^{-1}(\mu_0 - \mu_1)}{2} + \log \frac{P_Y(0)}{P_Y(1)}$

It could also be rewritten as

$$w^{T}(x - x_{0}) = 0,$$
where $w = \Sigma^{-1}(\mu_{0} - \mu_{1})$ and $x_{0} = \frac{\mu_{0} + \mu_{1}}{2} - \frac{1}{(\mu_{0} - \mu_{1})^{T} \Sigma^{-1}(\mu_{0} - \mu_{1})} \log \frac{P_{Y}(0)}{P_{Y}(1)}(\mu_{0} - \mu_{1})$

Gaussian Distribution Transformation

Let $x \sim N(\mu, \Sigma)$, and let $y = A^T x$, for some matrix A. Then, $y \sim N(A^T \mu, A^T \Sigma A)$. A special case of this is the whitening transform $A_w = \Phi \Lambda^{-1/2}$, where Φ is the matrix of orthonormal eigenvectors of Σ , and Λ is the diagonal matrix of eigenvalues of Σ .

Sigmoid

Suppose that $g_1(x) = 1 - g_0(x)$. Then, we can rewrite

$$g_0(x) = \frac{1}{1 + \frac{P_{X|Y}(x|1)P_Y(1)}{P_{X|Y}(x|0)P_Y(0)}} = \frac{1}{1 + \exp\{d_0(x, \mu_0) - d_1(x, \mu_1) + \alpha_0 - \alpha_1\}},$$

where $d(x,y) = (x-y)^T \Sigma^{-1} (x-y)$ and $\alpha_i = \log \left[(2\pi)^d |\Sigma_i| \right] - 2 \log P_Y(i)$.

Maximum Likelihood Estimation

Solve for

$$\theta^* = \underset{\Theta}{\operatorname{arg \, max}} P_{X;\Theta}(\mathcal{D}; \theta) = \underset{\Theta}{\operatorname{arg \, max}} \log P_{X|\Theta}(\mathcal{D}; \theta).$$

Consider the Gaussian example:

Given a sample $\mathcal{D} = \{x_1, \dots, x_n\}$ of independent points, where $P_X(x_i) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{1}{2}(x_i - \mu)^T \Sigma^{-1}(x_i - \mu)}$.

Then, the likelihood $L(x_1, \ldots, x_n | \mu, \sigma) = \prod_{i=1}^n P_X(x_i)$. We take the gradient of the natural log of L with respect to μ and get

$$\nabla_{\mu}(\log L) = \nabla_{\mu} \left(-\frac{1}{2} \log[(2\pi)^{d} |\Sigma|] - \frac{1}{2} \sum_{i=1}^{n} (x_{i} - \mu)^{T} \Sigma^{-1} (x_{i} - \mu) \right)$$
$$= \sum_{i=1}^{n} \Sigma^{-1} (x_{i} - \mu) = \sum_{i=1}^{n} x_{i} - \sum_{i=1}^{n} \mu = 0.$$

Thus, we get $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i$. By taking the Hessian, we get $\nabla_{\mu}^2(\log L) = -\sum_{i=1}^{n} \Sigma^{-1} = -n\Sigma^{-1}$. Since the covariance matrix Σ is positive definite, $-n\Sigma^{-1}$ is negative definite. Thus $\hat{\mu}$ is the maximum point.

In addition, the MLE of the covariance matrix is

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

Bias and Variance

$$\begin{split} Bias(\hat{\theta}) &= E[\hat{\theta} - \theta], \quad Var(\hat{\theta}) = E\left\{(\hat{\theta} - E[\hat{\theta}])^2\right\}, \\ MSE(\hat{\theta}) &= E\left[(\hat{\theta} - \theta)^2\right] = Var(\hat{\theta}) + Bias^2(\hat{\theta}). \end{split}$$

Least Squares

Consider an overdetermined system $\Phi\theta = z$, where we attempt to minimize $||z - \Phi\theta||$, the least square solution is

$$\theta^* = (\Phi^T \Phi)^{-1} \Phi^T z.$$

For a overdetermined system $W\Phi\theta = Wz$, where we attempt to minimize $(z - \Phi\theta)^T W^T W(z - \Phi\theta)$, the least square solution is

$$\theta^* = (\Phi^T W^T W \Phi)^{-1} \Phi^T W^T W z.$$

Bayesian Estimation

Pick i if

$$i^*(x) = \arg\max_{i} P_{X|Y,T}(x|i, \mathcal{D}_i) P_Y(i),$$

where the class conditional is the predictive distribution

$$P_{X|Y,T}(x|i,\mathcal{D}_i) = \int P_{X|Y,\Theta}(x|i,\theta)P_{\Theta|Y,T}(\theta|i,\mathcal{D}_i) d\theta = E_{\Theta|Y,T}[P_{X|i,\Theta}(x|\theta) \mid T = \mathcal{D}_i].$$

For the multivariate Gaussian case, suppose

$$P_{T|\mu}(\mathcal{D}|\mu) = \mathcal{G}(\mathcal{D}, \mu, \Sigma), \quad P_{\mu}(\mu) = \mathcal{G}(\mu, \mu_0, \Sigma_0),$$

for known Σ, μ_0, Σ_0 . The posterior distribution is $P_{\mu|T}(\mu|\mathcal{D}) = \mathcal{G}(\mu, \mu_n, \Sigma_n)$, where

$$\Sigma_{n} = \Sigma_{0} A^{-1} \frac{1}{n} \Sigma \Rightarrow \Sigma_{n}^{-1} = n \Sigma^{-1} + \Sigma_{0}^{-1},$$

$$\mu_{n} = \Sigma_{0} A^{-1} \mu_{ML} + \frac{1}{n} \Sigma A^{-1} \mu_{0},$$

$$A = \Sigma_{0} + \frac{1}{n} \Sigma.$$

Then, the predictive distribution is

$$P_{X|T}(x|\mathcal{D}) = \int P_{X|\mu}(x|\mu)P_{\mu|T}(\mu|\mathcal{D}) d\mu$$

$$= \int \mathcal{G}(x,\mu,\Sigma)\mathcal{G}(\mu,\mu_n,\Sigma_n) d\mu$$

$$= \int \mathcal{G}(x-\mu,0,\Sigma)\mathcal{G}(\mu,\mu_n,\Sigma_n) d\mu$$

$$= \mathcal{G}(x,0,\Sigma) * \mathcal{G}(x,\mu_n,\Sigma_n) = \mathcal{G}(x,\mu_n,\Sigma+\Sigma_n).$$

Note that for non-informative prior, $\lim_{|\Sigma_0|\to\infty}\mu_n=\mu_{ML}$ and $\lim_{|\Sigma_0|\to\infty}\Sigma_n=\frac{1}{n}\Sigma=\Sigma_{ML}$, so

$$P_{X|T}(x|\mathcal{D}) = \mathcal{G}(x, \mu_n, \Sigma + \Sigma_n) = \mathcal{G}\left(x, \mu_{ML}, \left(1 + \frac{1}{n}\right)\Sigma\right).$$

MAP Estimation

$$\theta_{MAP} = \underset{\theta}{\operatorname{arg max}} P_{\Theta|T}(\theta|\mathcal{D}) = \underset{\theta}{\operatorname{arg max}} P_{T|\Theta}(\mathcal{D}|\theta) P_{\Theta}(\theta),$$

and this makes the predictive distribution equal to

$$P_{X|T}(x|\mathcal{D}) = P_{X|\Theta}(x|\theta_{MAP}) = \mathcal{G}(x,\mu_{ML},\Sigma)$$

Note that for the MAP estimator approaches the ML estimator as the sample size increases, i.e. $\theta_{MAP} \to \theta_{ML}$ as $n \to \infty$.

Expectation-maximization

1. write down the likelihood of the complete data (can drop terms irrelevant to Z and Ψ)

$$P_{X,Z}(\mathcal{D},z;\Psi) = \left(\prod_{i=1}^{n} P_{X|Z}(x_i|z;\Psi)\right) P_Z(z;\Psi).$$

2. **E-step**: write down the Q function

$$Q(\Psi; \Psi^{(n)}) = E_{Z|X;\Psi^{(n)}}[\log P_{X,Z}(\mathcal{D}, z; \Psi) \mid \mathcal{D}].$$

3. **M-step**: update Ψ , i.e.

$$\Psi^{(n+1)} = \arg\max_{\Psi} Q(\Psi; \Psi^{(n)}).$$

EM for Mixtures

Represent the class variable as $z = e_j = (\underbrace{0, \dots, 1_j, \dots, 0})^T$. The complete data log likelihood is

$$\log P_{X,Z}(\mathcal{D}, \{z_1, \dots, z_n\}; \Psi) = \log \prod_{i=1}^n \prod_{j=1}^C [P_{X|Z}(x|e_j, \Psi)\pi_j]^{z_{ij}} = \sum_{i,j} z_{ij} \log [P_{X|Z}(x|e_j, \Psi)\pi_j].$$

Thus, in E-step,

$$Q(\Psi; \Psi^{(n)}) = \sum_{i,j} h_{ij} \log[P_{X|Z}(x|e_j, \Psi)\pi_j]$$

where $h_{ij} = E_{Z|X;\Psi^{(n)}}[z_{ij}|\mathcal{D}]$. Hence, we only have to compute

$$h_{ij} = E_{Z|X;\Psi^{(n)}}[z_{ij}|\mathcal{D}] = P_{Z|X}(z_{ij} = 1|x_i;\Psi^{(n)}) = P_{Z|X}(e_j|x_i;\Psi^{(n)})$$

In M-step, we compute

$$\Psi^{(n+1)} = \underset{\Psi}{\operatorname{arg max}} \sum_{i,j} h_{ij} \log[P_{X|Z}(x|e_j, \Psi)\pi_j].$$

For Gaussian mixure, we may solve for h_{ij} first then take the Lagrangian $L = Q(\Psi; \Psi^{(n)}) + \lambda \left(\sum_{j=1}^{C} \pi_j - 1\right)$ to solve for the parameters. Here are the results:

$$h_{ij} = \frac{\mathcal{G}\left(x_i, \mu_j^{(n)}, \sigma_j^{(n)}\right) \pi_j^{(n)}}{\sum_k^C \mathcal{G}\left(x_i, \mu_k^{(n)}, \sigma_k^{(n)}\right) \pi_k^{(n)}} \qquad \qquad \pi_j^{(n+1)} = \frac{1}{n} \sum_{i=1}^n h_{ij}$$
$$\mu_j^{(n+1)} = \frac{\sum_i^n h_{ij} x_i}{\sum_i^n h_{ij}} \qquad \qquad \sigma_j^{2(n+1)} = \frac{\sum_i^n h_{ij} (x_i - \mu_j)^2}{\sum_i^n h_{ij}}$$

MAP-EM

1. **E-step**: compute

$$E_{Z|X,\Psi}[\log P_{\Psi|X,Z}(\Psi|\mathcal{D},z) \mid \mathcal{D}, \Psi^{(n)}] \Rightarrow Q(\Psi|\Psi^{(n)}) + \log P_{\Psi}(\Psi)$$
 (only need to compute Q)

2. M-step: compute

$$\Psi^{(n+1)} = \underset{\Psi}{\operatorname{arg\,max}} \{ Q(\Psi | \Psi^{(n)}) + \log P_{\Psi}(\Psi) \}.$$