Machine Learning 2024 Spring

HW2: Classification

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Methodology

Training data $D \equiv \{(x_1, t_1), (x_2, t_2), ..., (x_N, t_N)\}$, where t_n 's are represented in the 1-of-K format (one hot encoding).

Probabilistic Generative Model

In generative models, we compute (infer) the class-conditional densities $p(x|C_k)$ for each class C_k , as well as the class priors $p(C_k)$, and then use them to compute posterior class probabilities $p(C_k|x)$ through Bayes' theorem.

$$p(C_k|x) = \frac{p(x, C_k)}{\sum_{i=1}^{K} p(x, C_i)} = \frac{p(x|C_k)p(C_k)}{\sum_{i=1}^{K} p(x|C_i)p(C_i)} = \frac{p(x|C_k)p(C_k)}{p(x)}$$

Using the posterior (class) probabilities, we can determine class membership for each new input x. Such classifiers are called Bayesian Classifiers. This approach explicitly or implicitly models the distribution of inputs as well as outputs.

Class prior:

$$p(C_k) = \frac{N_k}{\sum_i N_i} = \frac{N_k}{N}$$

Class-conditional probability distributions (Gaussian distribution with the same covariance matrix but different mean vectors):

$$p(x|C_k) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2} (x - \mu_k)^T \Sigma^{-1} (x - \mu_k)\right\}$$

where

$$\mu_k = \frac{1}{N_k} \sum_{x_n \in C_k} x_n$$

and

$$\Sigma = \frac{1}{N} \sum_{k=1}^{K} N_k S_k$$

where

$$S_k = \frac{1}{N_k} \sum_{x_n \in C_k} (x_n - \mu_k) (x_n - \mu_k)^T$$

Probabilistic Discriminative Model

In the discriminative model, we directly model the conditional probability $p(C_i|x)$ without explicitly modeling the joint distribution. Here, we define the conditional probability as:

$$p(C_i|x) = y_k(x) = \frac{\exp(a_k(x) - a_1(x))}{\sum_{j=1}^{K} \exp(a_j(x) - a_1(x))}$$

where

$$a_k(x) = w_k^T \phi(x)$$

where

$$\phi(x) = [\phi_0(x), \phi_1(x), ..., \phi_{M-1}(x)]^T$$

$$\phi_0(x) = 1, \phi_0(x) = x_1, \phi_0(x) = x_2$$

 x_1 : the offensive value of one data point

 x_2 : the defensive value of one data point

and

$$w_k = [w_{k,0}, w_{k,1}, \dots, w_{k,M-1}]^T$$

Define

$$W = [w_1^T, w_2^T, ..., w_K^T]^T$$

Gradient Descent method

$$W^{(new)} = W^{(old)} - \eta \nabla E(W^{(old)})$$

where

$$\nabla E(W) = \left[\left(\nabla_{w_1} E(W) \right)^T, \left(\nabla_{w_2} E(W) \right)^T, \dots, \left(\nabla_{w_K} E(W) \right)^T \right]^T$$

$$\nabla_{w_j} E(W) = \sum_{n=1}^N \left(y_j (x_n; w_j) - t_{nj} \right) \phi(x_n)$$

**Extra (updating the weights using Adagrad):

$$\forall d \colon W_d^{(new)} = W_d^{(old)} - \frac{\eta}{\sqrt{z_d + \epsilon}} \nabla E(W_d^{(old)})$$

where $\forall d: z_d \leftarrow z_d + \nabla E(W_d^{(old)})^2$

Newton-Raphson method

$$W^{(new)} = W^{(old)} - H^{-1} \nabla E(W^{(old)})$$

where Hessian matrix, $H = \nabla \nabla E(W)$

where

$$\nabla_{w_k} \nabla_{w_j} E(W) = \sum_{n=1}^N y_k(x_n; w_k) \left(I_{kj} - y_j(x_n; w_j) \right) \phi(x_n) \phi(x_n)^T$$

In theory, since $\nabla_{w_k} \nabla_{w_j} E(W) = \nabla_{w_j} \nabla_{w_k} E(W)$, H is symmetric matrix.

Confusion Matrix and Accuracy

Confusion Matrix =
$$\begin{bmatrix} T_0 & F_{01} & F_{02} & F_{03} \\ F_{10} & T_1 & F_{12} & F_{13} \\ F_{20} & F_{21} & T_2 & F_{23} \\ F_{30} & F_{31} & F_{32} & T_3 \end{bmatrix}$$

where

 T_i : The number of samples in class i that are actually predicted as i by the model.

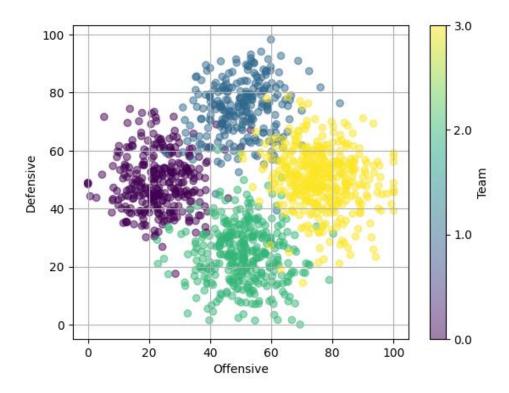
 F_{ij} : The number of samples in class i that are actually predicted as j by the model.

Accuracy =
$$\frac{\sum_{i=0}^{3} T_i}{\sum_{i=0}^{3} (T_i + \sum_{i=0}^{3} F_{ij})} \times 100\%$$

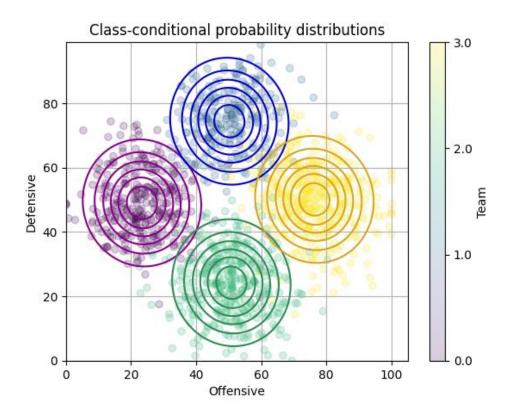
Cross-entropy error function

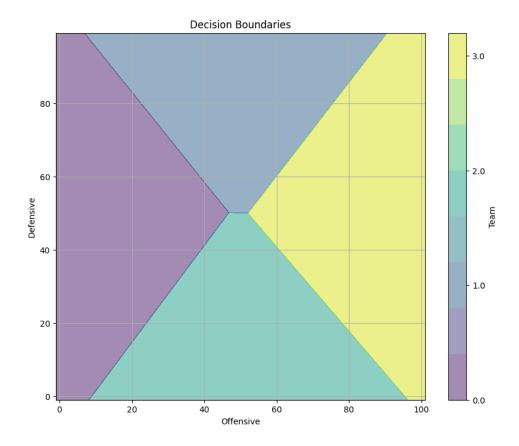
$$-E(w_1, w_2, ..., w_K) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_k(x_n; w_k)$$

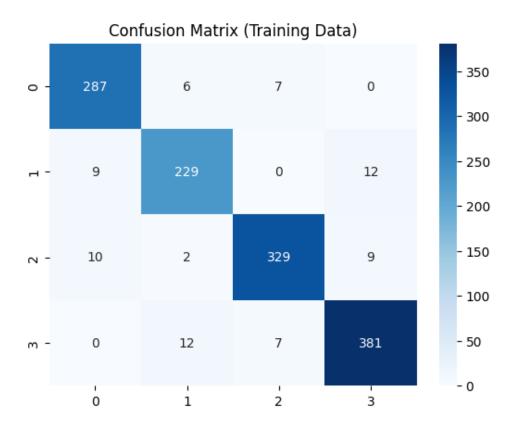
Part I



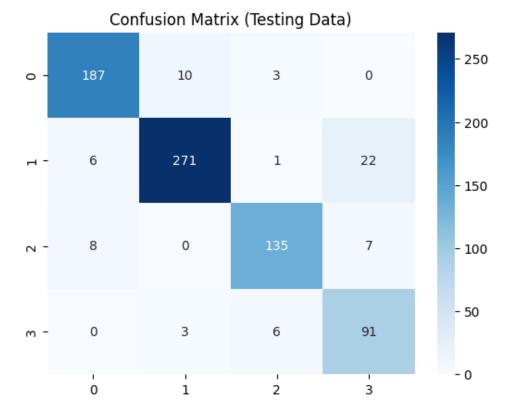
Generative Model







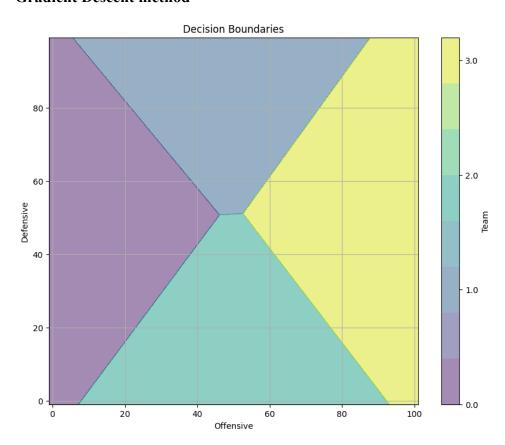
Accuracy (Training Data): 94.3076923076923

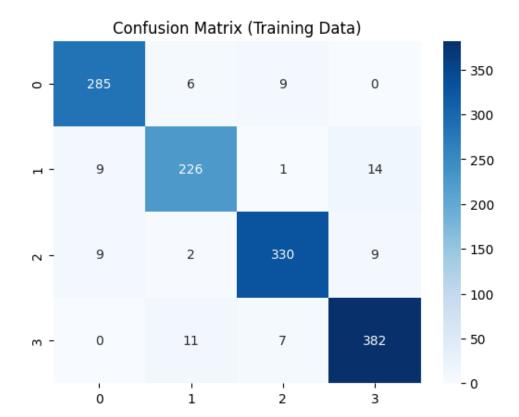


Accuracy (Testing Data): 91.2

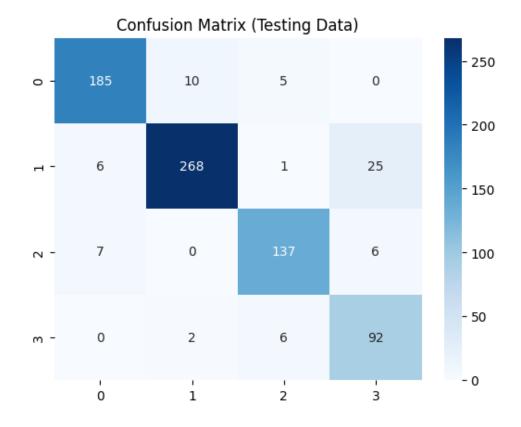
Discriminative Model

Gradient Descent method

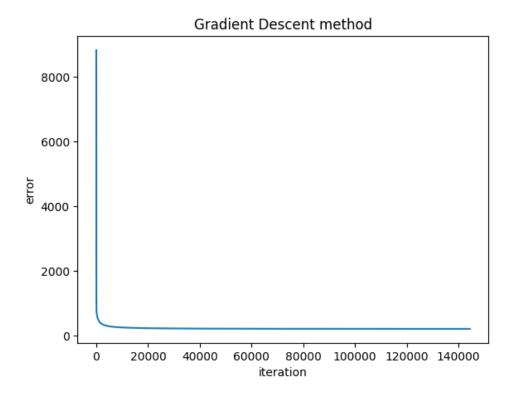




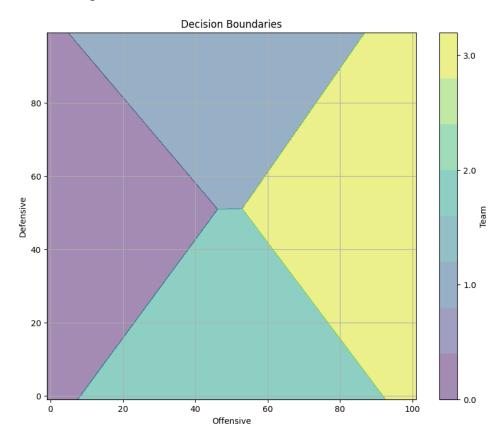
Accuracy (Training Data): 94.07692307692308

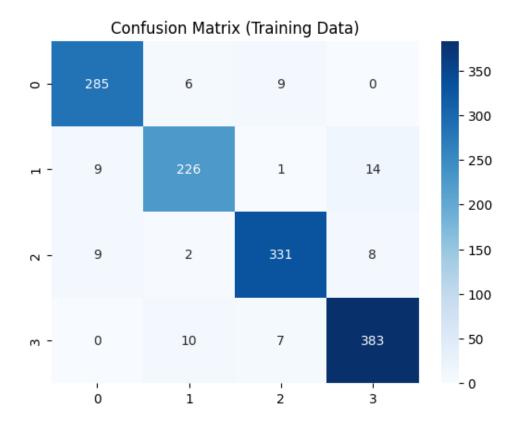


Accuracy (Testing Data): 90.9333333333333

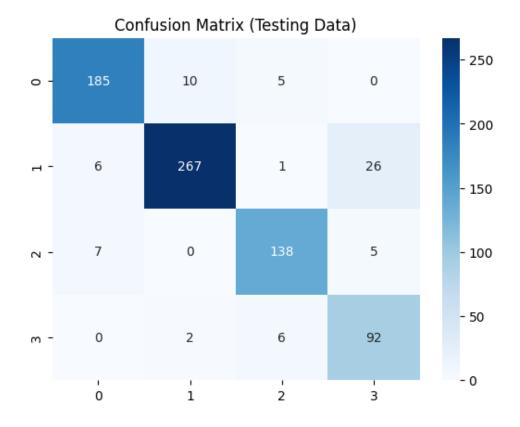


Newton-Raphson method

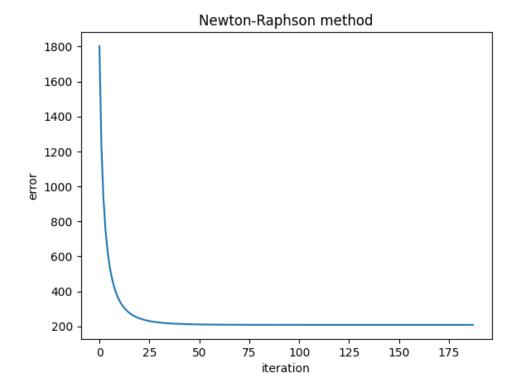




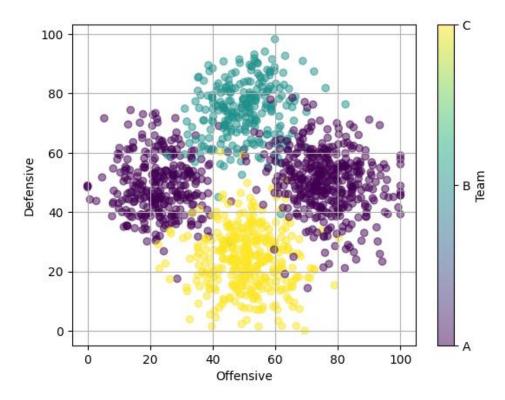
Accuracy (Training Data): 94.23076923076923



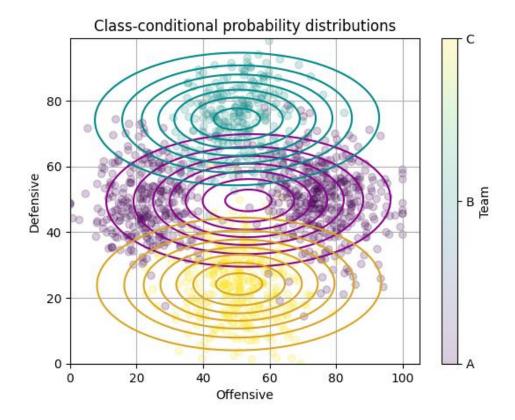
Accuracy (Testing Data): 90.93333333333333

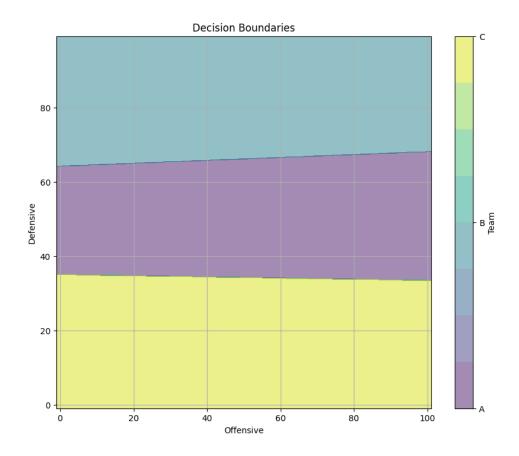


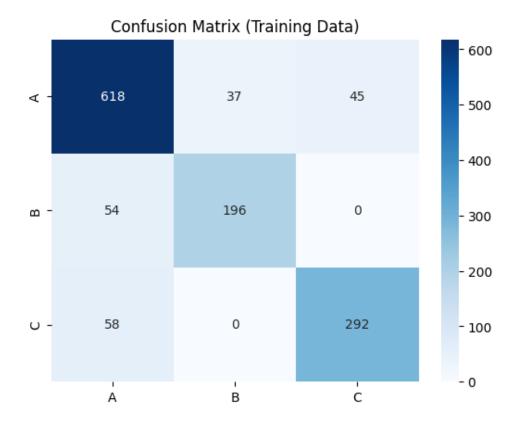
Part II



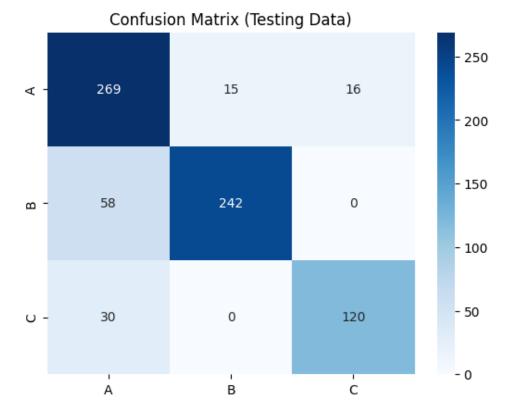
Generative Model







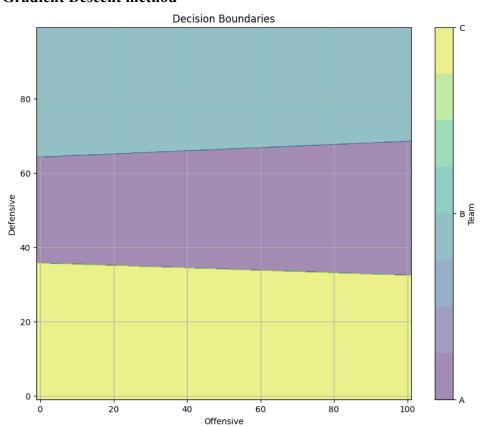
Accuracy (Training Data): 85.07692307692308

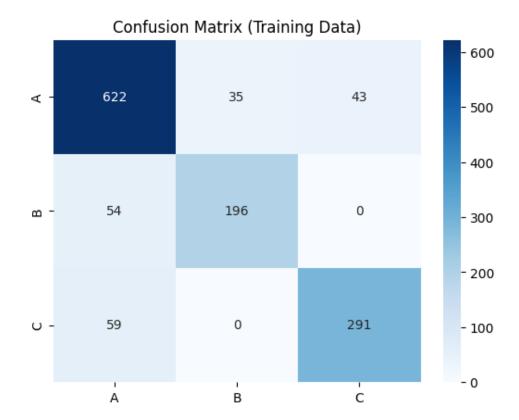


Accuracy (Testing Data): 84.1333333333333

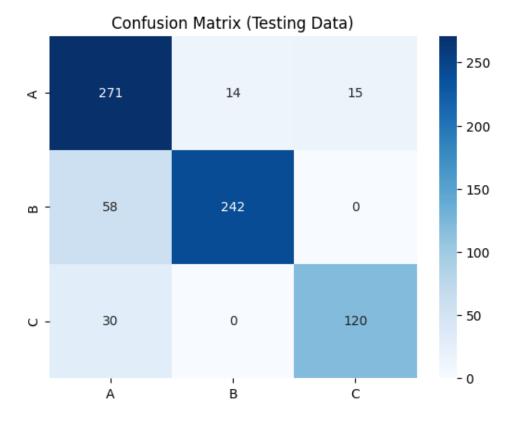
Discriminative Model

Gradient Descent method

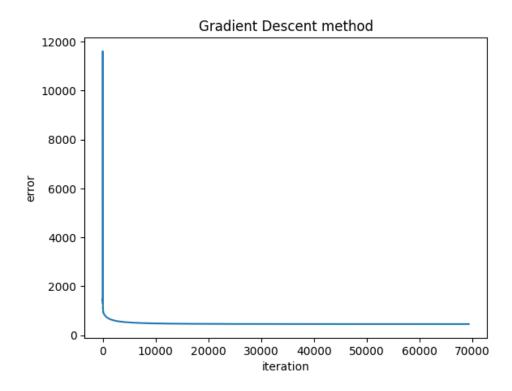




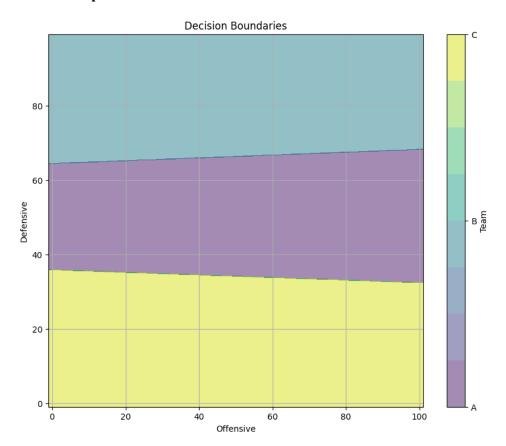
Accuracy (Training Data): 85.3076923076923

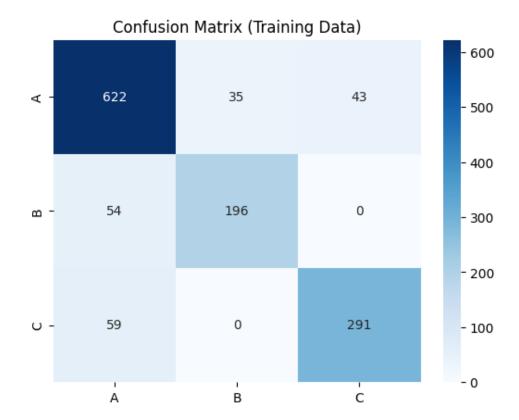


Accuracy (Testing Data): 84.4

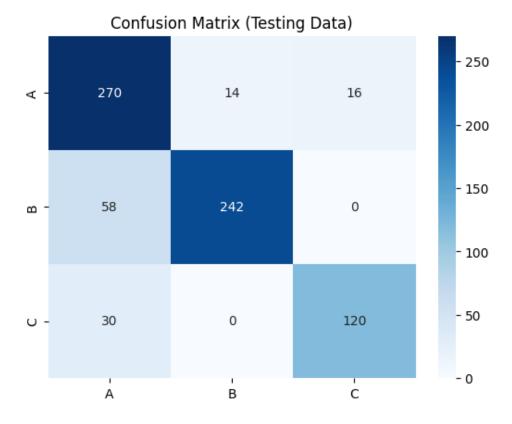


Newton-Raphson method

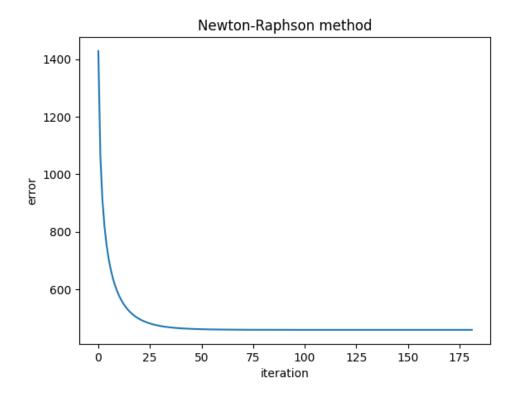




Accuracy (Training Data): 85.3076923076923



Accuracy (Testing Data): 84.2666666666667



Discussion

| Aspect | Generative model | Discriminative model |
|------------|---|--|
| Objective | Learn the joint probability distribution $p(x, C_k)$ then evaluate $p(C_k x)$ | Directly learn the conditional probability distribution $p(C_k x)$ |
| Focus | Models how data is generated from | Models the decision boundary |
| | each class | between classes |
| Data | Requires assumptions about the data | Does not require assumptions |
| Assumption | distribution | about the data distribution |

| Aspect | Gradient Descent method | Newton-Raphson method |
|-------------|---|---|
| Туре | Iterative Optimization Method | |
| Update Rule | Adjusts parameters in the direction of steepest descent (negative gradient) | Uses second-order derivative information to adjust parameters |
| Convergence | Slower | Faster (due to use of second-order information) |
| Complexity | Simple to implement | More complex due to the computation of the Hessian matrix |

In Part I, the generative model achieves slightly higher accuracy than the discriminative model on both the training and testing datasets. Generative models make assumptions about the underlying distribution of the data and model the joint probability of features and labels, which might be beneficial when the assumptions hold true. In this case, assuming Gaussian distributions might have captured the data's structure effectively. Discriminative models, on the other hand, directly model the decision boundary between classes. They don't make assumptions about the data distribution and can sometimes lead to better performance, especially with complex or high-dimensional data.

In Part II, the discriminative model achieves slightly higher accuracy than the generative model on both the training and testing datasets. Part II involves a different classification task where the teams are grouped based on overall performance ratings rather than being classified individually. Discriminative models might be more effective in capturing complex decision boundaries and relationships between features and labels, especially when the classes are not easily separable. The discriminative model might be better suited for this task because it directly models the decision boundary between the classes without making assumptions about the underlying data distribution.

The accuracy of both models dropped slightly in Part II compared to Part I. This could be due to the change in the distribution of data points after modifying the team labels (size of data points for class A [Team 0 and 3 in Part I] is much larger than the size of others (class B and class C)).