Machine Learning - Classification

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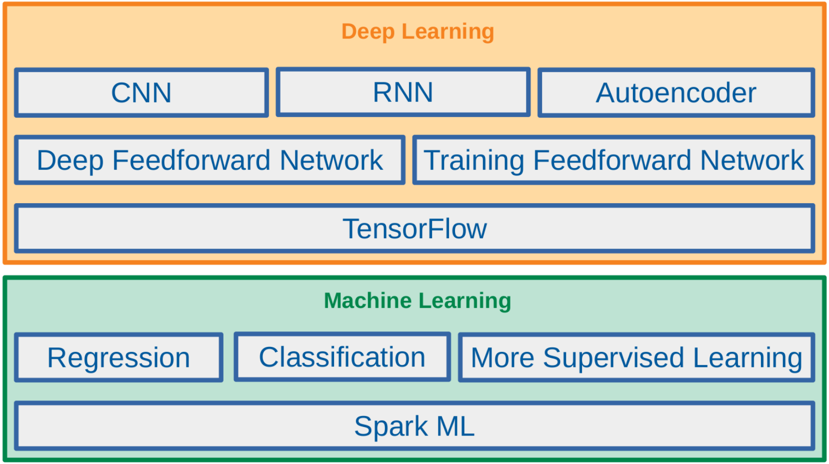
The Course Web Page

https://id2223kth.github.io

Where Are We?


Deep Learning
CNN
RNN
Autoencoder
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
Classification
More Supervised Learning
Spark ML

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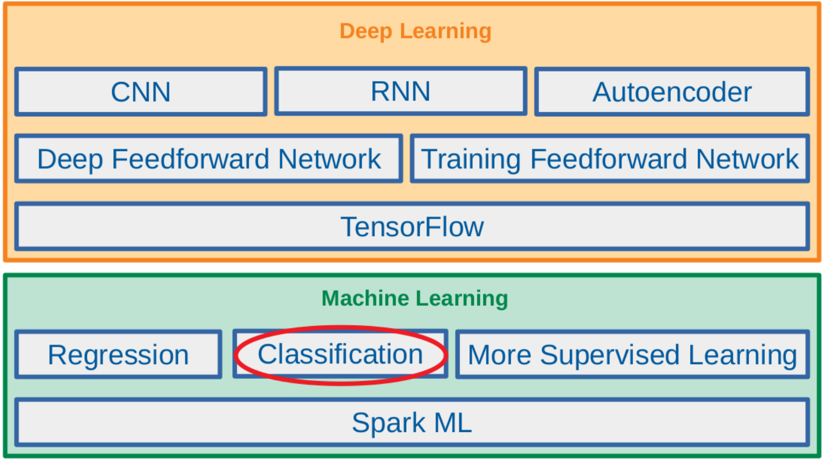
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Let's Start with an Example

Example (1/4)

- Given the dataset of `m` cancer tests.

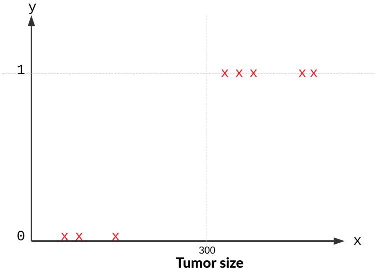
Tumor size	Cancer
330	1
120	0
400	1
⋮	⋮

- Predict the risk of cancer, as a function of the tumor size?

Example (2/4)

Tumor size	Cancer
330	1
120	0
400	1
⋮	⋮

$$\mathbf{x} = \begin{bmatrix} 330 \\ 120 \\ 400 \\ \vdots \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}$$

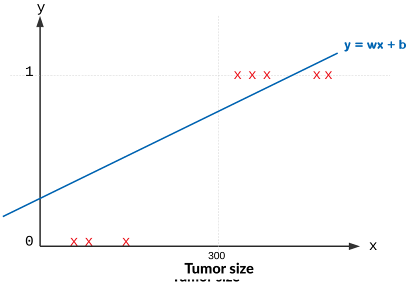


- $\mathbf{x}^{(\mathtt{i})} \in \mathbb{R}$: $\mathtt{x}_1^{(\mathtt{i})}$ is the tumor size of the $\mathtt{i}$th instance in the training set.

Example (3/4)

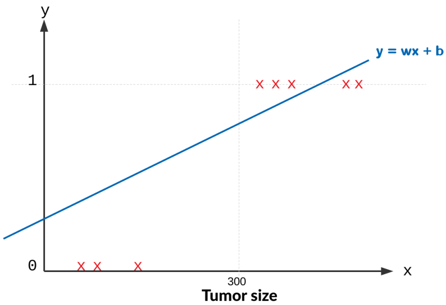
Tumor size	Cancer
330	1
120	0
400	1
⋮	⋮

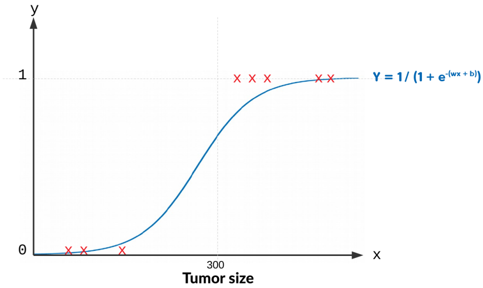
$$\mathbf{x} = \begin{bmatrix} 330 \\ 120 \\ 400 \\ \vdots \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 1 \\ \vdots \end{bmatrix}$$



- Predict the risk of cancer $\hat{y}$ as a function of the tumor sizes x_1, i.e., $\hat{y} = f(x_1)$
- E.g., what is $\hat{y}$, if $x_1 = 500$?
- As an initial choice: $\hat{y} = f_w(\mathbf{x}) = w_0 + w_1 x_1$
- Bad model!

Example (4/4)



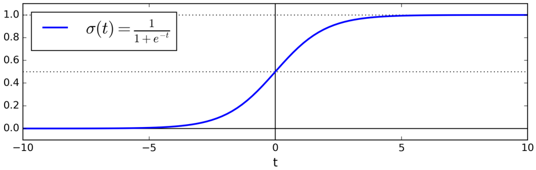


- A better model $\hat{y} = \frac{1}{1+e^{-(w_0+w_1x_1)}}$

Sigmoid Function

- The sigmoid function, denoted by $\sigma(.)$, outputs a number between 0 and 1.

$$\sigma(\mathtt{t}) = \frac{1}{1 + \mathtt{e}^{-\mathtt{t}}}$$

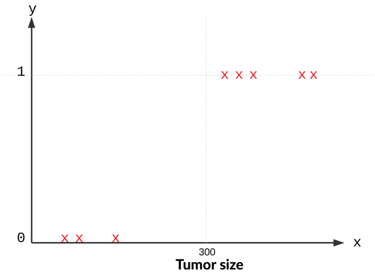


- When $\mathtt{t} < 0$, then $\sigma(\mathtt{t}) < 0.5$
- when $\mathtt{t} \geq 0$, then $\sigma(\mathtt{t}) \geq 0.5$

Binomial Logistic Regression

Binomial Logistic Regression (1/2)

- Our goal: to build a system that takes input $\mathbf{x} \in \mathbb{R}^n$ and predicts output $\hat{y} \in \{0, 1\}$.
- To specify which of 2 categories an input $\mathbf{x}$ belongs to.



Binomial Logistic Regression (2/2)

- Linear regression: the model computes the weighted sum of the input features (plus a bias term).

$$\hat{y} = w_0x_0 + w_1x_1 + w_2x_2 + \cdots + w_nx_n = \mathbf{w}^\intercal\mathbf{x}$$

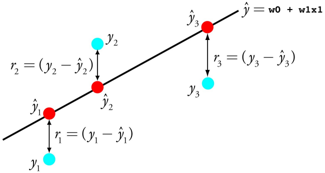
- Binomial logistic regression: the model computes a weighted sum of the input features (plus a bias term), but it outputs the logistic of this result.

$$z = w_0x_0 + w_1x_1 + w_2x_2 + \cdots + w_nx_n = \mathbf{w}^\intercal\mathbf{x}$$

$$\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}} = \frac{1}{1 + e^{-\mathbf{w}^\intercal\mathbf{x}}}$$

How to Learn Model Parameters $\mathbf{w}$?

Linear Regression - Cost Function



- One reasonable model should make $\hat{y}$ close to y, at least for the training dataset.
- Cost function $J(\mathbf{w})$: the mean squared error (MSE)

$$\mathrm{cost}(\hat{y}^{(i)}, y^{(i)}) = (\hat{y}^{(i)} - y^{(i)})^2$$

$$J(\mathbf{w}) = \frac{1}{m}\sum_{i}^{m} \mathrm{cost}(\hat{y}^{(i)}, y^{(i)}) = \frac{1}{m}\sum_{i}^{m}(\hat{y}^{(i)} - y^{(i)})^2$$

Binomial Logistic Regression - Cost Function (1/5)

- Naive idea: minimizing the Mean Squared Error (MSE)

$$\mathtt{cost}(\hat{y}^{(i)}, y^{(i)}) = (\hat{y}^{(i)} - y^{(i)})^2$$

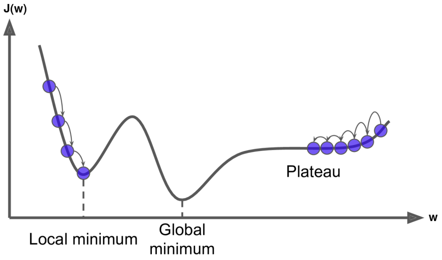
$$J(\mathbf{w}) = \frac{1}{m}\sum_{i}^{m}\mathtt{cost}(\hat{y}^{(i)}, y^{(i)}) = \frac{1}{m}\sum_{i}^{m}(\hat{y}^{(i)} - y^{(i)})^2$$

$$J(\mathbf{w}) = \mathtt{MSE}(\mathbf{w}) = \frac{1}{m}\sum_{i}^{m}\left(\frac{1}{1+e^{-\mathbf{w}^\intercal \mathbf{x}^{(i)}}} - y^{(i)}\right)^2$$

- This cost function is a non-convex function for parameter optimization.

Binomial Logistic Regression - Cost Function (2/5)

- What do we mean by non-convex?
- If a line joining two points on the curve, crosses the curve.
- The algorithm may converge to a local minimum.
- We want a convex logistic regression cost function $J(\mathbf{w})$.



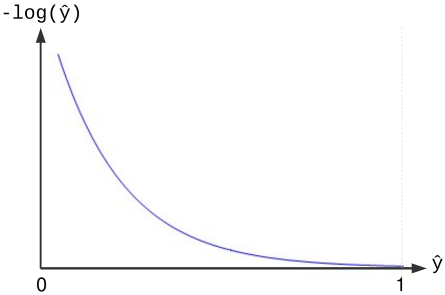
Binomial Logistic Regression - Cost Function (3/5)

- The predicted value $\hat{y} = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^\mathsf{T}\mathbf{x}}}$
- $\texttt{cost}(\hat{y}^{(i)}, y^{(i)}) = ?$
- The $\texttt{cost}(\hat{y}^{(i)}, y^{(i)})$ should be
  - Close to 0, if the predicted value $\hat{y}$ will be close to true value y.
  - Large, if the predicted value $\hat{y}$ will be far from the true value y.

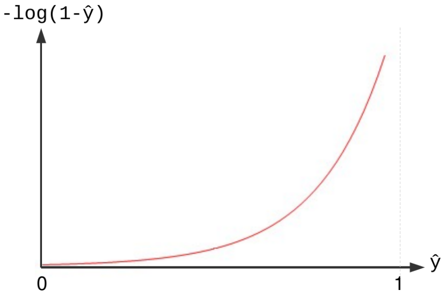
$$\texttt{cost}(\hat{y}^{(i)}, y^{(i)}) = \begin{cases} -\texttt{log}(\hat{y}^{(i)}) & \text{if} \quad y^{(i)} = 1 \\ -\texttt{log}(1 - \hat{y}^{(i)}) & \text{if} \quad y^{(i)} = 0 \end{cases}$$

Binomial Logistic Regression - Cost Function (4/5)

$$\mathtt{cost}(\hat{y}^{(i)}, y^{(i)}) = \begin{cases} -\log(\hat{y}^{(i)}) & \text{if} \quad y^{(i)} = 1 \\ -\log(1 - \hat{y}^{(i)}) & \text{if} \quad y^{(i)} = 0 \end{cases}$$



when $y = 1$



when $y = 0$

Binomial Logistic Regression - Cost Function (5/5)

- We can define $\mathtt{J}(\mathbf{w})$ as below

$$\mathtt{cost}(\hat{\mathtt{y}}^{(\mathtt{i})}, \mathtt{y}^{(\mathtt{i})}) = \begin{cases} -\mathtt{log}(\hat{\mathtt{y}}^{(\mathtt{i})}) & \text{if} \quad \mathtt{y}^{(\mathtt{i})} = 1 \\ -\mathtt{log}(1 - \hat{\mathtt{y}}^{(\mathtt{i})}) & \text{if} \quad \mathtt{y}^{(\mathtt{i})} = 0 \end{cases}$$

$$\mathtt{J}(\mathbf{w}) = \frac{1}{\mathtt{m}} \sum_{\mathtt{i}}^{\mathtt{m}} \mathtt{cost}(\hat{\mathtt{y}}^{(\mathtt{i})}, \mathtt{y}^{(\mathtt{i})}) = -\frac{1}{\mathtt{m}} \sum_{\mathtt{i}}^{\mathtt{m}} (\mathtt{y}^{(\mathtt{i})} \mathtt{log}(\hat{\mathtt{y}}^{(\mathtt{i})}) + (1 - \mathtt{y}^{(\mathtt{i})}) \mathtt{log}(1 - \hat{\mathtt{y}}^{(\mathtt{i})}))$$

How to Learn Model Parameters $\mathbf{w}$?

- We want to choose $\mathbf{w}$ so as to minimize $J(\mathbf{w})$.
- An approach to find $\mathbf{w}$: gradient descent
  - Batch gradient descent
  - Stochastic gradient descent
  - Mini-batch gradient descent

Binomial Logistic Regression Gradient Descent (1/3)

- Goal: find $\mathbf{w}$ that minimizes $\mathtt{J}(\mathbf{w}) = -\frac{1}{\mathtt{m}}\sum_{\mathtt{i}}^{\mathtt{m}}(\mathtt{y}^{(\mathtt{i})}\mathtt{log}(\hat{\mathtt{y}}^{(\mathtt{i})}) + (1 - \mathtt{y}^{(\mathtt{i})})\mathtt{log}(1 - \hat{\mathtt{y}}^{(\mathtt{i})}))$.
- Start at a random point, and repeat the following steps, until the stopping criterion is satisfied:
  1. Determine a descent direction $\frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}}$
  2. Choose a step size η
  3. Update the parameters: $\mathtt{w}^{(\mathtt{next})} = \mathtt{w} - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}}$ (simultaneously for all parameters)

Binomial Logistic Regression Gradient Descent (2/3)

- 1. Determine a descent direction $\frac{\partial J(\mathbf{w})}{\partial w}$.

$$\hat{y} = \sigma(\mathbf{w}^\intercal \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^\intercal \mathbf{x}}}$$

$$J(\mathbf{w}) = \frac{1}{m}\sum_{i}^{m} \mathrm{cost}(\hat{y}^{(i)}, y^{(i)}) = -\frac{1}{m}\sum_{i}^{m}(y^{(i)}\log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)}))$$

$$\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial w_j} &= \frac{1}{m}\sum_{i}^{m} -(y^{(i)}\frac{1}{\hat{y}^{(i)}} - (1 - y^{(i)})\frac{1}{1 - \hat{y}^{(i)}})\frac{\partial \hat{y}^{(i)}}{\partial w_j} \\
&= \frac{1}{m}\sum_{i}^{m} -(y^{(i)}\frac{1}{\hat{y}^{(i)}} - (1 - y^{(i)})\frac{1}{1 - \hat{y}^{(i)}})\hat{y}^{(i)}(1 - \hat{y}^{(i)})\frac{\partial \mathbf{w}^\intercal \mathbf{x}}{\partial w_j} \\
&= \frac{1}{m}\sum_{i}^{m} -(y^{(i)}(1 - \hat{y}^{(i)}) - (1 - y^{(i)})\hat{y}^{(i)})x_j \\
&= \frac{1}{m}\sum_{i}^{m}(\hat{y}^{(i)} - y^{(i)})x_j
\end{aligned}$$

Binomial Logistic Regression Gradient Descent (3/3)

- 2. Choose a step size η
- 3. Update the parameters: $\mathtt{w}_\mathtt{j}^{(\mathtt{next})} = \mathtt{w}_\mathtt{j} - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_\mathtt{j}}$
  - $0 \leq \mathtt{j} \leq \mathtt{n}$, where $\mathtt{n}$ is the number of features.

Binomial Logistic Regression Gradient Descent - Example (1/4)

Tumor size	Cancer
330	1
120	0
400	1

$$\mathbf{X} = \left[\begin{array}{c|c} 1 & 330 \\ 1 & 120 \\ 1 & 400 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

- Predict the risk of cancer $\hat{y}$ as a function of the tumor sizes x_1.
- E.g., what is $\hat{y}$, if $x_1 = 500$?

Binomial Logistic Regression Gradient Descent - Example (2/4)

$$\mathbf{X} = \left[\begin{array}{c|c} 1 & 330 \\ 1 & 120 \\ 1 & 400 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

$$\hat{y} = \sigma(w_0 + w_1 x_1) = \frac{1}{1 + e^{-(w_0 + w_1 x_1)}}$$

$$J(\mathbf{w}) = -\frac{1}{m}\sum_{i}^{m}(y^{(i)}\log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)}))$$

$$\begin{aligned}\frac{\partial J(\mathbf{w})}{\partial w_0} &= \frac{1}{3}\sum_{i}^{3}(\hat{y}^{(i)} - y^{(i)})x_0 \\ &= \frac{1}{3}[(\frac{1}{1 + e^{-(w_0 + 330 w_1)}} - 1) + (\frac{1}{1 + e^{-(w_0 + 120 w_1)}} - 0) + (\frac{1}{1 + e^{-(w_0 + 400 w_1)}} - 1)]\end{aligned}$$

Binomial Logistic Regression Gradient Descent - Example (3/4)

$$\mathbf{X} = \left[\begin{array}{c|c} 1 & 330 \\ 1 & 120 \\ 1 & 400 \end{array}\right] \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

$$\hat{y} = \sigma(w_0 + w_1 x_1) = \frac{1}{1 + e^{-(w_0 + w_1 x_1)}}$$

$$J(\mathbf{w}) = -\frac{1}{m} \sum_{i}^{m} (y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}))$$

$$\frac{\partial J(\mathbf{w})}{\partial w_1} = \frac{1}{3} \sum_{i}^{3} (\hat{y}^{(i)} - y^{(i)}) x_1$$

$$= \frac{1}{3} [330(\frac{1}{1 + e^{-(w_0 + 330 w_1)}} - 1) + 120(\frac{1}{1 + e^{-(w_0 + 120 w_1)}} - 0) + 400(\frac{1}{1 + e^{-(w_0 + 400 w_1)}} - 1)]$$

Binomial Logistic Regression Gradient Descent - Example (4/4)

$$\mathtt{w}_0^{(\mathtt{next})} = \mathtt{w}_0 - \eta \frac{\partial \mathrm{J}(\mathbf{w})}{\partial \mathtt{w}_0}$$

$$\mathtt{w}_1^{(\mathtt{next})} = \mathtt{w}_1 - \eta \frac{\partial \mathrm{J}(\mathbf{w})}{\partial \mathtt{w}_1}$$

Binomial Logistic Regression in Spark

```scala
case class cancer(x1: Long, y: Long)

val trainData = Seq(cancer(330, 1), cancer(120, 0), cancer(400, 1)).toDF
val testData = Seq(cancer(500, 0)).toDF
```

```scala
import org.apache.spark.ml.feature.VectorAssembler

val va = new VectorAssembler().setInputCols(Array("x1")).setOutputCol("features")

val train = va.transform(trainData)
val test = va.transform(testData)
```

```scala
import org.apache.spark.ml.classification.LogisticRegression

val lr = new LogisticRegression().setFeaturesCol("features").setLabelCol("y")
    .setMaxIter(10).setRegParam(0.3).setElasticNetParam(0.8)

val lrModel = lr.fit(train)
lrModel.transform(test).show
```

Binomial Logistic Regression
Probabilistic Interpretation

Probability and Likelihood (1/2)

- Let $\mathtt{X} : \{\mathtt{x}^{(1)}, \mathtt{x}^{(2)}, \cdots, \mathtt{x}^{(\mathtt{m})}\}$ be a discrete random variable drawn independently from a distribution probability $\mathtt{p}$ depending on a parameter θ.
  - For six tosses of a coin, $\mathtt{X} : \{\mathtt{h}, \mathtt{t}, \mathtt{t}, \mathtt{t}, \mathtt{h}, \mathtt{t}\}$, $\mathtt{h}$: head, and $\mathtt{t}$: tail.
  - Suppose you have a coin with probability θ to land heads and $(1 - \theta)$ to land tails.

- $\mathtt{p}(\mathtt{X} \mid \theta = \frac{2}{3})$ is the probability of $\mathtt{X}$ given $\theta = \frac{2}{3}$.

- $\mathtt{p}(\mathtt{X} = \mathtt{h} \mid \theta)$ is the likelihood of θ given $\mathtt{X} = \mathtt{h}$.

- Likelihood ($\mathtt{L}$): a function of the parameters (θ) of a probability model, given specific observed data, e.g., $\mathtt{X} = \mathtt{h}$.

$$\mathtt{L}(\theta) = \mathtt{p}(\mathtt{X} \mid \theta)$$

Probability and Likelihood (2/2)

- If samples in $\mathtt{X}$ are independent we have:

$$\begin{aligned}\mathtt{L}(\theta) = \mathtt{p}(\mathtt{X} \mid \theta) &= \mathtt{p}(\mathtt{x}^{(1)}, \mathtt{x}^{(2)}, \cdots, \mathtt{x}^{(\mathtt{m})} \mid \theta) \\ &= \mathtt{p}(\mathtt{x}^{(1)} \mid \theta)\mathtt{p}(\mathtt{x}^{(2)} \mid \theta) \cdots \mathtt{p}(\mathtt{x}^{(\mathtt{m})} \mid \theta) = \prod_{\mathtt{i}=1}^{\mathtt{m}} \mathtt{p}(\mathtt{x}^{(\mathtt{i})} \mid \theta)\end{aligned}$$

Likelihood and Log-Likelihood

- The Likelihood product is prone to numerical underflow.

$$\mathtt{L}(\theta) = \mathtt{p}(\mathtt{X} \mid \theta) = \prod_{\mathtt{i}=1}^{\mathtt{m}} \mathtt{p}(\mathtt{x}^{(\mathtt{i})} \mid \theta)$$

- To overcome this problem we can use the logarithm of the likelihood.
  - Transforms a product into a sum.

$$\log(\mathtt{L}(\theta)) = \log(\mathtt{p}(\mathtt{X} \mid \theta)) = \sum_{\mathtt{i}=1}^{\mathtt{m}} \log \mathtt{p}(\mathtt{x}^{(\mathtt{i})} \mid \theta)$$

- Negative Log-Likelihood: $-\log \mathtt{L}(\theta) = -\sum_{\mathtt{i}=1}^{\mathtt{m}} \log \mathtt{p}(\mathtt{x}^{(\mathtt{i})} \mid \theta)$

Binomial Logistic Regression and Log-Likelihood (1/2)

- Let's consider the value of $\hat{y}^{(i)}$ as the probability:

$$\begin{cases} p(y^{(i)} = 1 \mid \mathbf{x}^{(i)}; \mathbf{w}) = \hat{y}^{(i)} \\ p(y^{(i)} = 0 \mid \mathbf{x}^{(i)}; \mathbf{w}) = 1 - \hat{y}^{(i)} \end{cases} \Rightarrow p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) = (\hat{y}^{(i)})^{y^{(i)}}(1 - \hat{y}^{(i)})^{(1-y^{(i)})}$$

- So the likelihood is:

$$L(\mathbf{w}) = p(y \mid \mathbf{x}; \mathbf{w}) = \prod_{i=1}^{m} p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) = \prod_{i=1}^{m} (\hat{y}^{(i)})^{y^{(i)}}(1 - \hat{y}^{(i)})^{(1-y^{(i)})}$$

- And the negative log-likelihood:

$$-\log(L(\mathbf{w})) = -\sum_{i=1}^{m} \log p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) = -\sum_{i=1}^{m} y^{(i)}\log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)})$$

Binomial Logistic Regression and Log-Likelihood (2/2)

- The negative log-likelihood:

$$-\log(L(\mathbf{w})) = -\sum_{i=1}^{m} \log p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) = -\sum_{i=1}^{m} y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})$$

- This equation is the same as the the logistic regression cost function.

$$J(\mathbf{w}) = \frac{1}{m} \sum_{i}^{m} (y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}))$$

- Minimize the negative log-likelihood to minimize the cost function $J(\mathbf{w})$.

Binomial Logistic Regression and Cross-Entropy (1/2)

- Negative log-likelihood is also called the cross-entropy
- Coss-entropy: quantify the difference (error) between two probability distributions.
- How close is the predicted distribution to the true distribution?

$$\mathtt{H}(\mathtt{p}, \mathtt{q}) = -\sum_{\mathtt{j}} \mathtt{p}_{\mathtt{j}} \mathtt{log}(\mathtt{q}_{\mathtt{j}})$$

- Where $\mathtt{p}$ is the true distriution, and $\mathtt{q}$ is the predicted distribution.

Binomial Logistic Regression and Cross-Entropy (2/2)

$$H(p, q) = -\sum_j p_j \log(q_j)$$

- The true probability distribution: $p(y = 1) = y$ and $p(y = 0) = 1 - y$
- The predicted probability distribution: $q(y = 1) = \hat{y}$ and $q(y = 0) = 1 - \hat{y}$
- $p \in \{y, 1 - y\}$ and $q \in \{\hat{y}, 1 - \hat{y}\}$
- So, the cross-entropy of p and q is nothing but the logistic cost function.

$$H(p, q) = -\sum_j p_j \log(q_j) = -(y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})) = \text{cost}(y, \hat{y})$$

$$J(\mathbf{w}) = \frac{1}{m}\sum_i^m \text{cost}(y, \hat{y}) = \frac{1}{m}\sum_i^m H(p, q) = -\frac{1}{m}\sum_i^m (y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)}))$$

- Minimize the cross-entropy to minimize the cost function $J(\mathbf{w})$.

Multinomial Logistic Regression

Multinomial Logistic Regression

- Multinomial classifiers can distinguish between more than two classes.
- Instead of $\mathtt{y} \in \{0, 1\}$, we have $\mathtt{y} \in \{1, 2, \cdots, \mathtt{k}\}$.

Binomial vs. Multinomial Logistic Regression (1/2)

- In a binomial classifier, $y \in \{0, 1\}$, the estimator is $\hat{y} = p(y = 1 \mid \mathbf{x}; \mathbf{w})$.
  - We find one set of parameters $\mathbf{w}$.

$$\mathbf{w}^\mathsf{T} = [w_0, w_1, \cdots, w_n]$$

- In multinomial classifier, $y \in \{1, 2, \cdots, k\}$, we need to estimate the result for each individual label, i.e., $\hat{y}_j = p(y = j \mid \mathbf{x}; \mathbf{w})$.
  - We find k set of parameters $\mathbf{W}$.

$$\mathbf{W} = \begin{bmatrix} [w_{0,1}, w_{1,1}, \cdots, w_{n,1}] \\ [w_{0,2}, w_{1,2}, \cdots, w_{n,2}] \\ \vdots \\ [w_{0,k}, w_{1,k}, \cdots, w_{n,k}] \end{bmatrix} = \begin{bmatrix} \mathbf{w}_1^\mathsf{T} \\ \mathbf{w}_2^\mathsf{T} \\ \vdots \\ \mathbf{w}_k^\mathsf{T} \end{bmatrix}$$

Binomial vs. Multinomial Logistic Regression (2/2)

- In a binary class, $y \in \{0, 1\}$, we use the sigmoid function.

$$\mathbf{w}^\mathsf{T}\mathbf{x} = w_0 x_0 + w_1 x_1 + \cdots + w_n x_n$$

$$\hat{y} = p(y = 1 \mid \mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^\mathsf{T}\mathbf{x}}}$$

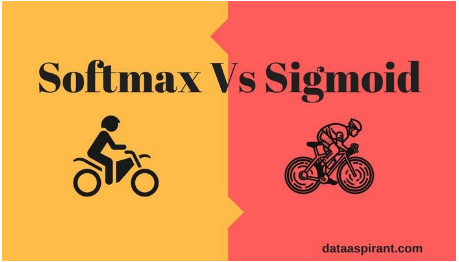
- In multiclasses, $y \in \{1, 2, \cdots, k\}$, we use the softmax function.

$$\mathbf{w}_j^\mathsf{T}\mathbf{x} = w_{0,j} x_0 + w_{1,j} x_1 + \cdots + w_{n,j} x_n, 1 \leq j \leq k$$

$$\hat{y}_j = p(y = j \mid \mathbf{x}; \mathbf{w}_j) = \sigma(\mathbf{w}_j^\mathsf{T}\mathbf{x}) = \frac{e^{\mathbf{w}_j^\mathsf{T}\mathbf{x}}}{\sum_{i=1}^{k} e^{\mathbf{w}_i^\mathsf{T}\mathbf{x}}}$$

Sigmoid vs. Softmax

- Sigmoid function: $\sigma(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}}$
- Softmax function: $\sigma(\mathbf{w}_j^\top \mathbf{x}) = \frac{e^{\mathbf{w}_j^\top \mathbf{x}}}{\sum_{i=1}^{k} e^{\mathbf{w}_i^\top \mathbf{x}}}$
  - Calculate the probabilities of each target class over all possible target classes.
  - The softmax function for two classes is equivalent the sigmoid function.



How Does Softmax Work? - Step 1

- For each instance $\mathbf{x}^{(i)}$, computes the score $\mathbf{w}_j^\intercal \mathbf{x}^{(i)}$ for each class j.

$$\mathbf{w}_j^\intercal \mathbf{x}^{(i)} = w_{0,j} x_0^{(i)} + w_{1,j} x_1^{(i)} + \cdots + w_{n_j} x_n^{(i)}$$

- Note that each class j has its own dedicated parameter vector $\mathbf{w}_j$.

$$\mathbf{W} = \begin{bmatrix} [w_{0,1}, w_{1,1}, \cdots, w_{n,1}] \\ [w_{0,2}, w_{1,2}, \cdots, w_{n,2}] \\ \vdots \\ [w_{0,k}, w_{1,k}, \cdots, w_{n,k}] \end{bmatrix} = \begin{bmatrix} \mathbf{w}_1^\intercal \\ \mathbf{w}_2^\intercal \\ \vdots \\ \mathbf{w}_k^\intercal \end{bmatrix}$$

How Does Softmax Work? - Step 2

- For each instance $\mathbf{x}^{(i)}$, apply the softmax function on its scores: $\mathbf{w}_1^T\mathbf{x}^{(i)}, \cdots, \mathbf{w}_k^T\mathbf{x}^{(i)}$
- Estimates the probability that the instance $\mathbf{x}^{(i)}$ belongs to class j.

$$\hat{y}_j^{(i)} = p(y^{(i)} = j \mid \mathbf{x}^{(i)}; \mathbf{w}_j) = \sigma(\mathbf{w}_j^T\mathbf{x}^{(i)}) = \frac{e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^T\mathbf{x}^{(i)}}}$$

- k: the number of classes.
- $\mathbf{w}_j^T\mathbf{x}^{(i)}$: the scores of class j for the instance $\mathbf{x}^{(i)}$.
- $\sigma(\mathbf{w}_j^T\mathbf{x}^{(i)})$: the estimated probability that $\mathbf{x}^{(i)}$ belongs to class j.

How Does Softmax Work? - Step 3

- Predicts the class with the highest estimated probability.

Softmax Model Estimation and Prediction - Example (1/2)

- Assume we have a training set consisting of $\mathtt{m} = 4$ instances from $\mathtt{k} = 3$ classes.

$$\begin{aligned}
\mathbf{x}^{(1)} &\rightarrow \mathtt{class1}, \mathbf{y}^{(1)\intercal} = [1\ 0\ 0] \\
\mathbf{x}^{(2)} &\rightarrow \mathtt{class2}, \mathbf{y}^{(2)\intercal} = [0\ 1\ 0] \\
\mathbf{x}^{(3)} &\rightarrow \mathtt{class3}, \mathbf{y}^{(3)\intercal} = [0\ 0\ 1] \\
\mathbf{x}^{(4)} &\rightarrow \mathtt{class3}, \mathbf{y}^{(4)\intercal} = [0\ 0\ 1]
\end{aligned}
\qquad
\mathbf{Y} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

- Assume training set $\mathbf{X}$ and random parameters $\mathbf{W}$ are as below:

$$\mathbf{X} = \left[\begin{array}{c|cc} 1 & 0.1 & 0.5 \\ 1 & 1.1 & 2.3 \\ 1 & -1.1 & -2.3 \\ 1 & -1.5 & -2.5 \end{array}\right]
\qquad
\mathbf{W} = \begin{bmatrix} 0.01 & 0.1 & 0.1 \\ 0.1 & 0.2 & 0.3 \\ 0.1 & 0.2 & 0.3 \end{bmatrix}$$

Softmax Model Estimation and Prediction - Example (2/2)

- Now, let's compute the softmax activation:

$$\hat{y}_j^{(i)} = p(y^{(i)} = j \mid \mathbf{x}^{(i)}; \mathbf{w}_j) = \sigma(\mathbf{w}_j^\mathsf{T}\mathbf{x}^{(i)}) = \frac{e^{\mathbf{w}_j^\mathsf{T}\mathbf{x}^{(i)}}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\mathsf{T}\mathbf{x}^{(i)}}}$$

$$\hat{\mathbf{Y}} = \begin{bmatrix} \hat{\mathbf{y}}^{(1)\mathsf{T}} \\ \hat{\mathbf{y}}^{(2)\mathsf{T}} \\ \hat{\mathbf{y}}^{(3)\mathsf{T}} \\ \hat{\mathbf{y}}^{(4)\mathsf{T}} \end{bmatrix} = \begin{bmatrix} 0.29 & 0.34 & 0.36 \\ 0.21 & 0.33 & 0.46 \\ 0.43 & 0.33 & 0.24 \\ 0.45 & 0.33 & 0.22 \end{bmatrix} \quad \text{the predicted classes} = \begin{bmatrix} 3 \\ 3 \\ 1 \\ 1 \end{bmatrix} \quad \text{The correct classes} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

- They are terribly wrong.
- We need to update the weights based on the cost function.
- What is the cost function?

Multinomial Logistic Regression - Cost Function (1/2)

- The objective is to have a model that estimates a high probability for the target class, and consequently a low probability for the other classes.
- Cost function: the cross-entropy between the correct classes and predicted class for all classes.

$$J(\mathbf{w}_j) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{j=1}^{k} y_j^{(i)} \log(\hat{y}_j^{(i)})$$

- $y_j^{(i)}$ is 1 if the target class for the ith instance is j, otherwise, it is 0.

Multinomial Logistic Regression - Cost Function (2/2)

- If there are two classes ($k = 2$), this cost function is equivalent to the logistic regression's cost function.

$$J(\mathbf{w}) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}\log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)})]$$

How to Learn Model Parameters $\mathbf{W}$?

- Goal: find $\mathbf{W}$ that minimizes $\mathtt{J}(\mathbf{W})$.
- Start at a random point, and repeat the following steps, until the stopping criterion is satisfied:
  1. Determine a descent direction $\frac{\partial \mathtt{J}(\mathbf{W})}{\partial \mathtt{w}}$
  2. Choose a step size η
  3. Update the parameters: $\mathtt{w}^{(\mathtt{next})} = \mathtt{w} - \eta \frac{\partial \mathtt{J}(\mathbf{W})}{\partial \mathtt{w}}$ (simultaneously for all parameters)

Multinomial Logistic Regression in Spark

```
val training = spark.read.format("libsvm").load("multiclass_data.txt")
```

```
import org.apache.spark.ml.classification.LogisticRegression

val lr = new LogisticRegression().setMaxIter(10).setRegParam(0.3).setElasticNetParam(0.8)
val lrModel = lr.fit(training)
```

```
println(s"Coefficients: \n${lrModel.coefficientMatrix}")
println(s"Intercepts: \n${lrModel.interceptVector}")
```

Performance Measures

Performance Measures

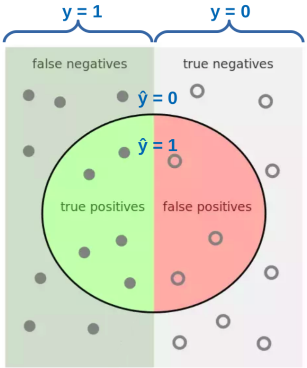
- Evaluate the performance of a model.
- Depends on the application and its requirements.
- There are many different types of classification algorithms, but the evaluation of them share similar principles.

Evaluation of Classification Models (1/3)

- In a classification problem, there exists a true output y and a model-generated predicted output $\hat{y}$ for each data point.
- The results for each instance point can be assigned to one of four categories:
  - True Positive (TP)
  - True Negative (TN)
  - False Positive (FP)
  - False Negative (FN)

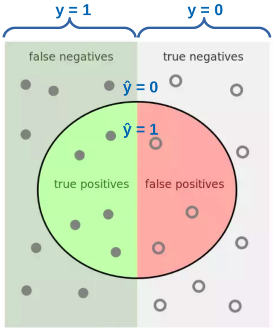
Evaluation of Classification Models (2/3)

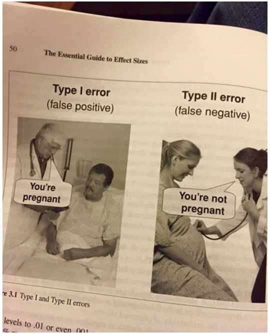
- True Positive (TP): the label y is positive and prediction $\hat{y}$ is also positive.
- True Negative (TN): the label y is negative and prediction $\hat{y}$ is also negative.



Evaluation of Classification Models (3/3)

- False Positive (FP): the label y is negative but prediction $\hat{y}$ is positive (type I error).
- False Negative (FN): the label y is positive but prediction $\hat{y}$ is negative (type II error).





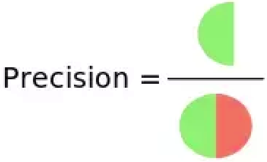
Why Pure Accuracy Is Not A Good Metric?

- Accuracy: how close the prediction is to the true value.
- Assume a highly unbalanced dataset
- E.g., a dataset where 95% of the data points are not fraud and 5% of the data points are fraud.
- A a naive classifier that predicts not fraud, regardless of input, will be 95% accurate.
- For this reason, metrics like precision and recall are typically used.

Precision

- It is the accuracy of the positive predictions.

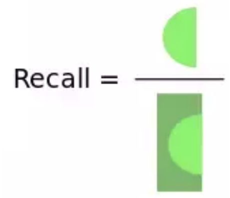
$$\texttt{Precision} = \mathrm{p}(\mathrm{y} = 1 \mid \hat{\mathrm{y}} = 1) = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$



Recall

- Is is the ratio of positive instances that are correctly detected by the classifier.
- Also called sensitivity or true positive rate (TPR).

$$\mathtt{Recall} = p(\hat{y} = 1 \mid y = 1) = \frac{\mathtt{TP}}{\mathtt{TP} + \mathtt{FN}}$$



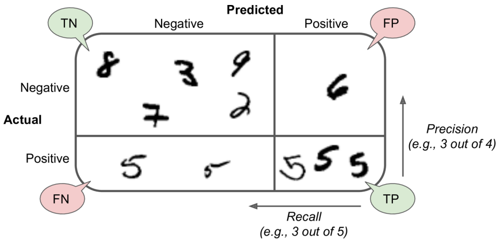
F1 Score

- $F1$ score: combine precision and recall into a single metric.
- The $F1$ score is the harmonic mean of precision and recall.
- Whereas the regular mean treats all values equally, the harmonic mean gives much more weight to low values.
- $F1$ only gets high score if both recall and precision are high.

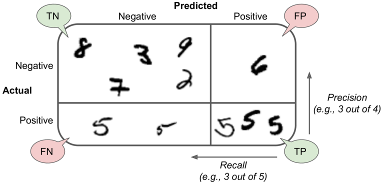
$$\mathtt{F1} = \frac{2}{\frac{1}{\mathtt{precision}} + \frac{1}{\mathtt{recall}}}$$

Confusion Matrix

- The confusion matrix is $\mathtt{K} \times \mathtt{K}$, where $\mathtt{K}$ is the number of classes.
- It shows the number of correct and incorrect predictions made by the classification model compared to the actual outcomes in the data.



Confusion Matrix - Example



$$\mathrm{TP} = 3, \mathrm{TN} = 5, \mathrm{FP} = 1, \mathrm{FN} = 2$$

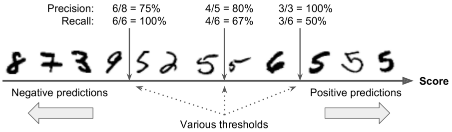
$$\mathrm{Precision} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}} = \frac{3}{3+1} = \frac{3}{4}$$

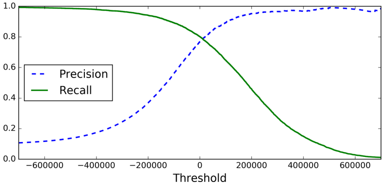
$$\mathrm{Recall\ (TPR)} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} = \frac{3}{3+2} = \frac{3}{5}$$

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{TN} + \mathrm{FP}} = \frac{1}{5+1} = \frac{5}{6}$$

Precision-Recall Tradeoff

- Precision-recall tradeoff: increasing precision reduces recall, and vice versa.
- Assume a classifier that detects number 5 from the other digits.
  - If an instance score is greater than a threshold, it assigns it to the positive class, otherwise to the negative class.
- Raising the threshold (move it to the arrow on the right), the false positive (the 6) becomes a true negative, thereby increasing precision.
- Lowering the threshold increases recall and reduces precision.

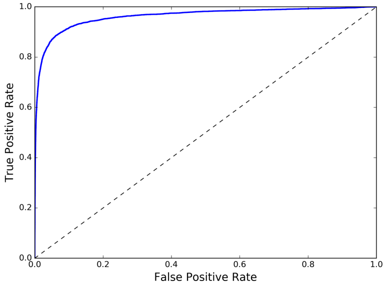




The ROC Curve (1/2)

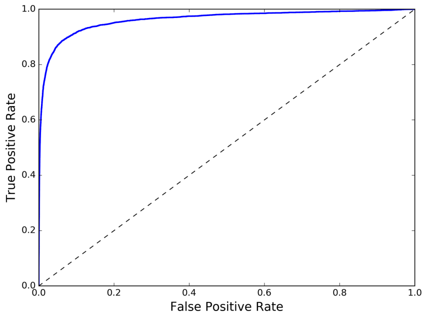
- True positive rate (TPR) (recall): $p(\hat{y} = 1 \mid y = 1)$
- False positive rate (FPR): $p(\hat{y} = 1 \mid y = 0)$

- The receiver operating characteristic (ROC) curves summarize the trade-off between the TPR and FPR for a model using different probability thresholds.



The ROC Curve (2/2)

- Here is a tradeoff: the higher the TPR, the more FPR the classifier produces.
- The dotted line represents the ROC curve of a purely random classifier.
- A good classifier moves toward the top-left corner.
- Area under the curve (AUC)



Binomial Logistic Regression Measurements in Spark

```scala
val lr = new LogisticRegression()
val lrModel = lr.fit(training)
```

```scala
val trainingSummary = lrModel.binarySummary

// obtain the objective per iteration.
val objectiveHistory = trainingSummary.objectiveHistor
objectiveHistory.foreach(loss => println(loss))

// obtain the ROC as a dataframe and areaUnderROC.
val roc = trainingSummary.roc
roc.show()
println(s"areaUnderROC: ${trainingSummary.areaUnderROC}")

// set the model threshold to maximize F-Measure
val fMeasure = trainingSummary.fMeasureByThreshold
val maxFMeasure = fMeasure.select(max("F-Measure")).head().getDouble(0)
val bestThreshold = fMeasure.where($"F-Measure" === maxFMeasure)
  .select("threshold").head().getDouble(0)
lrModel.setThreshold(bestThreshold)
```

Multinomial Logistic Regression in Spark (1/2)

```scala
val trainingSummary = lrModel.summary

// for multiclass, we can inspect metrics on a per-label basis
println("False positive rate by label:")
trainingSummary.falsePositiveRateByLabel.zipWithIndex.foreach { case (rate, label) =>
  println(s"label $label: $rate")
}

println("True positive rate by label:")
trainingSummary.truePositiveRateByLabel.zipWithIndex.foreach { case (rate, label) =>
  println(s"label $label: $rate")
}
```

Multinomial Logistic Regression in Spark (2/2)

```scala
println("Precision by label:")
trainingSummary.precisionByLabel.zipWithIndex.foreach { case (prec, label) =>
  println(s"label $label: $prec")
}

println("Recall by label:")
trainingSummary.recallByLabel.zipWithIndex.foreach { case (rec, label) =>
  println(s"label $label: $rec")
}

val accuracy = trainingSummary.accuracy
val falsePositiveRate = trainingSummary.weightedFalsePositiveRate
val truePositiveRate = trainingSummary.weightedTruePositiveRate
val fMeasure = trainingSummary.weightedFMeasure
val precision = trainingSummary.weightedPrecision
val recall = trainingSummary.weightedRecall
```

Summary

Summary

- Binomial logistic regression
  - $y \in \{0, 1\}$
  - Sigmoid function
  - Minimize the cross-entropy
- Multinomial logistic regression
  - $y \in \{1, 2, \cdots, k\}$
  - Softmax function
  - Minimize the cross-entropy
- Performance measurements
  - TP, TF, FP, FN
  - Precision, recall, F1
  - Threshold and ROC

Reference

- Ian Goodfellow et al., Deep Learning (Ch. 4, 5)
- Aurélien Géron, Hands-On Machine Learning (Ch. 3)
- Matei Zaharia et al., Spark - The Definitive Guide (Ch. 26)

Questions?