

Introduction to Machine Learning

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1. The pdf for two jointly Gaussian random variables X and Y is of the following form parameterized by the scalars m_1 , m_2 , σ_1 , σ_2 and ρ_{XY} :

$$f_{X,Y}(x,y) = \frac{\exp \left\{ \frac{-1}{2(1-\rho_{XY}^2)} \left[\left(\frac{x-m_1}{\sigma_1} \right)^2 - 2\rho_{XY} \left(\frac{x-m_1}{\sigma_1} \right) \left(\frac{y-m_2}{\sigma_2} \right) + \left(\frac{y-m_2}{\sigma_2} \right)^2 \right] \right\}}{2\pi\sigma_1\sigma_2\sqrt{1-\rho_{XY}^2}}. \quad (1)$$

The pdf for multivariate jointly Gaussian random variable $Z \in \mathbb{R}^k$ is of the following form parameterized by $\mu \in \mathbb{R}^k$ and $\Sigma \in \mathbb{R}^{k \times k}$.

$$f_Z(z) = \frac{\exp \left\{ -\frac{1}{2}(z - \mu)^T \Sigma^{-1} (z - \mu) \right\}}{\sqrt{(2\pi)^k |\Sigma|}}. \quad (2)$$

Suppose $Z = [X, Y]^T$, i.e., $z = [x, y]^T$.

- (a) Find μ , Σ^{-1} and Σ in terms of m_1 , m_2 , σ_1 , σ_2 and ρ_{XY} .
- (b) Suppose $\rho_{XY} = 0$, what is Σ in this case? Can you write $f_{X,Y}(x, y)$ as the product of two single variate Gaussian distributions? Are X and Y independent?

2. The Gaussian Discriminant Analysis (GDA) models the class conditional distribution as multivariate Gaussian, i.e, $P(X|Y) \sim \mathcal{N}(\mu_Y, \Sigma)$. Suppose we want to enforce the **Naive Bayes (NB) assumption**, i.e. $P(X_i|Y, X_j) = P(X_i|Y), \forall j \neq i$, to GDA. Show that all off diagonal elements of Σ equal to 0: $\Sigma_{i,j} = 0, \forall i \neq j$ with the **NB assumption**.

3. Consider the classification problem for two classes, C_0 and C_1 . In the generative approach, we model the class-conditional distribution $P(x|C_0)$ and $P(x|C_1)$, as well as the class priors $P(C_0)$ and $P(C_1)$. The posterior probability for class C_0 can be written as

$$P(C_0|x) = \frac{P(x|C_0)P(C_0)}{P(x|C_0)P(C_0) + P(x|C_1)P(C_1)}.$$

- (a) Show that $P(C_0|x) = \sigma(a)$ where $\sigma(a)$ is the *sigmoid* function defined by

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

Find a in terms of $P(x|C_0)$, $P(x|C_1)$, $P(C_0)$ and $P(C_1)$.

- (b) In the GDA model, we have the class conditional distribution as follows

$$P(x|C_0) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_0)^T \Sigma^{-1}(x - \mu_0)\right),$$

$$P(x|C_1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1)\right).$$

Suppose we are able to find the maximum likelihood estimation of $\mu_0, \mu_1, \Sigma, P(C_0)$, and $P(C_1)$. Show that $a = w^T x + b$ for some w and b . Find w and b in terms of $\mu_0, \mu_1, \Sigma, P(C_0)$, and $P(C_1)$. This shows that the decision boundary is linear.

- (c) In (b), we modeled the class conditional distribution with same covariance matrix Σ . Now let us consider two classes that have difference covariance matrix as follows

$$P(x|C_0) = \frac{1}{(2\pi)^{n/2}|\Sigma_0|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_0)^T \Sigma_0^{-1}(x - \mu_0)\right),$$

$$P(x|C_1) = \frac{1}{(2\pi)^{n/2}|\Sigma_1|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_1)^T \Sigma_1^{-1}(x - \mu_1)\right).$$

Suppose we are able to find the maximum likelihood estimation of $\mu_0, \mu_1, \Sigma_0, \Sigma_1, P(C_0)$, and $P(C_1)$. Show that $a = x^T A x + w^T x + b$ for some A, w and b . Find w and b in terms of $\mu_0, \mu_1, \Sigma_0, \Sigma_1, P(C_0)$, and $P(C_1)$. This shows that the decision boundary is quadratic.

4. We are given a training set $\{(x^{(i)}, y^{(i)}); i = \{1, \dots, m\}\}$, where $x^{(i)} \in R^n$ and $y^{(i)} \in \{0, 1\}$. We consider the Gaussian Discriminant Analysis (GDA) model, which models $P(x|y)$ using multivariate Gaussian. Writing out the model, we have:

$$P(y = 1) = \phi = 1 - P(y = 0)$$

$$P(x|y = 0) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_0)^T \Sigma^{-1}(x - \mu_0)\right)$$

$$P(x|y = 1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_1)^T \Sigma^{-1}(x - \mu_1)\right)$$

The log-likelihood of the data is given by:

$$L(\phi, \mu_0, \mu_1, \Sigma) = \ln P(x^{(1)}, \dots, x^{(m)}, y^{(1)}, \dots, y^{(m)}) = \ln \prod_{i=1}^m P(x^{(i)}|y^{(i)})P(y^{(i)}).$$

In this exercise, we want to maximize $L(\phi, \mu_0, \mu_1, \Sigma)$ with respect to ϕ, μ_0 . The maximization over Σ is left for discussion.

- (a) Write down the explicit expression for $P(x^{(1)}, \dots, x^{(m)}, y^{(1)}, \dots, y^{(m)})$ and $L(\phi, \mu_0, \mu_1, \Sigma)$.
- (b) Find the maximum likelihood estimate for ϕ . How do you know such ϕ is the “best” but not the “worst”? Hint: Show that the second derivative of $L(\phi, \mu_0, \mu_1, \Sigma)$ with respect to ϕ is negative.
- (c) Find the maximum likelihood estimate for μ_0 . How do you know such μ_0 is the “best” but not the “worst”? Hint: Show that the Hessian Matrix of $L(\phi, \mu_0, \mu_1, \Sigma)$ with respect to μ_0 is negative definite. You may use the following: if A is positive definite, then A^{-1} is also positive definite. Also B is negative definite if $-B$ is positive definite.

5. In this exercise, you will implement a binary classifier using the Gaussian Discriminant Analysis (GDA) model in MATLAB. The data is given in *data.csv*. The first two columns are the feature values and the last column contains the class labels.
- (a) Visualization. Plot the data from different classes in different colors. Is the data linearly separable?
 - (b) In the GDA model, we assume the class label follows a Bernoulli distribution and we model the class conditional distribution as multivariate Gaussian with same covariance matrix (Σ) and different means (μ_0 and μ_1). Find the maximum likelihood estimate of the parameters $P(y = 0)$ (parameter for the Bernoulli distribution), μ_0 , μ_1 and Σ given this data set.
 - (c) Using the result you find in Question 3 and your ML estimate of model parameters, find the decision boundary parameterized by $w^T x + b = 0$. Report w , b and plot the decision boundary on the same plot.
 - (d) Visualize your results by plotting the contour of the two distributions $P(x, y = 0)$ and $P(x, y = 1)$. For consistency, set 'LevelList' ('level' for python) to `logspace(-3,-1,7)`. Does your decision boundary pass through the points where the two distributions have equal probabilities ? Explain why.