Logistic Regression & Discriminative Classifier

Dr. Jianlin Cheng

Department of Electrical Engineering and Computer Science
University of Missouri, Columbia
Fall, 2019

Slides Adapted from Book and CMU, Stanford Machine Learning Courses
Naïve Bayes Recap...

- Optimal Classifier: \[ f^*(x) = \arg \max_y P(y|x) \]

- NB Assumption: \[ P(X_1 \ldots X_d|Y) = \prod_{i=1}^{d} P(X_i|Y) \]

- NB Classifier: \[ f_{NB}(x) = \arg \max_y \prod_{i=1}^{d} P(x_i|y) P(y) \]

- Assume parametric form for \( P(X_i|Y) \) and \( P(Y) \)
  - Estimate parameters using MLE/MAP and plug in
Generative vs. Discriminative Classifiers

Generative classifiers (e.g. Naïve Bayes)

- Assume some functional form for $P(X,Y)$ (or $P(X|Y)$ and $P(Y)$)
- Estimate parameters of $P(X|Y)$, $P(Y)$ directly from training data
- Use Bayes rule to calculate $P(Y|X)$

Why not learn $P(Y|X)$ directly? Or better yet, why not learn the decision boundary directly?

Discriminative classifiers (e.g. Logistic Regression)

- Assume some functional form for $P(Y|X)$ or for the decision boundary
- Estimate parameters of $P(Y|X)$ directly from training data
Logistic Regression

Assumes the following functional form for $P(Y | X)$:

$$P(Y = 0 | X, w) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1 | X, w) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

Logistic function applied to a linear function of the data

Logistic function (or Sigmoid):

$$\frac{1}{1 + \exp(-z)}$$

Features can be discrete or continuous!
Logistic Regression is a Linear Classifier!

Assumes the following functional form for $P(Y|X)$:

$$P(Y = 0|X, w) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$P(Y = 1|X, w) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

Decision boundary:

$$P(Y = 1|X) \geq P(Y = 0|X)$$

$$w_0 + \sum_i w_i X_i \geq 0$$

(Linear Decision Boundary)
Machine Learning Problems to Practice

- An example - Iris data: http://archive.ics.uci.edu/ml/machine-learning-databases/iris/
Logistic Regression is a Linear Classifier!

Assumes the following functional form for $P(Y \mid X)$:

$$P(Y = 0 \mid X) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow P(Y = 1 \mid X) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}$$

$$\Rightarrow \frac{P(Y = 1 \mid X)}{P(Y = 0 \mid X)} = \exp(w_0 + \sum_i w_i X_i) \ \overset{\text{if}}{\Rightarrow} \ 1$$

$$\Rightarrow w_0 + \sum_i w_i X_i \ \overset{\text{if}}{\Rightarrow} \ 0$$
Logistic Regression for more than 2 classes

- Logistic regression in more general case, where $Y \in \{y_1, \ldots, y_K\}$

For $k < K$

$$P(Y = y_k | X) = \frac{\exp(w_{k0} + \sum_{i=1}^{d} w_{ki}X_i)}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{d} w_{ji}X_i)}$$

For $k = K$ (normalization, so no weights for this class)

$$P(Y = y_K | X) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{d} w_{ji}X_i)}$$

Is the decision boundary still linear?
Training Logistic Regression

We’ll focus on binary classification:

\[
P(Y = 0|X, w) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)}
\]

\[
P(Y = 1|X, w) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)}
\]

How to learn the parameters \( w_0, w_1, \ldots w_d \)?

Training Data \( \{(X^{(j)}, Y^{(j)})\}_{j=1}^{n} \) \( X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)}) \)

Maximum Likelihood Estimates

\[
\hat{w}_{MLE} = \arg \max_w \prod_{j=1}^{n} P(X^{(j)}, Y^{(j)} | w)
\]

But there is a problem ...

Don’t have a model for \( P(X) \) or \( P(X|Y) \) - only for \( P(Y|X) \)
Training Logistic Regression

How to learn the parameters $w_0, w_1, \ldots, w_d$?

Training Data \[ \{ (X^{(j)}, Y^{(j)}) \}_{j=1}^n \] \[ X^{(j)} = (X_1^{(j)}, \ldots, X_d^{(j)}) \]

Maximum (Conditional) Likelihood Estimates

\[ \hat{w}_{MCLE} = \arg \max_w \prod_{j=1}^n P(Y^{(j)} | X^{(j)}, w) \]

Discriminative philosophy — Don’t waste effort learning $P(X)$, focus on $P(Y|X)$ — that’s all that matters for classification!
Expressing Conditional log Likelihood

\[ P(Y = 0|X, w) = \frac{1}{1 + \exp(w_0 + \sum_i w_i X_i)} \]

\[ P(Y = 1|X, w) = \frac{\exp(w_0 + \sum_i w_i X_i)}{1 + \exp(w_0 + \sum_i w_i X_i)} \]

\[ l(w) \equiv \ln \prod_j P(y^j|x^j, w) \]

\[ = \sum_j \left[ y^j (w_0 + \sum_i^d w_i x_i^j) - \ln(1 + \exp(w_0 + \sum_i^d w_i x_i^j)) \right] \]
\[
p(0 | \omega) = \prod_{j=1}^{n} p(y_j^0 | x_j^0, \omega) = \prod_{j=1}^{n} p(y_j^0 = 1 | x_j^0, \omega) p(y_j^0 = 0 | x_j^0, \omega)^{1 - y_j^0} = \prod_{j=1}^{n} \left( \frac{\exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right)^{y_j^0} \left( \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right)^{1 - y_j^0}
\]

\[
\ell(\omega) = \ln p(0 | \omega) = \sum_{j=1}^{n} \left[ y_j^0 \left( \frac{\exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right)^{y_j^0} \left( \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right)^{1 - y_j^0} - \ln \left( \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right) \right]
\]

\[
\frac{\partial \ell(\omega)}{\partial w_i} = \sum_{j=1}^{n} \left[ x_i^0 \frac{\exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} - \frac{\exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right]
\]

\[
= \sum_{j=1}^{n} x_i^0 \left( y_j^0 - \frac{\exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)}{1 + \exp(w_0 + \sum_{i=1}^{d} w_i x_i^0)} \right)
\]

\[
= \sum_{j=1}^{n} x_i^0 \left( y_j^0 - p(y_j^0 = 1 | x_j^0, \omega) \right)
\]
Maximizing Conditional log Likelihood

\[
\max_w l(w) \equiv \ln \prod_j P(y_j^j|x_j^j, w) \\
= \sum_j y_j^j (w_0 + \sum_i^d w_i x_i^j) - \ln (1 + \exp(w_0 + \sum_i^d w_i x_i^j))
\]

Good news: \( l(w) \) is concave function of \( w \) → no locally optimal solutions

Bad news: no closed-form solution to maximize \( l(w) \)

Good news: concave functions easy to optimize (unique maximum)
Optimizing concave/convex function

- Conditional likelihood for Logistic Regression is concave
- Maximum of a concave function = minimum of a convex function

Gradient Ascent (concave)/ Gradient Descent (convex)

Gradient:
\[ \nabla_w l(w) = \left[ \frac{\partial l(w)}{\partial w_0}, \ldots, \frac{\partial l(w)}{\partial w_n} \right]' \]

Update rule:
\[ \Delta w = \eta \nabla_w l(w) \]
\[ w_i(t+1) \leftarrow w_i(t) + \eta \frac{\partial l(w)}{\partial w_i} \bigg|_t \]
Gradient Ascent/Descent for Concave and Convex function
Calculate Partial Derivative – A Beautiful Result

\[
\frac{\partial l(w)}{\partial w_i} = \sum_j y^j x^j_i \left( y^j - \frac{\exp(w_o + \sum_1^d w_i x^j_i)}{1 + \exp(w_o + \sum_1^d w_i x^j_i)} \right)
\]

\[
\frac{\partial l(w)}{\partial w_i} = \sum_j x^j_i (y^j - P(y^j = 1|x^j, w))
\]
Gradient Ascent for Logistic Regression

Gradient ascent algorithm: iterate until change $< \varepsilon$

$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \sum_j [y^j - \hat{P}(Y^j = 1 \mid x^j, w^{(t)})]$$

For $i=1,...,d,$

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \hat{P}(Y^j = 1 \mid x^j, w^{(t)})]$$

repeat

- Gradient ascent is simplest of optimization approaches
  - e.g., Newton method, Conjugate gradient ascent, IRLS (see Bishop 4.3.3)
Effect of step-size $\eta$

Large $\eta$ ==> Fast convergence but larger residual error
Also possible oscillations

Small $\eta$ ==> Slow convergence but small residual error
That’s all M(C)LE. How about MAP?

\[ p(w \mid Y, X) \propto P(Y \mid X, w)p(w) \]

- One common approach is to define priors on \( w \)
  - Normal distribution, zero mean, identity covariance
  - “Pushes” parameters towards zero
- Corresponds to **Regularization**
  - Helps avoid very large weights and overfitting
  - More on this later in the semester

- M(C)AP estimate

\[
  w^* = \arg \max_w \ln \left[ p(w) \prod_{j=1}^{n} P(y^j \mid x^j, w) \right]
\]
Large weights → Overfitting

\[
\begin{align*}
1 & \quad \frac{1}{1 + e^{-x}} \\
1 & \quad \frac{1}{1 + e^{-2x}} \\
1 & \quad \frac{1}{1 + e^{-100x}}
\end{align*}
\]

- Large weights lead to overfitting:

- Penalizing high weights can prevent overfitting...
  - again, more on this later in the semester
M(C)AP – Regularization

- Regularization

\[
\text{arg} \max_w \ln \left[ p(w) \prod_{j=1}^{n} P(y^j | x^j, w) \right]
\]

\[
p(w) = \prod_i \frac{1}{\kappa \sqrt{2\pi}} \frac{-w_i^2}{e^{2\kappa^2}}
\]

Zero-mean Gaussian prior

\[
w^* = \text{arg} \max_w \sum_{j=1}^{n} \ln P(y^j | x^j, w) - \sum_{i=1}^{d} \frac{w_i^2}{2\kappa^2}
\]

Penalizes large weights
Calculate Partial Derivative – A Beautiful Result

\[
l(w) = \sum_{j=1}^{n} \ln P(y^j \mid x^j, w) - \sum_{i=1}^{d} \frac{w_i^2}{2\kappa^2}
\]

\[
\frac{\partial l(w)}{\partial w_i} = \sum_j x_i^j (y^j - P(y^j = 1 \mid x^j, w)) - \frac{w_i}{k^2}
\]
Gradient Ascent for Logistic Regression

Gradient ascent algorithm: iterate until change $< \varepsilon$

$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \sum_j [y_j - \hat{P}(Y_j = 1 | x_j, w^{(t)})]$$

For $i=1,...,d$,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y_j - \hat{P}(Y_j = 1 | x_j, w^{(t)})]$$

repeat

- Gradient ascent is simplest of optimization approaches
  - e.g., Newton method, Conjugate gradient ascent, IRLS (see Bishop 4.3.3)