CS5805 : Machine Learning I
Lecture #9

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COLLEGE OF ENGINEERING
COMPUTER SCIENCE
VIRGINIA TECH

Generative v.s Discriminative Model

- Two type of probabilistic classification models:

Generative Model

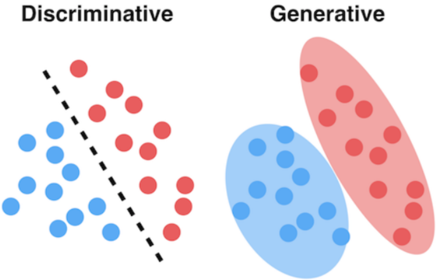
- A Generative model can generate new data instances.
- A statistical model of **joint probability distribution** P(X,Y) on given observable X and target Y.
- Examples : **GANs**, **Naïve Bayes** and **Bayesian Networks**.
- A model of conditional probability of observable X, given a target Y, $P(X|Y = y)$

Discriminative Model

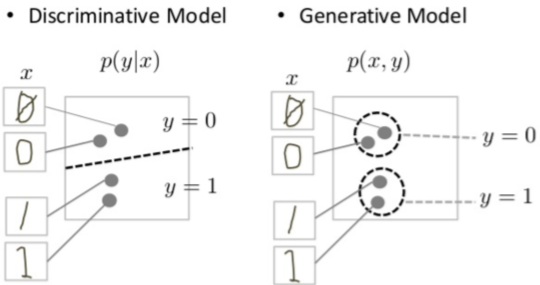
- Discriminative models the **decision boundary between classes**.
- A model of **conditional probability** $P(Y|X = x)$ of the target Y, given an observation x.
- Example : **Logistic Regression**. Capture the process of generating Y given X

Generative versus Discriminative

- Discriminative models draw boundaries in the data space.
- Generative try to model how data is placed throughout the space.
- If an accurate data distribution $p(x|y)$ (x : features and y: class) is achievable, then generative model perform better than discriminative model. Otherwise discriminative model will be used.
- Generative models are prone to outliers.



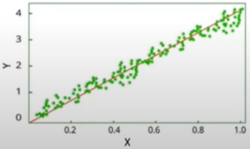
Generative versus Discriminative



Type of Regression

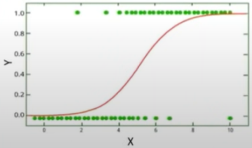
Linear Regression

- When there is a linear relationship between independent and dependent variables.



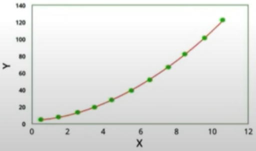
Logistic Regression

- When the dependent variable is categorical (0/ 1, True/ False, Yes/ No, A/B/C) in nature.



Polynomial Regression

- When the power of independent variable is more than 1.



Logistic Regression

- Logistic regression is a classification model that is very easy to implement and performs very well on linearly separable classes.
- It is one of the most widely used algorithms for classification in industry.
- Logistic regression is a linear model for binary classification.
- To explain the idea behind logistic regression as a probabilistic model for binary classification, let define **Odds** in a favor or a particular event:

$$\frac{P(t=1|\mathbf{z})}{P(t=0|\mathbf{z})}$$

- For classifying a test record, it suffices to predict if the odds is > 1 or < 1.

Odds Ratio in Logistic Regression

- Suppose that seven out of 10 male dogs are admitted to an obedience school while three of 10 female dogs are admitted. The probabilities for admitting male dogs (p) and probability of not being admitted male dogs (q) are:

$$p = \frac{7}{10}, q = \frac{3}{10}$$

- Same probabilities for female :

$$p = \frac{3}{10}, q = \frac{7}{10}$$

- logit: A logit is defined as the log base e of the odds.

$$logit(p) = \log_e(\frac{p}{q})$$

	Admitted	Not admitted
Male	7	3
Female	3	7

Odds Ratio in Logistic Regression

- Now we can use the probabilities to compute the odds of admission for both males and females:

$$odds(male) = \frac{0.7}{0.3} = 2.33, odds(female) = \frac{0.3}{0.7} = 0.42$$

- Next, we compute the odds ratio for admission,

$$odds\_ratio = \frac{2.33}{0.42} = 5.44$$

- Thus, for a <u>male</u>, the odds of being admitted are $\boxed{5.44}$ times as large as the odds for a female being admitted.

Logistic function

- The goal is to predict the target class t from an input $z = w^T x + b$.

Logistic function

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- The probability $P(t = 1|z)$ that input z is classified as class $t = 1$ is represented by the output y of the logistic function computed as

$$y = Pr(t = 1|z) = \sigma(z) = \frac{1}{1 + e^{-z}}$$

where z is the multiple linear regression.

Logistic Regression

- Logistic Regression Model :

$$\frac{P(t=1|\mathbf{z})}{P(t=0|\mathbf{z})} = e^{\mathbf{z}} = e^{\mathbf{w}^T\mathbf{x}+b}$$

where $\mathbf{w}$, b are parameters to be learned during training.

Logistic Regression

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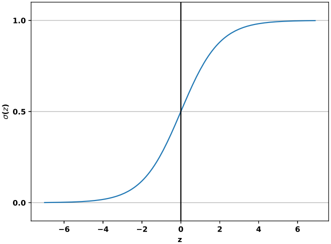
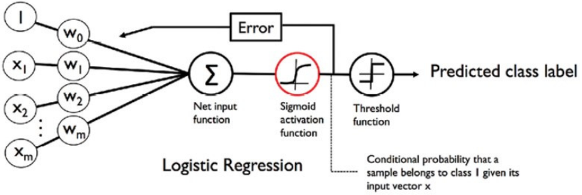
- Sigmoid Function:



Logistic Regression Diagram

- The output of the sigmoid function is then interpreted as the probability of a particular example belonging to class 1, $\sigma(\mathbf{z}) = P(y = 1|\mathbf{x}, \mathbf{w}, b)$
- If the output is 80% for Iris-versicolor flower , therefore, the probability that this flower is an Iris-setosa flower can be calculated as or 20% percent.



Logistic Regression Diagram

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- Logistic regression is used in weather forecasting, for example, not only to predict whether it will rain on a particular day but also to report the chance of rain.

Logistic Regression Diagram

- There are many applications where we are not only interested in the predicted class labels, but where the estimation of the class-membership probability is particularly useful.
- Logistic regression is used in weather forecasting, for example, not only to predict whether it will rain on a particular day but also to report the chance of rain.
- Similarly, logistic regression can be used to predict the chance that a patient has a particular disease given certain symptoms, which is why logistic regression enjoys great popularity in the field of medicine.

Predicted probability

- Let us consider a predictor x and a binary (or Bernoulli) variable y.
- Assuming there exist some relationship between x and y, an ideal model would predict:

$$P(y|x) = \begin{cases} 1: & \text{if y=1} \\ 0: & \text{if y=0} \end{cases}$$

- By using logistic regression, this unknown probability function is modeled as

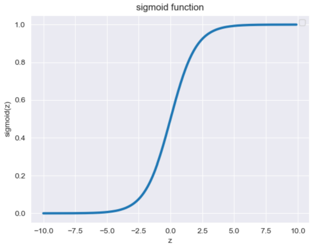
$$\hat{P}(y=1|z) = \sigma(z) = \frac{1}{1+e^{-w^T x}} = \begin{cases} 1: & \text{if } \sigma(z) \geq 0.5 \\ 0: & \text{otherwise} \end{cases}$$

- The predicted probability can then simply be converted into a binary outcome via a threshold function:
- If we look at the preceding plot of the sigmoid function, this is equivalent to the following:

Predicted probability

- If we look at the preceding plot of the sigmoid function, this is equivalent to the following:

$$\hat{y} = \begin{cases} 1: & \text{if } z \geq 0 \\ 0: & \text{otherwise} \end{cases}$$



Learning the weights of the logistic cost function

- Maximize the likelihood of observing training record.
- Likelihood of a single record $(\mathbf{x}_i, y_i)$:

$$\begin{aligned}\ell(\mathbf{w}) &= \hat{P}(y_i|\mathbf{x};\mathbf{w}) \\ &= \hat{P}(1|\mathbf{x}_i,\mathbf{w})^y \times \hat{P}(0|\mathbf{x}_i,\mathbf{w})^{1-y}\end{aligned}$$

- Likelihood of entire training data :

$$\begin{aligned}\ell(\mathbf{w}) &= \prod_{i=1}^{n} \hat{P}(y_i|\mathbf{x}_i,\mathbf{w}) \\ &= \prod_{i=1}^{n} \hat{P}(1|\mathbf{x}_i,\mathbf{w})^{y_i} \times \hat{P}(0|\mathbf{x}_i,\mathbf{w})^{1-y_i}\end{aligned}$$

Logistic Regression Model

- The goal is to find $\mathbf{w}$ that maximizes likelihood function. In practice, we minimizes negative of the (natural) log of likelihood function (**Cross-entropy Function**) (Let $t_i \rightarrow$ target and $y_i = \sigma(z_i)$

$$
\begin{aligned}
J(\mathbf{w}) &= -\sum_{i=1}^{n} [y_i \log(y_i) + (1 - y_i) \log(1 - y_i)] \\
&= -\sum_{i=1}^{n} [y_i \log(\sigma(z_i)) + (1 - y_i) \log(1 - \sigma(z_i))]
\end{aligned}
$$

Logistic Regression Model

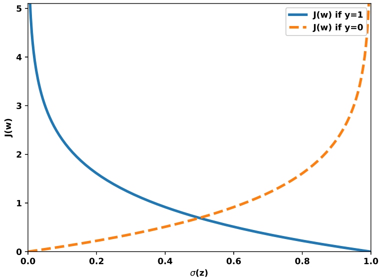
- Learn $\mathbf{w}^*$ that minimize cross-entropy.
- For a single training example, we can see that the first term is zero if $y = 0$ and the second term becomes zero if $y = 1$

$$J(\mathbf{w}) \quad = -\sum_{i=1}^{n} \left[y_i \log(\hat{P}(1|\mathbf{x}_i, \mathbf{w})) + (1 - y_i) \log(\hat{P}(0|\mathbf{x}_i, \mathbf{w})) \right]$$

$$J(\mathbf{w}) = \begin{cases} -\log(P(1\hat{|}\mathbf{x}_i, \mathrm{w}) & \text{if } y_i = 1 \\ -\log(1 - P(1\hat{|}\mathbf{x}_i, \mathrm{w}) & \text{if } y_i = 0 \end{cases}$$

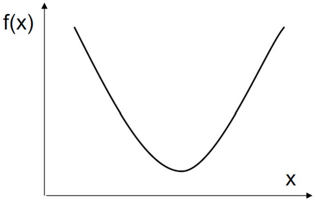
Logistic Regression Model

- It can be observed that the cost function $\rightarrow 0$ (continuous line) if we correctly predict that an example belongs to class 1.
- Similarly, we can see on the y-axis that the cost also approaches 0 if we correctly predict $y = 0$ (dashed line).
- However, if the prediction is wrong, the cost goes toward infinity.
- The main point is that we penalize wrong predictions with an increasingly larger cost.

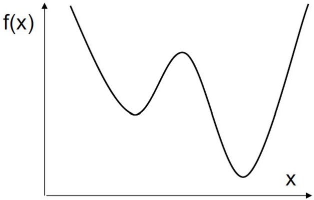


Learning Logistic Model as Convex Optimization

- The minimization of the cross-entropy function is a Convex optimization problem.
- A convex optimization problem:
  - Every local minima is a global minima.
  - Can be solved using standard optimization techniques such as Gradient Descend or Newton's Method.
  - Start with initial solution of model parameters.
  - Update parameters in direction of steepest descend.
  - Converge when gradient is 0 (local minima)



Convex

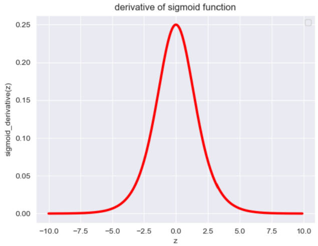


Non-convex

Derivative of Logistic function

- For the gradient descent optimization technique to minimize the logistic function, the derivative with respect to input z can be calculated as:

$$\frac{\partial y}{\partial z} = \frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1 - \sigma(z))$$



Gradient Descent Learning Algorithm for Logistic Regression

- Using calculus, optimum weights can be found by calculating the partial derivative of the log-likelihood function with respect to the jth weight:

$$\frac{\partial}{\partial_j} J(\mathbf{w}) = \left(y \frac{1}{\sigma(z)} - (1-y) \frac{1}{1-\sigma(\mathbf{z})}\right) \frac{\partial}{\partial w_j} \sigma(\mathbf{z})$$

- To update all weights simultaneously, we can write the general update rule as follows:

$$\mathbf{w} := \mathbf{w} + \Delta \mathbf{w}$$

where $\Delta \mathbf{w} = \eta \nabla J(\mathbf{w})$

- Maximizing log-likelihood is equal to minimizing the cost function $J(\mathbf{w})$. Hence:

$$\mathbf{w} := \mathbf{w} - \Delta \mathbf{w}$$

Characteristics of Logistic Regression

- Does not make any assumption about conditional probabilities and directly computes the posterior probability $P(Y|X)$
- Can handle interacting variables.
- Can handle irrelevant and redundant attributes, as long as we can avoid overfitting.
- Robust to high dimensional attributes as it does not involve computing density or distances of points.
- Cannot handle missing values
- Can only learn linear decision boundaries.

ROC curve

- A receiver operating characteristic curve (ROC) curve is a graphical plot that illustrates the performance of a classification model at all classification thresholds.
- This curve plots two parameters: True Positive Rate and False Positive Rate
- **True Positive Rate (TPR)** is a synonym for **recall**:

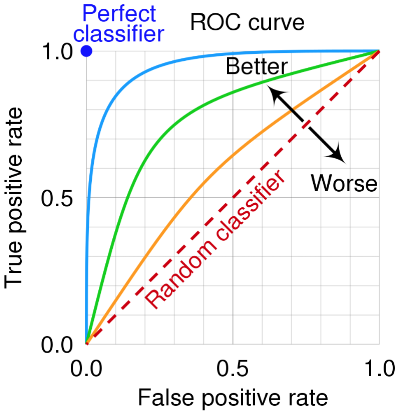
$$TPR = \frac{TP}{TP + FN}$$

- **False Positive Rate (FPR)** is defined as:

$$FPR = \frac{FP}{FP + TN}$$

ROC curve

- An ROC curve plots TPR versus FPR at different classification thresholds.
- Lowering the classification threshold classifies more items as positive, thus increasing both False Positive and True Positive.



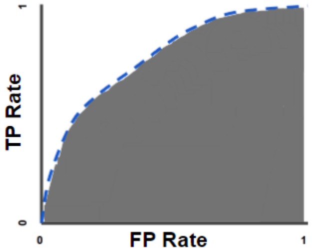
ROC curve example

- The result of model B is on the line. Random guess ACC = 50%.
- Model A performs better than B and C.
- Model C' performs the best.

A			B			C			C'		
TP=63	FN=37	100	TP=77	FN=23	100	TP=24	FN=76	100	TP=76	FN=24	100
FP=28	TN=72	100	FP=77	TN=23	100	FP=88	TN=12	100	FP=12	TN=88	100
91	109	200	154	46	200	112	88	200	88	112	200
TPR = 0.63			TPR = 0.77			TPR = 0.24			TPR = 0.76		
FPR = 0.28			FPR = 0.77			FPR = 0.88			FPR = 0.12		
PPV = 0.69			PPV = 0.50			PPV = 0.21			PPV = 0.86		
F1 = 0.66			F1 = 0.61			F1 = 0.23			F1 = 0.81		
ACC = 0.68			ACC = 0.50			ACC = 0.18			ACC = 0.82		

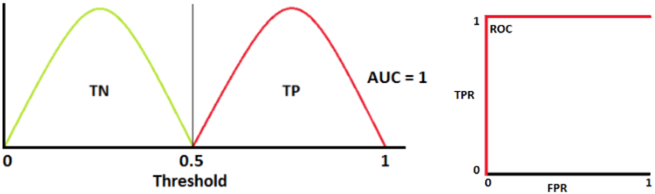
AUC curve

- To compute the points in an ROC curve., we could evaluate a logistic regression model many times with different classification thresholds.
- But this would be inefficient. There is an efficient sorting-based algorithm than can provide this information, called Area Under the ROC Curve (AUC).
- **AUC**measures the entire two-dimensional area underneath the entire ROC curve (think integral calculus) from (0,0) to (1,1)



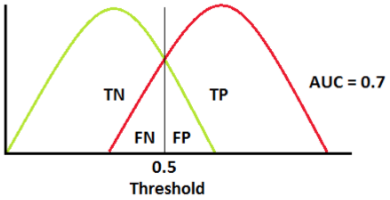
How to speculate about the performance of the model?

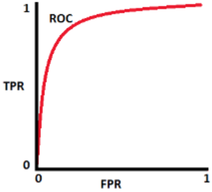
- An excellent model has AUC near to the 1 which means it has a good measure of separability.
- A poor model has an AUC near 0 which means it has the worst measure of separability. It is predicting 0s as 1s and 1s as 0s.
- And when AUC is 0.5, it means the model has no class separation capacity whatsoever.
- In an situation:



Understating of AUC

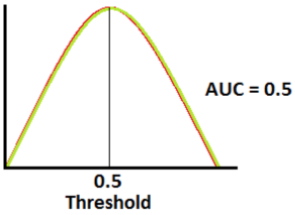
- When two distributions overlap, we introduce type 1 and type 2 errors.
- Depending upon the threshold, we can minimize or maximize them.
- When AUC is 0.7, it means there is a 70% chance that the model will be able to distinguish between positive class and negative class.

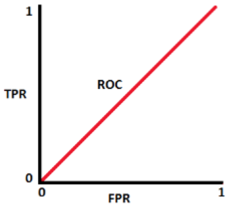




Understating of AUC

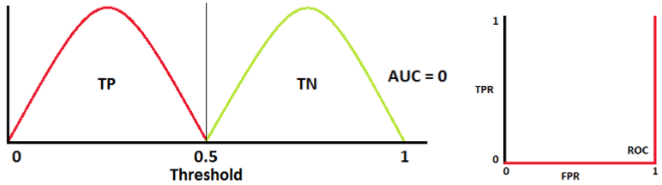
- This is the worst situation.
- When AUC is approximately 0.5, the model has no discrimination capacity to distinguish between positive class and negative class.





Understating of AUC

- When AUC is approximately 0, the model is actually reciprocating the classes.
- It means the model is predicting a negative class as a positive class and vice versa.



5 questions in data analytics