Logistic Regression

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Naïve Bayes Recap

- Classifier: $$f^*(x) = \arg\max_y P(y|x)$$
- NB Assumption: $$P(X_1 \dots X_d|Y) = \prod_{i=1}^{d} P(X_i|Y)$$
- 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

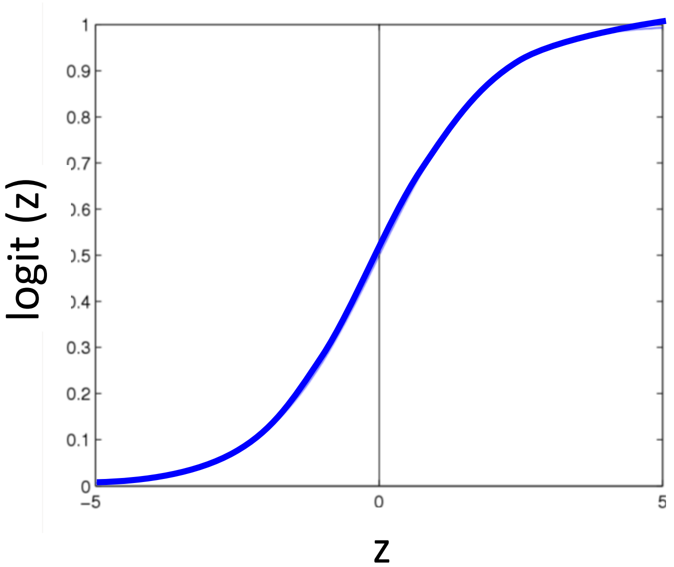
Assumes the following functional form for P(Y|X):

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

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):

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

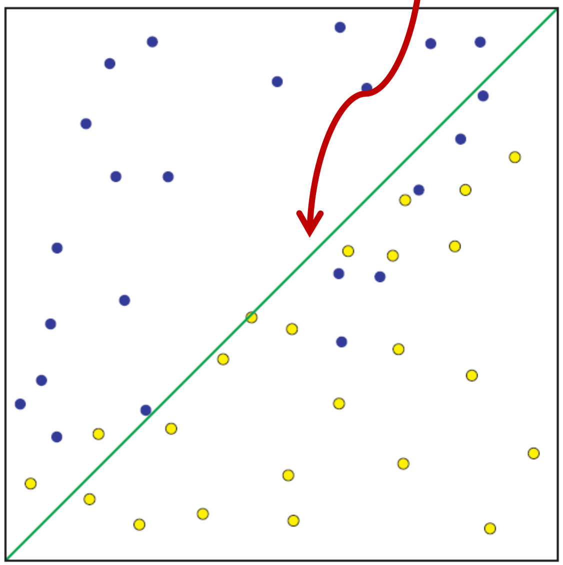
Decision boundary:

$$P(Y=1|X) > P(Y=0|X)\ ?$$

$$w_0 + \sum_i w_i X_i > 0\ ?$$

(Linear Decision Boundary)

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



Logistic Regression is a Linear Classifier!

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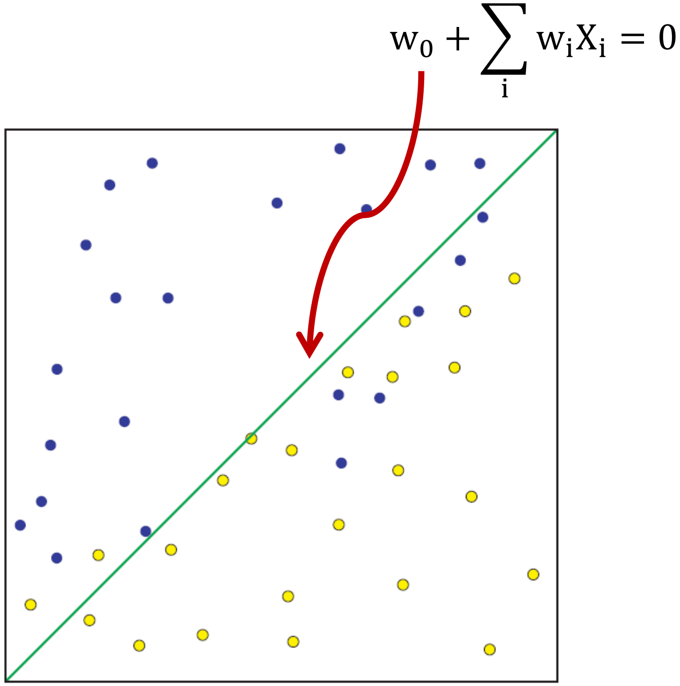
$$P(Y=1|X) = \frac{1}{1+\exp(-(w_0+\sum_i w_i X_i))} = \frac{\exp(w_0+\sum_i w_i X_i)}{\exp(w_0+\sum_i w_i X_i)+1}$$

Assumes a linear decision boundary: there are weights w_i s.t. when $w_0 + \sum_i w_i X_i > 0$, the example is more likely to be positive, and when this linear function is negative ($w_0 + \sum_i w_i X_i < 0$) the example is more likely to be negative.



$$w_0 + \sum_i w_i X_i = 0,\ P(Y=1|X) = \frac{1}{2}$$

$$w_0 + \sum_i w_i X_i \rightarrow \infty,\ P(Y=1|X) \rightarrow 1$$

$$w_0 + \sum_i w_i X_i \rightarrow -\infty,\ P(Y=1|X) \rightarrow 0$$

Logistic Regression is a Linear Classifier!

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

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

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

$$\Rightarrow \frac{P(Y=1|X)}{P(Y=0|X)} = \exp(w_0+\sum_i w_i X_i) > 1 \text{ ?}$$

$$\Rightarrow \boxed{w_0+\sum_i w_i X_i > 0 \text{ ?}}$$

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 $w_0, w_1, \dots, w_d$?

Training data: $\left\{\left(X^{(j)}, Y^{(j)}\right)\right\}_{j=1}^{n}$ $\quad X^{(j)} = \left(X_1^{(j)}, \dots, X_d^{(j)}\right)$

Maximum Likelihood Estimates:

$$\widehat{\mathbf{w}}_{MLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P\left(X^{(j)}, Y^{(j)} \middle| \mathbf{w}\right)$$

But there's 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 $\mathbf{w_0}$, $\mathbf{w1}$, … $\mathbf{w_d}$?

Training data: $\left\{\left(X^{(j)}, Y^{(j)}\right)\right\}_{j=1}^{n}$ $\quad X^{(j)} = \left(X_1^{(j)}, \ldots, X_d^{(j)}\right)$

Maximum (Conditional) Likelihood Estimates

$$\hat{\mathbf{w}}_{MCLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P\left(Y^{(j)} \middle| X^{(j)}, \mathbf{w}\right)$$

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

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

$$l(\mathbf{w}) \equiv \ln \prod_j P(y^j|\mathbf{x}^j, \mathbf{w})$$

$$= \sum_j \left[y^j \left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) - \ln\left(1 + \exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) \right) \right]$$

Maximizing Conditional log Likelihood

$$\max_{\mathbf{w}} \mathrm{l}(\mathbf{w}) \equiv \ln \prod_{j} P(y^j|\mathbf{x}^j, \mathbf{w})$$

$$= \sum_{j} \left[y^j \left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) - \ln\left(1 + \exp\left(w_0 + \sum_{i=1}^{d} w_i x_i^j \right) \right) \right]$$

Good news: $\mathrm{l}(\mathbf{w})$ is concave in w. Local optimum = global optimum

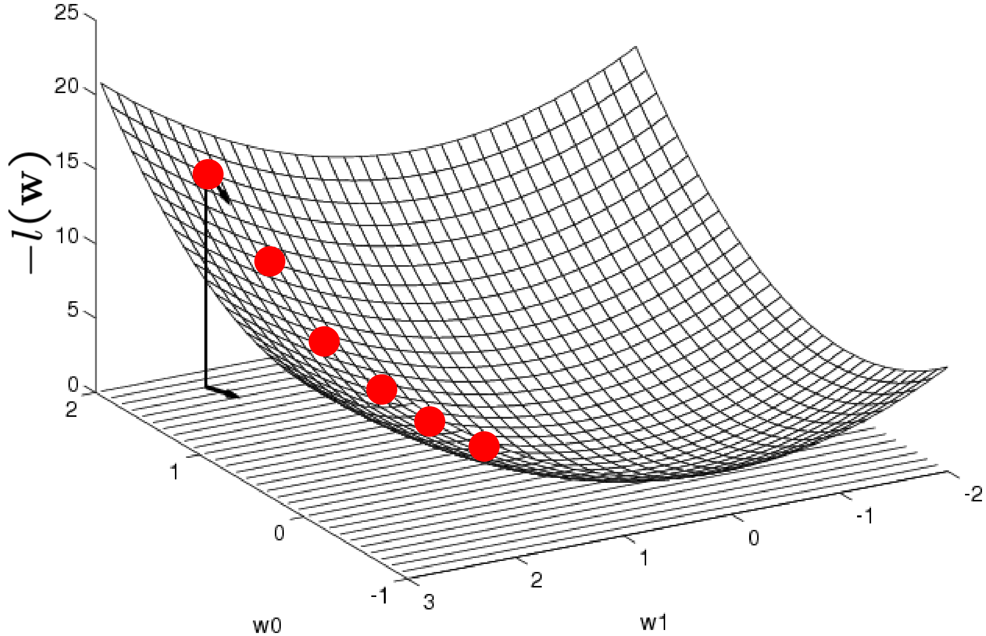
Bad news: no closed-form solution to maximize $l(\mathbf{w})$

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:

$$\nabla_{\mathbf{w}} l(\mathbf{w}) = \left[\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_d}\right]$$

Update rule: Learning rate, η>0

$$\Delta\mathbf{w} = \eta \nabla_{\mathbf{w}} l(\mathbf{w})$$

$$w_i^{(t+1)} = w_i^{(t)} + \eta \left.\frac{\partial l(\mathbf{w})}{\partial w_i}\right|_t$$

Gradient Ascent for Logistic Regression

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

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

For $i = 1, \ldots, d$:

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

repeat

Predict what current weight thinks label Y should be

look at actual labels of the examples, compare them to our current predictions, and then for each example j we multiply that difference by the feature value x_i^j and then add them up.

Gradient Ascent for Logistic Regression

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

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

For $i = 1, \ldots, d$:

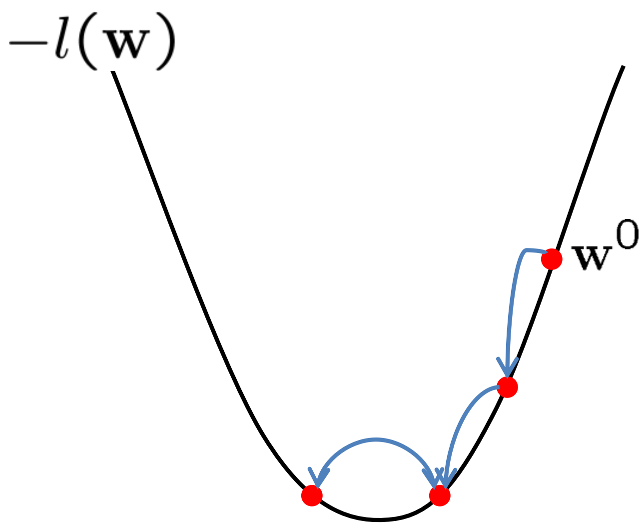
$$w_i^{(t+1)} = w_i^{(t)} + \eta \sum_j x_i^j [y^j - \underbrace{\hat{P}(Y^j = 1|\mathbf{x}^j, \mathbf{w}^{(t)})}]$$

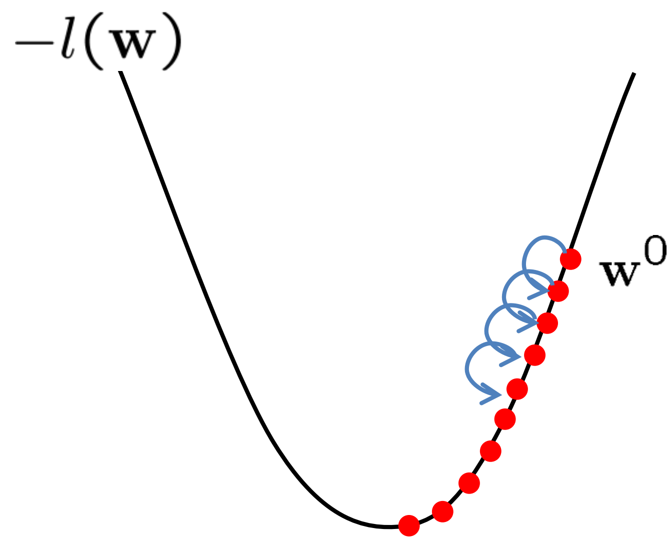
repeat

Predict what current weight thinks label Y should be

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

Effect of step-size η





Large η ⇒ Fast convergence but larger residual error
Also possible oscillations

Small η ⇒ Slow convergence but small residual error

That's all M(C)LE. How about MAP?

$$p(\mathbf{w} \mid Y, \mathbf{X}) \;\propto\; P(Y \mid \mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- 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

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \ln\left[p(\mathbf{w})\prod_{j=1}^{n} P\left(y^j \mid \mathbf{x}^j, \mathbf{w}\right)\right]$$

What you should know

- LR is a linear classifier: decision rule is a hyperplane
- LR optimized by conditional likelihood
  - no closed-form solution
  - concave $\Rightarrow$ global optimum with gradient ascent
  - Maximum conditional a posteriori corresponds to regularization