ECE M146 | Homework 6 Solution
Introduction to Machine Learning | Monday, May 20, 2019
Instructor: Lara Dolecek
TA: Zehui (Alex) Chen, Ruiyi (John) Wu

1. The Gaussian Discriminant Analysis (GDA) models the class conditional distribution as multivariate Gaussian, i.e, $P(x|y) \sim \mathbb{N}(\mu_y, \Sigma)$. 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 equals to 0: $\Sigma_{i,j} = 0, \forall i \neq j$ with the **NB assumption**.
Solution: By definition:

$$\begin{aligned}
\Sigma_{i,j} &= E\left[(x_i|y - E[x_i|y])\,(x_j|y - E[x_j|y])\right] \\
&= E\left[x_i x_j|y + E[x_i|y]E[x_j|y] - E[x_i|y]x_j|y - x_i|yE[x_j|y]\right] \\
&= 2E[x_i|y]E[x_j|y] - 2E[x_i|y]E[x_j|y] \\
&= 0.
\end{aligned}$$

The second last step comes from the NB assumption.

2. 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 $P(C_1)$.
Solution:

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

(b) In 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.
Solution: Omitted. This is a special case for the solution of (c).

(c) In (b), we model 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 $a = x^T Ax + w^T x + b$ 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.
Solution: We plug the class conditional distribution into the equation of a in (a). Simplify the equation and we have

$$a = \ln \frac{P(C_0)}{P(C_1)} + \ln \frac{|\Sigma_1|^{1/2}}{|\Sigma_0|^{1/2}} - \frac{1}{2}x^T\Sigma_0^{-1}x + \frac{1}{2}x^T\Sigma_1^{-1}x + x^T\Sigma_0^{-1}\mu_0 - x^T\Sigma_1^{-1}\mu_1 - \frac{\mu_0^T\Sigma_0^{-1}\mu_0}{2} + \frac{\mu_1^T\Sigma_1^{-1}\mu_1}{2}.$$

From above, we identify:

$$A = \frac{1}{2}\Sigma_1^{-1} - \frac{1}{2}\Sigma_0^{-1};$$

$$w = \Sigma_0^{-1}\mu_0 - \Sigma_1^{-1}\mu_1;$$

and

$$b = \ln\frac{P(C_0)}{P(C_1)} + \ln\frac{|\Sigma_1|^{1/2}}{|\Sigma_0|^{1/2}} - \frac{\mu_0^T\Sigma_0^{-1}\mu_0}{2} + \frac{\mu_1^T\Sigma_1^{-1}\mu_1}{2}.$$

3. We are given a training set $\{(x^{(i)}, y^{(i)}); i = \{1, \cdots, m\}\}$, 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:

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

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 $P(x^{(1)}, \cdots, x^{(m)}, y^{(1)}, \cdots, y^{(m)})$ and $L(\phi, \mu_0, \mu_1, \Sigma)$.
Solution:

$$\begin{aligned}
&P(x^{(i)}, \cdots, x^{(m)}, y^{(i)}, \cdots, y^{(m)} \\
&= \prod_{i=1}^{m} \left[\frac{1-\phi}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x^{(i)} - \mu_0)^T \Sigma^{-1} (x^{(i)} - \mu_0)\right)\right]^{1-y^{(i)}} \\
&\quad \times \left[\frac{\phi}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x^{(i)} - \mu_1)^T \Sigma^{-1} (x^{(i)} - \mu_1)\right)\right]^{y^{(i)}}
\end{aligned}$$

$$\begin{aligned}
&L(\phi, \mu_0, \mu_1, \Sigma) \\
&= \sum_{i=1}^{m} \left\{ (1 - y^{(i)}) \left[\ln(1-\phi) - \frac{n}{2}\ln(2\pi) - \frac{1}{2}\ln(|\Sigma|) - \frac{1}{2}(x^{(i)} - \mu_0)^T \Sigma^{-1} (x^{(i)} - \mu_0)\right] \right. \\
&\quad \left. + y^{(i)} \left[\ln(\phi) - \frac{n}{2}\ln(2\pi) - \frac{1}{2}\ln(|\Sigma|) - \frac{1}{2}(x^{(i)} - \mu_1)^T \Sigma^{-1} (x^{(i)} - \mu_1)\right] \right\}.
\end{aligned}$$

(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.
Solution: We only care about terms contains ϕ and treat other terms as constant:

$$L(\phi, \mu_0, \mu_1, \Sigma) = \sum_{i=1}^{m} \{y^{(i)} \ln(\phi) + (1 - y^{(i)}) \ln(1 - \phi)\} + const.$$

We set the derivative to 0:

$$\frac{\partial L}{\partial \phi} = \frac{N_1}{\phi} - \frac{N_0}{1-\phi} = 0.$$

where $N_1 = \sum_{i=1}^m y^{(i)}$ and $N_0 = \sum_{i=1}^m (1 - y^{(i)})$. We find $\phi = \frac{N_1}{N_0+N_1}$. Why not the "worst"? We take the second derivative.

$$\frac{\partial^2 L}{\partial \phi^2} = -\frac{N_1}{\phi^2} - \frac{N_0}{(1-\phi)^2} \le 0.$$

This shows that the log likelihood function is concave with respect to ϕ and therefore have a unique maximum.

(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.

Solution: We only care about terms contains μ_0 and treat other terms as constant:

$$\begin{aligned}
L(\phi, \mu_0, \mu_1, \Sigma) &= \sum_{i=1}^m \{-\frac{1}{2}(1 - y^{(i)})(x^{(i)} - \mu_0)^T \Sigma^{-1} (x^{(i)} - \mu_0)\} + const \\
&= -\sum_{i=1}^m [(1 - y^{(i)})(-\mu_0^T \Sigma^{-1} x^{(i)} + \frac{1}{2}\mu_0^T \Sigma^{-1} \mu_0)] + const.
\end{aligned}$$

. Taking the gradient with respect to μ_0:

$$\nabla_{\mu_0} J = -\sum_{i=1}^m [(1 - y^{(i)})(-\Sigma^{-1} x^{(i)} + \Sigma^{-1}\mu_0)].$$

Setting the gradient to 0, we get

$$\mu_0 = \frac{1}{N_0} \sum_{i=1}^m (1 - y^{(i)}) x^{(i)}.$$

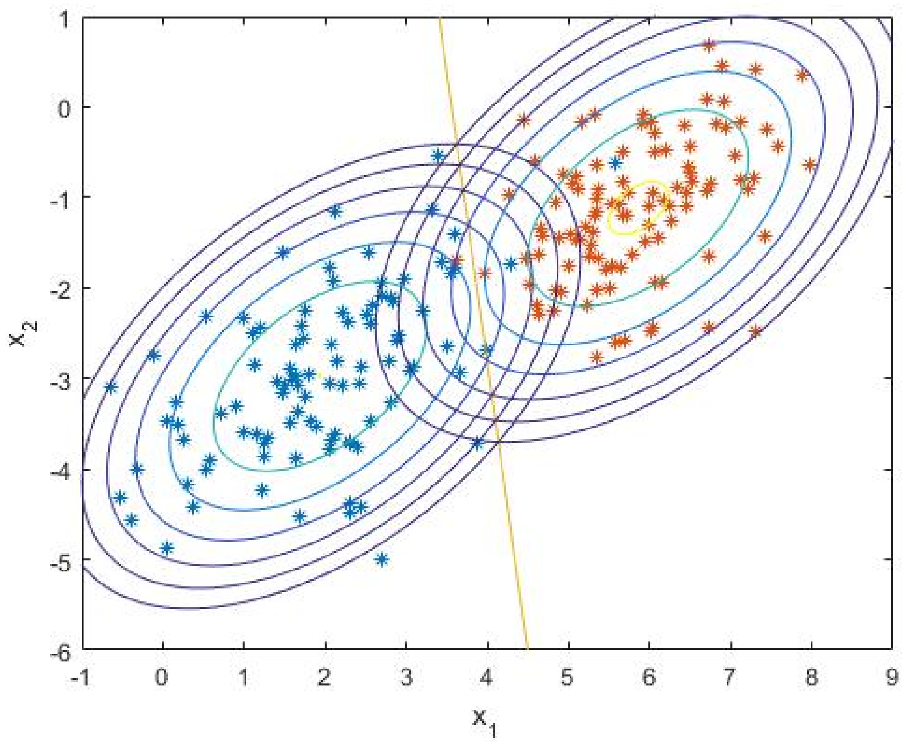
Why not "worst"? Let us calculate the Hessian matrix

$$\nabla^2_{\mu_0} J = -N_0 \Sigma^{-1}.$$

We know Σ is positive definite thus Σ^{-1} is also positive definite. The Hessian matrix is negative definite therefore there is a unique maximum.

4. 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?



   Solution: Not linearly separable.

   (b) In GDA model, we assume the class label follow 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 $P(y=0), \mu_0, \mu_1$ and Σ given this data set.
   Solution:

$$P(y=0) = 0.485, \mu_0 = \begin{bmatrix} 1.9348 \\ -2.9750 \end{bmatrix}, \mu_1 = \begin{bmatrix} 5.8565 \\ -1.1175 \end{bmatrix}, \Sigma = \begin{bmatrix} 1.1187 & 0.4520 \\ 0.4520 & 0.7137 \end{bmatrix}.$$

   (c) Using the result you find in Question 2 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.
   Solution:

$$w = \begin{bmatrix} -3.2979 \\ -0.5138 \end{bmatrix}, b = 11.7360.$$

   (d) Visualize your results by plotting the contour of the two distributions $P(x, y=0)$ and $P(x, y=1)$. For consistency, use *contour(X1,X2,Your Joint Probability Matrix,'LevelList', logspace(-3,-1,7))*. Your decision boundary should pass through

points where the two distribution have equal probabilities. Explain why?
Solution:
$P(x, y = 0) = P(x, y = 1)$ implies $P(y = 0|x) = P(y = 1|x)$. Therefore, the equal probability points on the plot correspond to the equal probability points for the two posterior distribution which is on the decision boundary defined by $w^T x + b = 0$.

5. Suppose we have a data set $\{x_1, \cdots, x_N\}$ and out goal is to partition the data set in to K clusters with μ_k representing the center of the k-th cluster. Recall that in K-means clustering we are attempting to minimize an objective function defined as follows:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|x_n - \mu_k\|_2^2,$$

where $r_{nk} \in \{0, 1\}$ and $r_{nk} = 1$ only if x_n is assigned to cluster k.

(a) What is the minimum value of the objective function when $K = n$ (the number of clusters equals to the number of samples)?
Solution: The minimum is 0 by assigning each x_i an unique cluster with the center also being x_i.

(b) Adding a regularization term, the objective function now becomes:

$$J = \sum_{k=1}^{K} \left[\lambda \|\mu_k\|_2^2 + \sum_{n=1}^{N} r_{nk} \|x_n - \mu_k\|_2^2 \right].$$

Consider the optimization of μ_k with all r_{nk} known. Find the optimal μ_k for

$$\text{argmin}_{\mu_k} \lambda \|\mu_k\|_2^2 + \sum_{n=1}^{N} r_{nk} \|x_n - \mu_k\|_2^2.$$

Solution: Let $f(\mu_k) = \lambda \|\mu_k\|_2^2 + \sum_{n=1}^{N} r_{nk} \|x_n - \mu_k\|_2^2$. Taking the gradient with respect to μ_k, we have:

$$\nabla f(\mu_k) = 2\lambda\mu_k - 2 \sum_{n=1}^{N} r_{nk}(x_n - \mu_k).$$

Letting the gradient to be 0, we get:

$$\mu_k^* = \frac{\sum_{n=1}^{N} r_{nk} x_n}{\lambda + \sum_{n=1}^{N} r_{nk}}.$$