Logistic Regression

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Discriminative Classifiers

Bayes Classifier:

$$\begin{aligned} f^*(x) &= \arg\max_{Y=y} P(Y=y|X=x) \\ &= \arg\max_{Y=y} P(X=x|Y=y)P(Y=y) \end{aligned}$$

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

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

Today we will see one such classifier – **Logistic Regression**

Logistic Regression

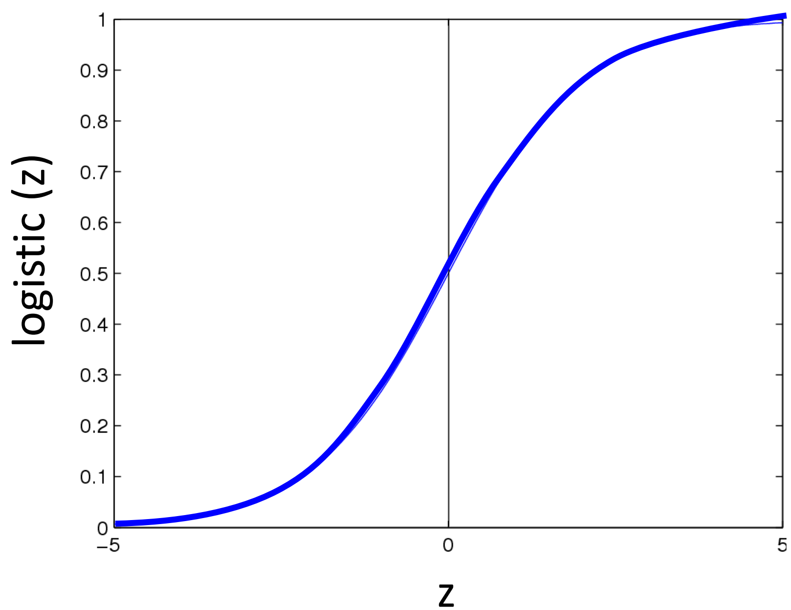
Not really regression

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

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

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):

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

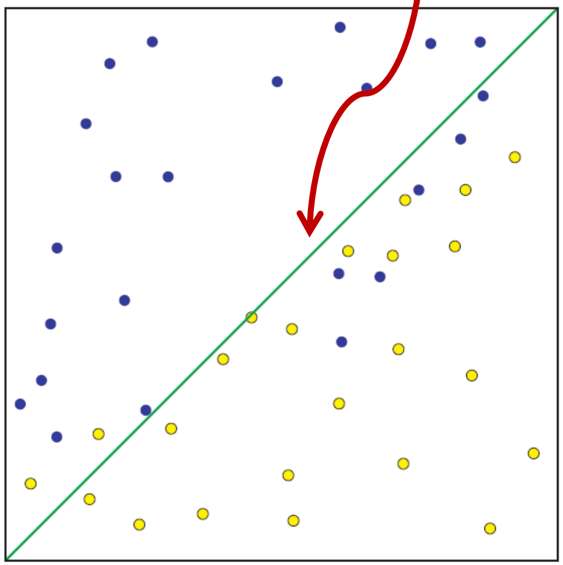
$$w_0 + \sum_i w_i X_i = 0$$

Decision boundary: Note - Labels are 0,1

$$P(Y=0|X) \underset{1}{\overset{0}{\gtrless}} P(Y=1|X)$$

$$w_0 + \sum_i w_i X_i \underset{0}{\overset{1}{\gtrless}} 0$$

(Linear Decision Boundary)



Logistic Regression is a Linear Classifier!

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

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

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

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

$$\Rightarrow \boxed{w_0 + \sum_i w_i X_i \underset{0}{\overset{1}{\gtrless}} 0}$$

Training Logistic Regression

How to learn the parameters w_0, w_1, … w_d? (d features)

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

Maximum Likelihood Estimates

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

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

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Maximum (Conditional) Likelihood Estimates

$$\widehat{\mathbf{w}}_{MCLE} = \arg\max_{\mathbf{w}} \prod_{j=1}^{n} P(Y^{(j)} \mid X^{(j)}, \mathbf{w})$$

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

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

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

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

Expressing Conditional log Likelihood

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$$\begin{aligned} l(\mathbf{w}) &\equiv \ln \prod_j P(y^j|\mathbf{x}^j,\mathbf{w}) \\ &= \sum_j \left[y^j (w_0 + \sum_i^d w_i x_i^j) - \ln(1+exp(w_0+\sum_i^d w_i x_i^j)) \right] \end{aligned}$$

Good news: $l(\mathbf{w})$ is concave function of **w** !

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

Good news: can use iterative optimization methods (gradient ascent)

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

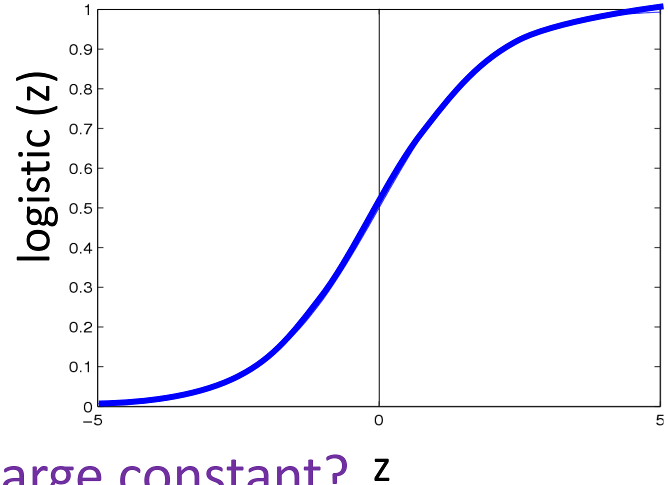
$$p(\mathbf{w} \mid Y, \mathbf{X}) \;\propto\; P(Y \mid \mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- Define priors on **w**
  - Common assumption: Normal distribution, zero mean, identity covariance
  - "Pushes" parameters towards zero

$$p(\mathbf{w}) = \prod_i \frac{1}{\kappa\sqrt{2\pi}} \; e^{\frac{-w_i^2}{2\kappa^2}}$$

Zero-mean Gaussian prior

Logistic function (or Sigmoid): $\dfrac{1}{1 + exp(-z)}$



➢ What happens if we scale z by a large constant?

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

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

$$p(\mathbf{w}) = \prod_i \frac{1}{\kappa\sqrt{2\pi}} \; e^{\frac{-w_i^2}{2\kappa^2}}$$

Zero-mean Gaussian prior

- M(C)AP estimate

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

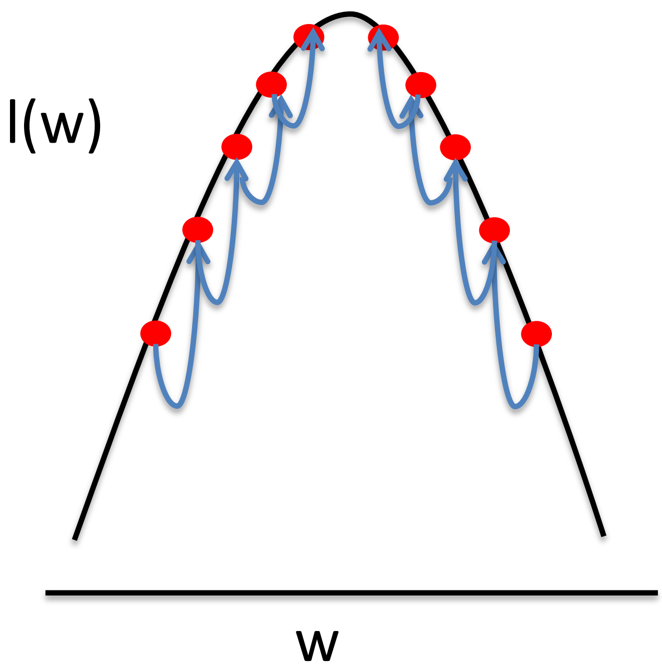
$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \sum_{j=1}^{n} \ln P(y^j \mid \mathbf{x}^j, \mathbf{w}) - \underbrace{\sum_{i=1}^{d} \frac{w_i^2}{2\kappa^2}}_{\text{Penalizes large weights}}$$

Still concave objective!

Iteratively optimizing concave function

- Conditional likelihood for Logistic Regression is concave
- Maximum of a concave function can be reached by

Gradient Ascent Algorithm



Initialize: Pick **w** at random

Gradient:

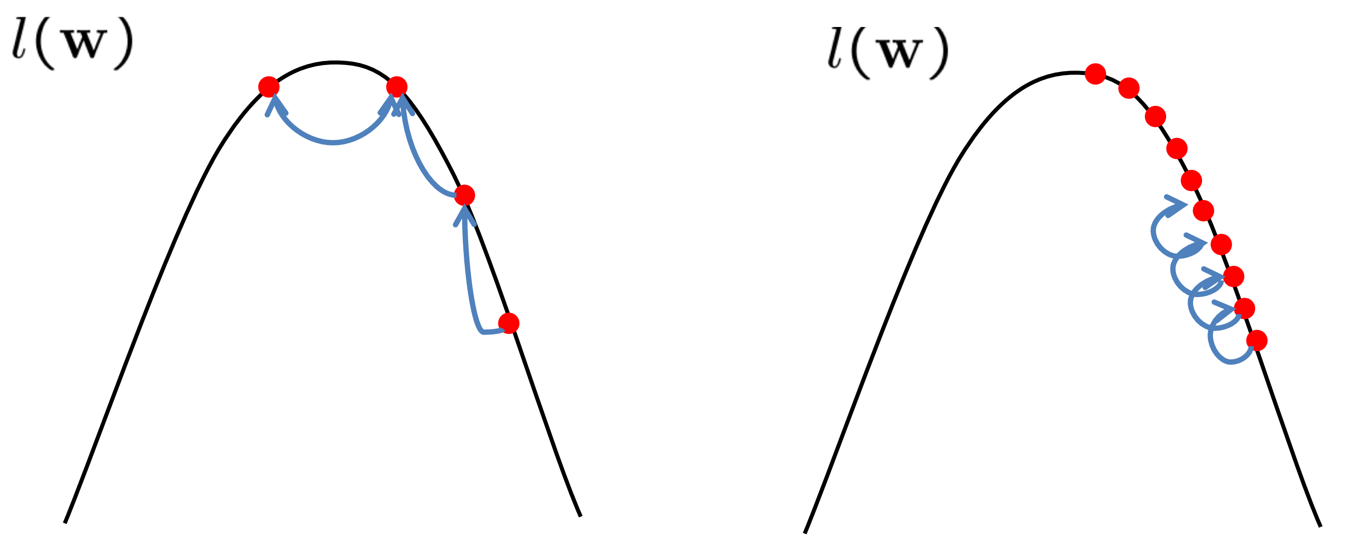
$$\nabla_{\mathbf{w}} l(\mathbf{w}) = [\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_d}]'$$

Update rule: **Learning rate, η>0**

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

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

Effect of step-size η



Large η => Fast convergence but larger residual error
Also possible oscillations

Small η => Slow convergence but small residual error

Gradient Ascent for M(C)LE

Gradient ascent rule for w_0:

$$w_0^{(t+1)} \leftarrow w_0^{(t)} + \eta \left.\frac{\partial l(\mathbf{w})}{\partial w_0}\right|_t$$

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

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$$\frac{\partial l(\mathbf{w})}{\partial w_0} = \sum_j \left[y^j - \underbrace{\frac{1}{1 + exp(w_0 + \sum_i^d w_i x_i^j)} \cdot exp(w_0 + \sum_i^d w_i x_i^j)} \right]$$

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

Gradient Ascent for M(C)LE
Logistic Regression

Gradient ascent algorithm: iterate until change < ε

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

For i=1,…,d,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \underbrace{\hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})}_{\text{Predict what current weight thinks label Y should be}}]$$

repeat

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

M(C)AP – Gradient

- Gradient

$$p(\mathbf{w}) = \prod_i \frac{1}{\kappa\sqrt{2\pi}} \; e^{\frac{-w_i^2}{2\kappa^2}}$$

Zero-mean Gaussian prior

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

$$\underbrace{\frac{\partial}{\partial w_i} \ln p(\mathbf{w})}_{\propto \frac{-w_i}{\kappa^2}} + \underbrace{\frac{\partial}{\partial w_i} \ln \left[\prod_{j=1}^{n} P(y^j \mid \mathbf{x}^j, \mathbf{w}) \right]}_{\text{Same as before}}$$

$$\propto \frac{-w_i}{\kappa^2}$$

Extra term Penalizes large weights

M(C)LE vs. M(C)AP

- Maximum conditional likelihood estimate

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

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

- Maximum conditional a posteriori estimate

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

$$\boxed{w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \left\{ -\frac{1}{\kappa^2} w_i^{(t)} + \sum_j x_i^j [y^j - P(Y = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})] \right\}}$$

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)

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

Predict $f^*(x) = \arg\max_{Y=y} P(Y = y|X = x)$

Is the decision boundary still linear?