Logistic Regression

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Classification Based on Probability

• Instead of just predicting the class, give the probability of the instance being that class
  – i.e., learn $p(y | x)$

• Comparison to perceptron:
  – Perceptron doesn’t produce probability estimate

• Recall that:
  \[
  0 \leq p(\text{event}) \leq 1 \\
  p(\text{event}) + p(\neg \text{event}) = 1
  \]
Logistic Regression

• Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)

• $h_\theta(x)$ should give $p(y = 1 \mid x; \theta)$
  - Want $0 \leq h_\theta(x) \leq 1$

• Logistic regression model:
  
  $h_\theta(x) = g(\theta^\top x)$
  
  $g(z) = \frac{1}{1 + e^{-z}}$
  
  $h_\theta(x) = \frac{1}{1 + e^{-\theta^\top x}}$
Interpretation of Hypothesis Output

\[ h_\theta(x) = \text{estimated } p(y = 1 \mid x; \theta) \]

Example: Cancer diagnosis from tumor size

\[ x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix} \]

\[ h_\theta(x) = 0.7 \]

→ Tell patient that 70% chance of tumor being malignant

Note that:

\[ p(y = 0 \mid x; \theta) + p(y = 1 \mid x; \theta) = 1 \]

Therefore,

\[ p(y = 0 \mid x; \theta) = 1 - p(y = 1 \mid x; \theta) \]

Based on example by Andrew Ng
Another Interpretation

• Equivalently, logistic regression assumes that

\[
\log \left( \frac{p(y = 1 \mid x; \theta)}{p(y = 0 \mid x; \theta)} \right) = \theta_0 + \theta_1 x_1 + \ldots + \theta_d x_d
\]

odds of \( y = 1 \)

**Side Note:** the odds in favor of an event is the quantity \( p / (1 - p) \), where \( p \) is the probability of the event

E.g., If I toss a fair dice, what are the odds that I will have a 6?

• In other words, logistic regression assumes that the log odds is a linear function of \( x \)
Logistic Regression

\[ h_\theta(x) = g(\theta^T x) \]

\[ g(z) = \frac{1}{1 + e^{-z}} \]

\[ \theta^T x \text{ should be large negative values for negative instances} \]

\[ \theta^T x \text{ should be large positive values for positive instances} \]

• Assume a threshold and...
  – Predict \( y = 1 \) if \( h_\theta(x) \geq 0.5 \)
  – Predict \( y = 0 \) if \( h_\theta(x) < 0.5 \)

Based on slide by Andrew Ng
Non-Linear Decision Boundary

- Can apply basis function expansion to features, same as with linear regression

\[
\mathbf{x} = \begin{bmatrix} 1 & x_1 & x_2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1 x_2 \\ x_1^2 \\ x_2^2 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ \vdots \end{bmatrix}
\]
Logistic Regression

• Given \( \{ (\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(n)}, y^{(n)}) \} \)

where \( \mathbf{x}^{(i)} \in \mathbb{R}^d, y^{(i)} \in \{0, 1\} \)

• Model: \( h_{\theta}(\mathbf{x}) = g(\mathbf{\theta}^\top \mathbf{x}) \)

\[
g(z) = \frac{1}{1 + e^{-z}}
\]

\[
\theta = \begin{bmatrix}
\theta_0 \\
\theta_1 \\
\vdots \\
\theta_d
\end{bmatrix}
\]

\[
\mathbf{x}^\top = \begin{bmatrix}
1 & x_1 & \ldots & x_d
\end{bmatrix}
\]
Logistic Regression Objective Function

• Can’t just use squared loss as in linear regression:

\[
J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right)^2
\]

– Using the logistic regression model

\[
h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}
\]

results in a non-convex optimization
Deriving the Cost Function via Maximum Likelihood Estimation

- Likelihood of data is given by:
  \[ l(\theta) = \prod_{i=1}^{n} p(y^{(i)} | x^{(i)}; \theta) \]

- So, looking for the \( \theta \) that maximizing the likelihood
  \[ \theta_{\text{MLE}} = \arg \max_{\theta} l(\theta) = \arg \max_{\theta} \prod_{i=1}^{n} p(y^{(i)} | x^{(i)}; \theta) \]

- Can take the log without changing the solution:
  \[ \theta_{\text{MLE}} = \arg \max_{\theta} \log \prod_{i=1}^{n} p(y^{(i)} | x^{(i)}; \theta) \]
  \[ = \arg \max_{\theta} \sum_{i=1}^{n} \log p(y^{(i)} | x^{(i)}; \theta) \]
Deriving the Cost Function via Maximum Likelihood Estimation

- Expand as follows:

\[ \theta_{\text{MLE}} = \arg \max_{\theta} \sum_{i=1}^{n} \log p(y^{(i)} | x^{(i)}; \theta) \]

\[ = \arg \max_{\theta} \sum_{i=1}^{n} \left[ y^{(i)} \log p(y^{(i)} = 1 | x^{(i)}; \theta) + (1 - y^{(i)}) \log \left( 1 - p(y^{(i)} = 1 | x^{(i)}; \theta) \right) \right] \]

- Substitute in model, and take negative to yield

**Logistic regression objective:**

\[ \min_{\theta} J(\theta) \]

\[ J(\theta) = - \sum_{i=1}^{n} \left[ y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log \left( 1 - h_\theta(x^{(i)}) \right) \right] \]
Intuition Behind the Objective

\[ J(\theta) = - \sum_{i=1}^{n} \left[ y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right] \]

- Cost of a single instance:

\[ \text{cost} (h_\theta(x), y) = \begin{cases} 
- \log(h_\theta(x)) & \text{if } y = 1 \\
- \log(1 - h_\theta(x)) & \text{if } y = 0
\end{cases} \]

- Can re-write objective function as

\[ J(\theta) = \sum_{i=1}^{n} \text{cost} \left( h_\theta(x^{(i)}), y^{(i)} \right) \]

Compare to linear regression: \[ J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left( h_\theta(x^{(i)}) - y^{(i)} \right)^2 \]
Intuition Behind the Objective

\[
\text{cost } (h_\theta(x), y) = \begin{cases} 
- \log(h_\theta(x)) & \text{if } y = 1 \\
- \log(1 - h_\theta(x)) & \text{if } y = 0 
\end{cases}
\]

Aside: Recall the plot of \( \log(z) \)
**Intuition Behind the Objective**

\[
\text{cost} \left( h_\theta(x), y \right) = \begin{cases} 
- \log(h_\theta(x)) & \text{if } y = 1 \\
- \log(1 - h_\theta(x)) & \text{if } y = 0 
\end{cases}
\]

If \( y = 1 \)

- Cost = 0 if prediction is correct
- As \( h_\theta(x) \to 0 \), cost \( \to \infty \)
- Captures intuition that larger mistakes should get larger penalties
  - e.g., predict \( h_\theta(x) = 0 \), but \( y = 1 \)

Based on example by Andrew Ng
Intuition Behind the Objective

\[
\text{cost} \left( h_\theta(x), y \right) = \begin{cases} 
- \log(h_\theta(x)) & \text{if } y = 1 \\
- \log(1 - h_\theta(x)) & \text{if } y = 0
\end{cases}
\]

If \(y = 0\)

- Cost = 0 if prediction is correct
- As \((1 - h_\theta(x)) \to 0\), cost \(\to \infty\)
- Captures intuition that larger mistakes should get larger penalties

Based on example by Andrew Ng
Regularized Logistic Regression

\[ J(\theta) = -\sum_{i=1}^{n} \left[ y^{(i)} \log h_{\theta}(x^{(i)}) + \left(1 - y^{(i)}\right) \log \left(1 - h_{\theta}(x^{(i)})\right) \right] \]

- We can regularize logistic regression exactly as before:

\[
J_{\text{regularized}}(\theta) = J(\theta) + \lambda \sum_{j=1}^{d} \theta_j^2
\]

\[
= J(\theta) + \lambda \|\theta_{[1:d]}\|_2^2
\]
Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\theta) = -\sum_{i=1}^{n} \left[ y^{(i)} \log h_{\theta}(\mathbf{x}^{(i)}) + \left(1 - y^{(i)}\right) \log \left(1 - h_{\theta}(\mathbf{x}^{(i)})\right) \right] + \lambda \|\theta_{[1:d]}\|_2^2$$

Want $$\min_{\theta} J(\theta)$$

- Initialize $$\theta$$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

simultaneous update for $$j = 0 \ldots d$$

Use the natural logarithm ($$\ln = \log_e$$) to cancel with the exp() in $$h_{\theta}(\mathbf{x})$$
Gradient Descent for Logistic Regression

\[ J_{\text{reg}}(\theta) = - \sum_{i=1}^{n} \left[ y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)})) \right] + \lambda \| \theta \|_2^2 \]

Want \( \min_{\theta} J(\theta) \)

- Initialize \( \theta \)
- Repeat until convergence (simultaneous update for \( j = 0 \ldots d \))

\[
\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right)
\]

\[
\theta_j \leftarrow \theta_j - \alpha \left[ \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \frac{\lambda}{n} \theta_j \right]
\]
Gradient Descent for Logistic Regression

- Initialize \( \theta \)
- Repeat until convergence

\[
\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right)
\]
\[
\theta_j \leftarrow \theta_j - \alpha \left[ \sum_{i=1}^{n} \left( h_\theta \left( x^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \frac{\lambda}{n} \theta_j \right]
\]

This looks IDENTICAL to linear regression!!!

- Ignoring the \( 1/n \) constant
- However, the form of the model is very different:

\[
h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}
\]
Multi-Class Classification

Binary classification:

Multi-class classification:

Disease diagnosis: healthy / cold / flu / pneumonia

Object classification: desk / chair / monitor / bookcase
Multi-Class Logistic Regression

• For 2 classes:

\[ h_\theta(x) = \frac{1}{1 + \exp(-\theta^T x)} = \frac{\exp(\theta^T x)}{1 + \exp(\theta^T x)} \]

- weight assigned to \( y = 0 \)
- weight assigned to \( y = 1 \)

• For \( C \) classes \( \{1, \ldots, C\} \):

\[ p(y = c \mid x; \theta_1, \ldots, \theta_C) = \frac{\exp(\theta_c^T x)}{\sum_{c=1}^{C} \exp(\theta_c^T x)} \]

- Called the softmax function
Multi-Class Logistic Regression

Split into One vs Rest:

• Train a logistic regression classifier for each class \( i \) to predict the probability that \( y = i \) with

\[
h_c(x) = \frac{\exp(\theta_c^T x)}{\sum_{c=1}^C \exp(\theta_c^T x)}
\]
Implementing Multi-Class Logistic Regression

• Use  \( h_c(x) = \frac{\exp(\theta^T_c x)}{\sum_{c=1}^C \exp(\theta^T_c x)} \) as the model for class c

• Gradient descent simultaneously updates all parameters for all models
  – Same derivative as before, just with the above \( h_c(x) \)

• Predict class label as the most probable label
  \[ \max_c h_c(x) \]