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 $p(y \mid x)$

• 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:

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

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

\[
h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}
\]
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, \( p(y = 0 \mid x; \theta) = 1 - p(y = 1 \mid x; \theta) \)
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

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

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

- 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 \( \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\} \)
  where \( x^{(i)} \in \mathbb{R}^d, y^{(i)} \in \{0, 1\} \)

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

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

\[ x^T = \begin{bmatrix} 1 & x_1 & \ldots & x_d \end{bmatrix} \]
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 maximizes 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:

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

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

• Substitute in model, and take negative to yield

Logistic regression objective:

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

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

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

- Cost of a single instance:

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

- Can re-write objective function as

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

Compare to linear regression:

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

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

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

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

If $y = 1$

- Cost = 0 if prediction is correct
- As $h_\theta(x) \rightarrow 0$, cost $\rightarrow \infty$
- 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

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

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

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

\[ \theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \quad \text{simultaneous update for } j = 0 \ldots d \]

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

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

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

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

\[
\begin{align*}
\theta_0 & \leftarrow \theta_0 - \alpha \sum_{i=1}^{n} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) \\
\theta_j & \leftarrow \theta_j - \alpha \left[ \sum_{i=1}^{n} \left( h_{\theta}(x^{(i)}) - y^{(i)} \right) x_j^{(i)} - \frac{\lambda}{n} \theta_j \right]
\end{align*}
\]
Gradient Descent for Logistic Regression

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

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

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

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

- 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 $h_c(x) = \frac{\exp(\theta_c^T x)}{\sum_{c=1}^{C} \exp(\theta_c^T x)}$ 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

$$\max_c h_c(x)$$