

CSE – 426 Homework 3

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1) Let $\{y^{(i)}\}_{i=1}^m$ be an I.I.D. sample from a multinomial distribution with unknown parameters $(\phi_1, \phi_2, \dots, \phi_k)$, where $y^{(i)} \in \{1, \dots, k\}$ and ϕ_j is the probability that a sample is equal to j . Find the MLE of $(\phi_1, \phi_2, \dots, \phi_k)$ from the observations. Your answer should include a log-likelihood function, the partial derivatives of the log-likelihood with respect to ϕ_j , $j = 1, \dots, k$, and then use the constraint that $\sum_j \phi_j = 1$ to find a formula for the MLE of ϕ_j in terms of the observations. [Hints: one way to solve for ϕ_j , $j = 1, \dots, k$, is to replace ϕ_k with $1 - \sum_{j \neq k} \phi_j$ and maximize the log-likelihood involving $\phi_1, \phi_2, \dots, \phi_{k-1}$ as an unconstrained optimization problem. The other approach is to maximize the log-likelihood with respect to all the k parameters, subject to the constraint that $\sum_j \phi_j = 1$. The Lagrangian method will then be used.] (Refer to PRML (2.32))

(Proof): To start, we can see that the probability distribution of y is defined as

$$P(y|\boldsymbol{\phi}) = \prod_{j=1}^k \phi_j^{1[y=j]}.$$

Now, we can derive the likelihood function

$$\begin{aligned} L(\boldsymbol{\phi}; \{y^{(i)}\}_{i=1}^m) &= \prod_{i=1}^m P(y^{(i)}|\boldsymbol{\phi}) = \prod_{i=1}^m \prod_{j=1}^k \phi_j^{1[y^{(i)}=j]} \\ &= \prod_{j=1}^k \phi_j^{\sum_{i=1}^m 1[y^{(i)}=j]}. \end{aligned}$$

Likewise, we can derive the log-likelihood function to be

$$\ell(\boldsymbol{\phi}) = \log L(\boldsymbol{\phi}) = \sum_{j=1}^k \log \phi_j \sum_{i=1}^m 1[y^{(i)} = j].$$

Setting up a Lagrangian, we have

$$\mathcal{L}(\boldsymbol{\phi}, \lambda) = \sum_{j=1}^k \log \phi_j \sum_{i=1}^m 1[y^{(i)} = j] + \lambda \left(\sum_{j=1}^k \phi_j - 1 \right).$$

In order to maximize this function, we will take the derivative with respect to ϕ_j and set it to zero:

$$\begin{aligned} \frac{\partial \mathcal{L}(\boldsymbol{\phi}, \lambda)}{\partial \phi_j} &= \frac{1}{\phi_j} \sum_{i=1}^m 1[y^{(i)} = j] + \lambda = 0 \\ \rightarrow \phi_j &= -\frac{\sum_{i=1}^m 1[y^{(i)} = j]}{\lambda}. \end{aligned}$$

Substituting this into the constraint, we have

$$\sum_{j=1}^k \phi_j = 1 \rightarrow -\frac{1}{\lambda} \sum_{j=1}^k \sum_{i=1}^m 1[y^{(i)} = j] = 1$$

$$\rightarrow \lambda = -\sum_{j=1}^k \sum_{i=1}^m 1[y^{(i)} = j] = -m.$$

Finally, substituting this back into the above equation, we have

$$\phi_j = \frac{\sum_{i=1}^m 1[y^{(i)} = j]}{m}.$$

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2) Let $y \in \{1, \dots, k\}$ be distributed according to a multinomial distribution with parameters $(\phi_1, \phi_2, \dots, \phi_k)$, where the probability of y taking j is ϕ_j . Let m observations be $\{y^{(1)}, \dots, y^{(m)}\}$, where $y^{(i)}$ is sampled from the multinomial. We know that MLE will estimate ϕ_j as $\sum_{i=1}^m \mathbb{I}[y^{(i)} = j]/m$. Prove that the Laplacian smoothing for multinomial distributions does generate a probability distribution over the set $\{1, \dots, k\}$.

[Hints: add a hallucinated sample to each class and follow the MLE of multinomial. You can use the conclusion about ϕ_j^{MLE} without proving it.]

(Proof): We are given the MLE of ϕ_j as

$$\phi_j^{MLE} = \frac{1}{m} \sum_{i=1}^m \mathbb{I}[y^{(i)} = j].$$

Laplacian smoothing will add 1 to the quantity $\sum_{i=1}^m \mathbb{I}[y^{(i)} = j]$, increasing m to $m + k$, where k is the number of classes. Thus, the Laplacian smoothing estimate of the MLE of ϕ_j is defined as

$$\phi_j^* = \frac{1}{m + k} \sum_{i=1}^m \mathbb{I}[y^{(i)} = j] + 1.$$

We can see that

$$\sum_{j=1}^k \phi_j^* = \frac{1}{m + k} \sum_{j=1}^k \sum_{i=1}^m \mathbb{I}[y^{(i)} = j] + 1 = \frac{m + k}{m + k} = 1.$$

And since we know that $\phi_j^* > 0, \forall j \in \{1, \dots, k\}$, we know that the Laplacian smoothing for the multinomial distribution does indeed generate a probability distribution over the set $\{1, \dots, k\}$. ■

3) Let the training data be $\mathbf{x}^{(1)} = [1, 0, 1]^T$, $y^{(1)} = 1$ and $\mathbf{x}^{(2)} = [0, 1, 1]^T$, $y^{(2)} = 0$. Assume the features and labels are all binary. First identify the parameters that need to be estimated for the Naïve Bayes classifier, then write down the log-likelihood of the training data. Lastly give an estimation of the parameters.

(Solution): Given a binary input vector \mathbf{x} , the Naïve Bayes model has the joint probability density

$$P(\mathbf{x}, y) = P(y)P(\mathbf{x}_1|y)P(\mathbf{x}_2|y) \dots P(\mathbf{x}_n|y) \\ = P(y) \prod_{j=1}^n P(\mathbf{x}_j|y).$$

Thus, each $P(\mathbf{x}_j|y)$ is a Bernoulli random variable parameterized by ϕ_{jy} . Then, given a sample $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^m$, the likelihood function is defined as

$$L(\boldsymbol{\phi}; \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^m) = \prod_{i=1}^m \prod_{j=1}^n P(y^{(i)})P(\mathbf{x}_j^{(i)}|y^{(i)})$$

Which yields the corresponding log-likelihood function

$$\ell(\boldsymbol{\phi}) = \sum_{i=1}^m \sum_{j=1}^n \left\{ \log P(y^{(i)}) + \log P(\mathbf{x}_j^{(i)}|y^{(i)}) \right\}.$$

For this problem, the likelihood function is

$$L(\boldsymbol{\phi}) = \prod_{i=1}^2 P(y^{(i)})P(\mathbf{x}_1^{(i)}|y^{(i)})P(\mathbf{x}_2^{(i)}|y^{(i)})P(\mathbf{x}_3^{(i)}|y^{(i)})$$

Which yields the corresponding log-likelihood function

$$\begin{aligned} \ell(\boldsymbol{\phi}) &= \log \left(\prod_{i=1}^2 P(y^{(i)})P(\mathbf{x}_1^{(i)}|y^{(i)})P(\mathbf{x}_2^{(i)}|y^{(i)})P(\mathbf{x}_3^{(i)}|y^{(i)}) \right) \\ &= \sum_{i=1}^2 \log \left(P(y^{(i)})P(\mathbf{x}_1^{(i)}|y^{(i)})P(\mathbf{x}_2^{(i)}|y^{(i)})P(\mathbf{x}_3^{(i)}|y^{(i)}) \right) \\ &= \sum_{i=1}^2 \left(\log P(y^{(i)}) + \log P(\mathbf{x}_1^{(i)}|y^{(i)}) + \log P(\mathbf{x}_2^{(i)}|y^{(i)}) + \log P(\mathbf{x}_3^{(i)}|y^{(i)}) \right). \end{aligned}$$

Since each of these probabilities are defined over a Bernoulli distribution such that $P(y) = \phi_1^y (1 - \phi_1)^{1-y}$ and $P(\mathbf{x}_j|y) = \phi_{j,y}^y (1 - \phi_{j,y})^{1-y}$, where $\phi_1 = P(Y = 1)$ and $\phi_{j,y} = P(\mathbf{x}_j = 1|Y = y)$. Then we can see that the log likelihood becomes:

$$\begin{aligned} \ell(\boldsymbol{\phi}) &= \sum_{i=1}^2 \left\{ \log \left[\phi_1^{y^{(i)}} (1 - \phi_1)^{1-y^{(i)}} \right] + \log \left[\phi_{1,y^{(i)}}^{y^{(i)}} (1 - \phi_{1,y^{(i)}})^{1-y^{(i)}} \right] \right. \\ &\quad \left. + \log \left[\phi_{2,y^{(i)}}^{y^{(i)}} (1 - \phi_{2,y^{(i)}})^{1-y^{(i)}} \right] + \log \left[\phi_{3,y^{(i)}}^{y^{(i)}} (1 - \phi_{3,y^{(i)}})^{1-y^{(i)}} \right] \right\}. \end{aligned}$$

Now, using the MLE of $\phi_y = P(Y = 1)$ is $\frac{\sum_i 1[y^{(i)}=y]}{m}$, and using the Laplacian smoothing estimate of MLE for ϕ_{jy} , which is $\frac{\sum_i 1[\mathbf{x}_j^{(i)}=1, y^{(i)}=y] + 1}{\sum_i 1[y^{(i)}=y] + 1}$, we can obtain the following parameter estimates for our training data:

$$\phi_1 = \frac{1[y^{(1)} = 1] + 1[y^{(2)} = 1]}{2} = \frac{1 + 0}{2} = \frac{1}{2}.$$

$$\begin{aligned}
\phi_{10} &= \frac{1[x_1^{(1)} = 1, y^{(1)} = 0] + 1[x_1^{(2)} = 1, y^{(2)} = 0] + 1}{1[y^{(1)} = 0] + 1[y^{(2)} = 0] + 1} = \frac{0 + 0 + 1}{0 + 1 + 1} = \frac{1}{2}. \\
\phi_{11} &= \frac{1[x_1^{(1)} = 1, y^{(1)} = 1] + 1[x_1^{(2)} = 1, y^{(2)} = 1] + 1}{1[y^{(1)} = 1] + 1[y^{(2)} = 1] + 1} = \frac{1 + 0 + 1}{1 + 0 + 1} = 1. \\
\phi_{20} &= \frac{1[x_2^{(1)} = 1, y^{(1)} = 0] + 1[x_2^{(2)} = 1, y^{(2)} = 0] + 1}{1[y^{(1)} = 0] + 1[y^{(2)} = 0] + 1} = \frac{0 + 1 + 1}{0 + 1 + 1} = 1. \\
\phi_{21} &= \frac{1[x_2^{(1)} = 1, y^{(1)} = 1] + 1[x_2^{(2)} = 1, y^{(2)} = 1] + 1}{1[y^{(1)} = 1] + 1[y^{(2)} = 1] + 1} = \frac{0 + 0 + 1}{1 + 0 + 1} = \frac{1}{2}. \\
\phi_{30} &= \frac{1[x_3^{(1)} = 1, y^{(1)} = 0] + 1[x_3^{(2)} = 1, y^{(2)} = 0] + 1}{1[y^{(1)} = 0] + 1[y^{(2)} = 0] + 1} = \frac{0 + 1 + 1}{0 + 1 + 1} = 1. \\
\phi_{31} &= \frac{1[x_3^{(1)} = 1, y^{(1)} = 1] + 1[x_3^{(2)} = 1, y^{(2)} = 1] + 1}{1[y^{(1)} = 1] + 1[y^{(2)} = 1] + 1} = \frac{1 + 0 + 1}{1 + 0 + 1} = 1.
\end{aligned}$$

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4) Given two training examples $\mathbf{x}^{(1)} = [2, 1]^T$, $y^{(1)} = 1$ and $\mathbf{x}^{(2)} = [1, -1]^T$, $y^{(2)} = -1$. Find the functional margin and geometric margin of the two training examples to the hyperplane $h(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$ with $\mathbf{w} = [1, -1]^T$ and $b = 2$. Compute the normal direction $\frac{\mathbf{w}}{\|\mathbf{w}\|}$ and the distance from the origin to the hyperplane $\frac{b}{\|\mathbf{w}\|}$. Then draw the two training examples and the hyperplane with its normal direction in \mathbb{R}^2 .

[Hints: use the formula in the SVM lecture notes to answer this question and there is no need to derive the formula. For drawing, hand-drawing is acceptable so long as the positions of the asked elements are approximately correct.]

(Solution): Given a hyperplane $h(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^T \mathbf{x} + b$, the geometric margin of the point \mathbf{x} is defined as

$$\gamma = \frac{y(\mathbf{w}^T \mathbf{x} + b)}{\|\mathbf{w}\|_2}.$$

Thus, the geometric margins of the two training examples are:

$$\begin{aligned}
\gamma^{(1)} &= \frac{y^{(1)}(\mathbf{w}^T \mathbf{x}^{(1)} + b)}{\|\mathbf{w}\|_2} = \frac{1(2 + (-1) + 2)}{\sqrt{1+1}} = \frac{3}{\sqrt{2}}. \\
\gamma^{(2)} &= \frac{y^{(2)}(\mathbf{w}^T \mathbf{x}^{(2)} + b)}{\|\mathbf{w}\|_2} = \frac{-1(1 + 1 + 2)}{\sqrt{1+1}} = -\frac{4}{\sqrt{2}}.
\end{aligned}$$

The functional margin of the point \mathbf{x} with label y is defined as

$$\hat{\gamma} = y(\mathbf{w}^T \mathbf{x} + b)$$

Thus, the functional margins of the two training examples are:

$$\begin{aligned}
\hat{\gamma}^{(1)} &= y^{(1)}(\mathbf{w}^T \mathbf{x}^{(1)} + b) = 1(2 + (-1) + 2) = 3. \\
\hat{\gamma}^{(2)} &= y^{(2)}(\mathbf{w}^T \mathbf{x}^{(2)} + b) = -1(1 + 1 + 2) = -4.
\end{aligned}$$

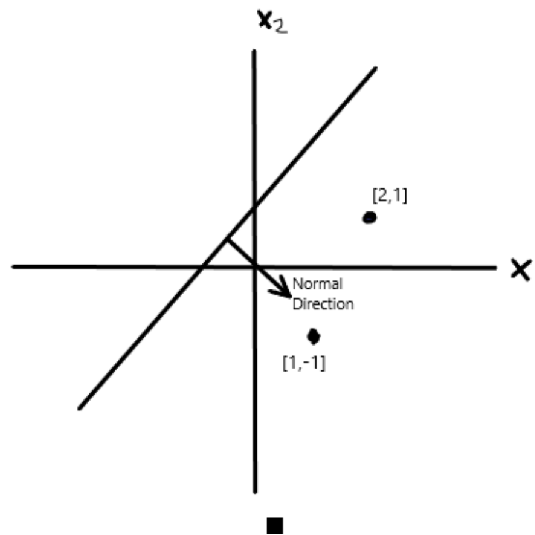
The normal direction is

$$\frac{\mathbf{w}}{\|\mathbf{w}\|_2} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

The distance from the origin to the hyperplane is

$$\frac{b}{\|\mathbf{w}\|_2} = \frac{2}{\sqrt{2}} = \sqrt{2}.$$

Here is the visual representation of the hyperplane with its normal direction and the two points:



5) (Graduate Only) Prove that GDA (Gaussian Discriminant Analysis) with two classes and the same Σ for both classes' Gaussians, leads to a logistic regression model. (Essentially, prove Eq. (4.66) and (4.67) in PRML).

(Proof): Recall that a logistic regression model is the parameterized function $h_{\theta}(\mathbf{x}) = \sigma(\theta^T \mathbf{x})$. Likewise, the GDA model uses Bayes rule to calculate the posterior distribution

$$P(y|\mathbf{x}) = \frac{P(y)P(\mathbf{x}|y)}{P(\mathbf{x})}$$

Where $P(\mathbf{x}|y)$ is the multivariate gaussian distribution

$$P(\mathbf{x}, y = c) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(\mathbf{x} - \mu_c)^T \Sigma^{-1} (\mathbf{x} - \mu_c)}.$$

Thus, we can restate our goal: Prove that $P(y|\mathbf{x})_{GDA} = \sigma(a)$, where a is some linear function.

To this end,

$$P(y = 1|\mathbf{x}) = \frac{P(y = 1)P(\mathbf{x}|y = 1)}{P(\mathbf{x})}$$

$$\begin{aligned}
&= \frac{P(y=1)P(\mathbf{x}|y=1)}{P(y=1)P(\mathbf{x}|y=1) + P(y=0)P(\mathbf{x}|y=0)} = \frac{1}{1 + \frac{P(y=0)P(\mathbf{x}|y=0)}{P(y=1)P(\mathbf{x}|y=1)}} \\
&= \frac{1}{1 + \exp\left\{\log \frac{P(y=0)P(\mathbf{x}|y=0)}{P(y=1)P(\mathbf{x}|y=1)}\right\}}.
\end{aligned}$$

Expanding out the contents of the exponent,

$$\begin{aligned}
&\log \frac{P(y=0)P(\mathbf{x}|y=0)}{P(y=1)P(\mathbf{x}|y=1)} = \log \frac{P(y=0)}{P(y=1)} + \log \frac{P(\mathbf{x}|y=0)}{P(\mathbf{x}|y=1)} \\
&= \log \frac{P(y=0)}{P(y=1)} + \log \frac{\frac{1}{(2\pi)^{n/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_0)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_0)}}{\frac{1}{(2\pi)^{n/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)}} \\
&= \log \frac{P(y=0)}{P(y=1)} + \log \left\{ e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_0)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_0) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)} \right\} \\
&= \log \frac{P(y=0)}{P(y=1)} + -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_0)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_0) + \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_1) \\
&= \log \frac{P(y=0)}{P(y=1)} + \mathbf{x}^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_0 - \mathbf{x}^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 + \frac{1}{2} \boldsymbol{\mu}_1^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 - \frac{1}{2} \boldsymbol{\mu}_0^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_0 \\
&= \{\mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)\}^T \mathbf{x} + \frac{1}{2} \boldsymbol{\mu}_1^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 - \frac{1}{2} \boldsymbol{\mu}_0^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_0 + \log \frac{P(y=0)}{P(y=1)} \\
&= \mathbf{w}^T \mathbf{x} + w_0.
\end{aligned}$$

Here, $\mathbf{w} = \{\mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)\}$ and $w_0 = \frac{1}{2} \boldsymbol{\mu}_1^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_1 - \frac{1}{2} \boldsymbol{\mu}_0^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_0 + \log \frac{P(y=0)}{P(y=1)}$.

Now, inserting this expression back into the following:

$$\frac{1}{1 + e^{\mathbf{w}^T \mathbf{x} + w_0}} = \frac{1}{1 + e^{\mathbf{w}^T \mathbf{x} + w_0}} = \sigma(a).$$

Where, $a = -\mathbf{w}^T \mathbf{x} - w_0$. Therefore, since a is a linear function, we have proven that GDA with two classes and the same covariance matrix for both classes, yields a logistic regression model. ■