Logistic Regression & Discriminative Classifier

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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

Example:
Drug dose response experiments

Logistic Regression

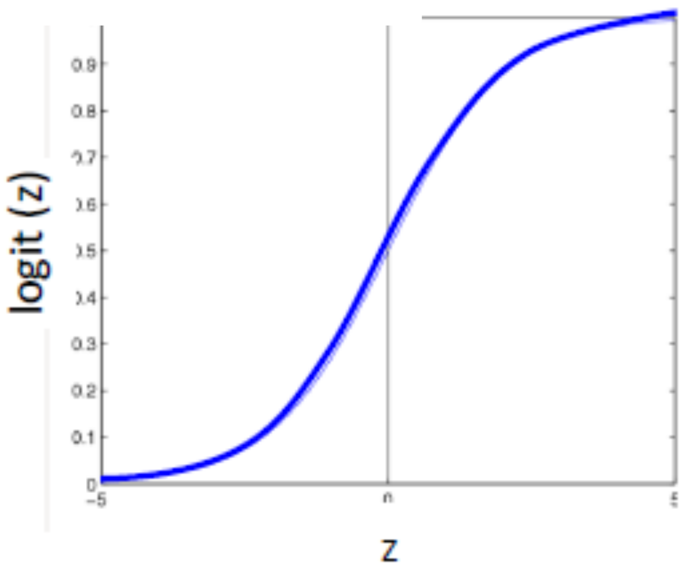
Assumes the following functional form for P(Y|X):

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

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

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!

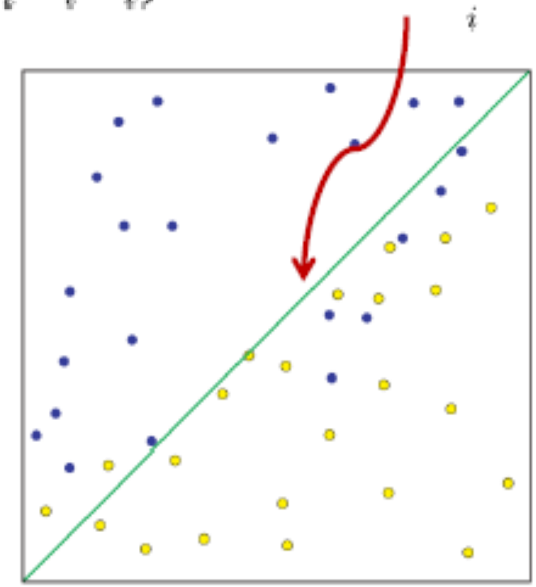
Logistic Regression is a Linear Classifier!

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

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

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

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



Decision boundary:

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

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

(Linear Decision Boundary)

Machine Learning Problems to Practice

UCI

Machine Learning Repository

- http://archive.ics.uci.edu/ml/index.php
- 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|X):

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

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

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

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

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:

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

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

How to learn the parameters w_0, w_1, … w_d?

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

How to learn the parameters w_0, w_1, … w_d?

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

Maximum (<u>Conditional</u>) 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

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

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

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

MLE Estimate

$$P(D|w) = \prod_{j=1}^{n} P(y^j|x^j,w) = \prod_{j=1}^{n} P(y^j=1|x^j,w)^{y^j} P(y^j=0|x^j,w)^{1-y^j}$$

$$= \prod_{j=1}^{n} \left(\frac{\exp(w_0+\sum_i w_i x_i^j)}{1+\exp(w_0+\sum_i w_i x_i^j)} \right)^{y^j} \left(\frac{1}{1+\exp(w_0+\sum_i w_i x_i^j)} \right)^{1-y^j}$$

$$l(w) = \ln P(D|w) = \sum_{j=1}^{n} \Big[y^j \big((w_0+\sum_i w_i x_i^j) - \ln(1+\exp(w_0+\sum_i w_i x_i^j)) \big) -$$

$$(1-y^j)\left(-\ln(1+\exp(w_0+\sum_i w_i x_i^j))\right) \Big]$$

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

$$\frac{\partial l(w)}{\partial w_i} = \sum_{j=1}^{n} \Big[x_i^j y^j - \frac{\exp(w_0+\sum_{i=1}^{d} w_i x_i^j)\cdot x_i^j}{1+\exp(w_0+\sum_{i=1}^{d} w_i x_i^j)} \Big]$$

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

$$= \sum_{j=1}^{n} x_i^j \left(y^j - P(y^j=1|x^j,w) \right)$$

Maximizing Conditional log Likelihood

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

$$= \sum_j y^j (w_0 + \sum_i^d w_i x_i^j) - \ln(1 + exp(w_0 + \sum_i^d w_i x_i^j))$$

Good news: $l(\mathbf{w})$ is concave function of $\mathbf{w}$ $\rightarrow$ no locally optimal solutions

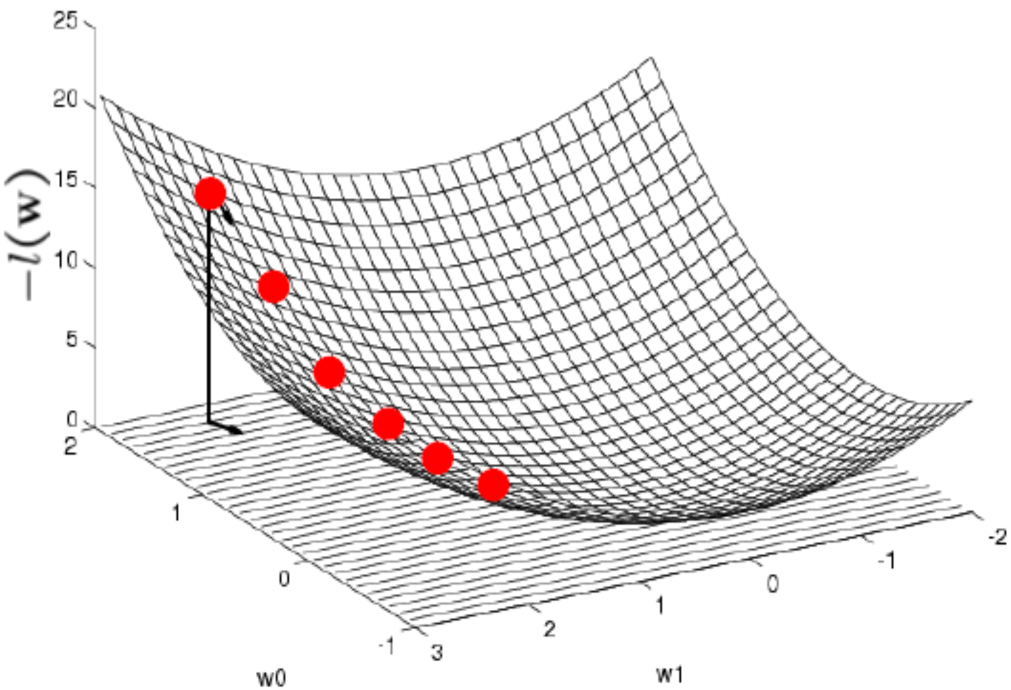
Bad news: no closed-form solution to maximize $l(\mathbf{w})$

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:

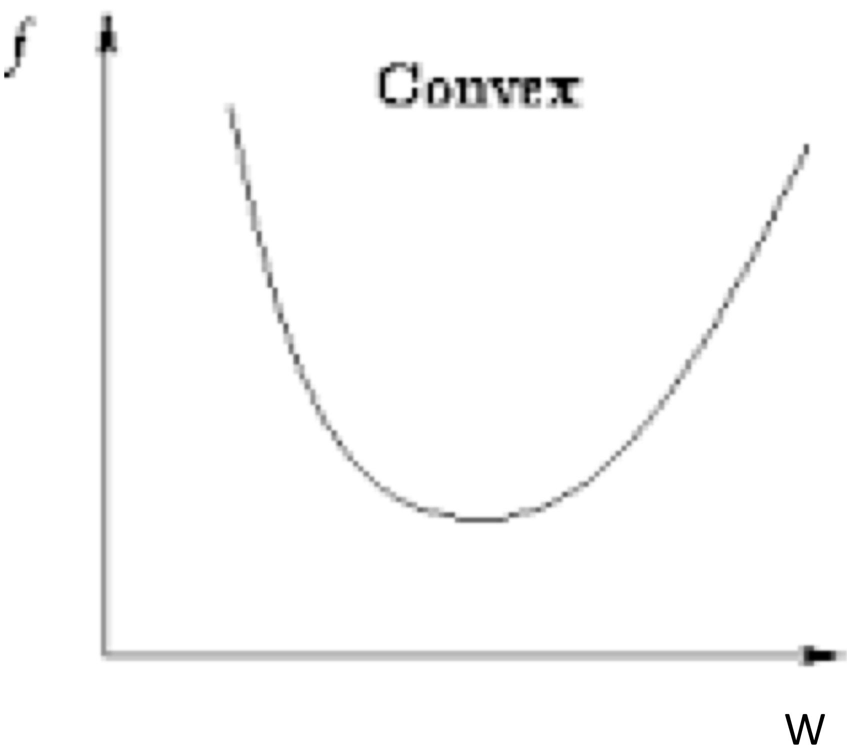
$$\nabla_{\mathbf{w}} l(\mathbf{w}) = [\frac{\partial l(\mathbf{w})}{\partial w_0}, \ldots, \frac{\partial l(\mathbf{w})}{\partial w_n}]'$$

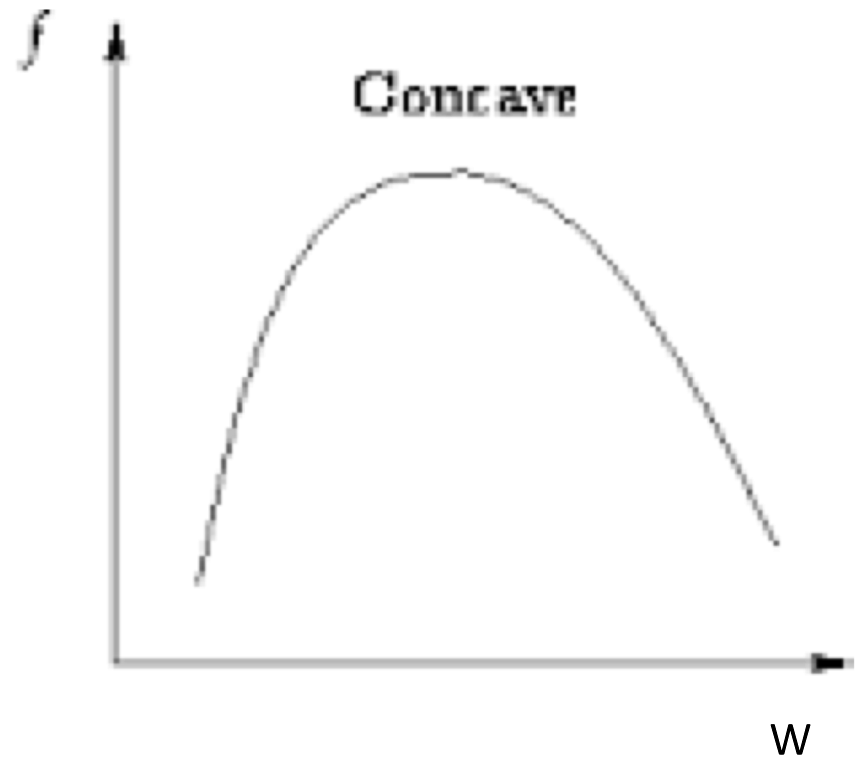
Update rule: Learning rate, η>0

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

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

Gradient Ascent/Descent for Concave and Convex function





Calculate Partial Derivative – A Beautiful Result

$$\frac{\partial l(w)}{\partial w_i} = \sum_j y^j x_i^j - \frac{\exp(w_o + \sum_1^d w_i x_i^j)\, x_i^j}{1 + \exp(w_o + \sum_1^d w_i x_i^j)} = \sum_j x_i^j (y^j - \frac{\exp(w_o + \sum_1^d w_i x_i^j)}{1 + \exp(w_o + \sum_1^d w_i x_i^j)})$$

$$\frac{\partial l(w)}{\partial w_i} = \sum_j x_i^j (y^j - P(y^j = 1 | x^j, w))$$

Gradient Ascent for Logistic Regression

Gradient ascent algorithm: iterate until change < ε

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

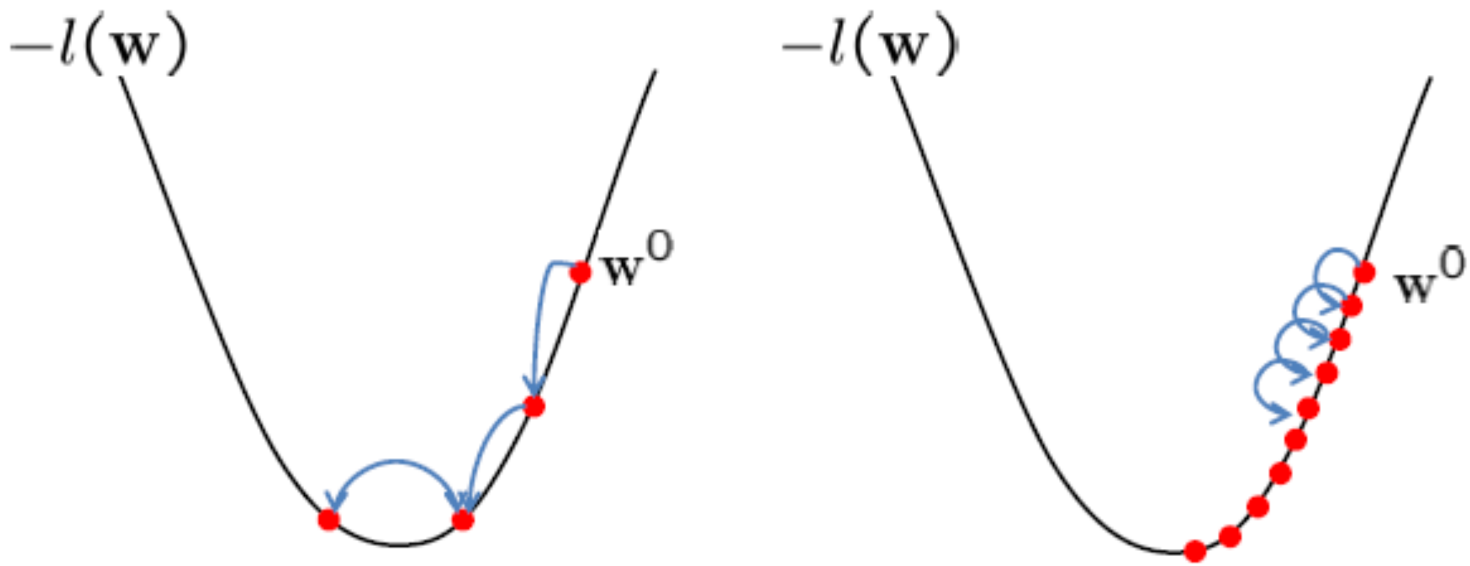
For i=1,…,d,

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

repeat

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

Effect of step-size η



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

Small η => Slow convergence but small residual error

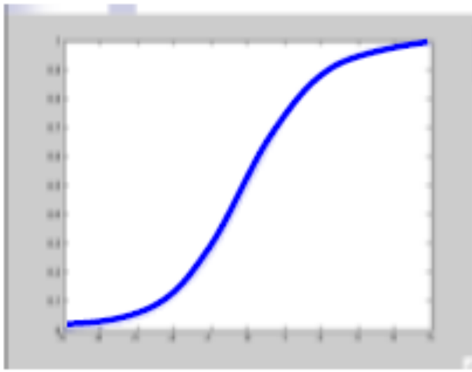
That's all M(C)LE. How about MAP?

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

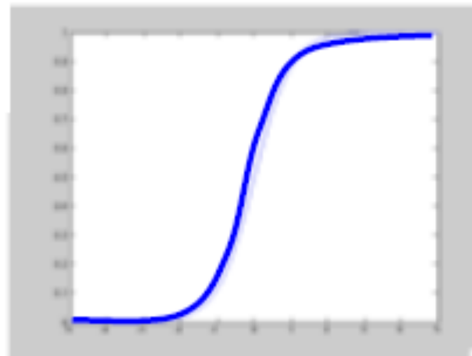
- One common approach is to define priors on **w**
  - Normal distribution, zero mean, identity covariance
  - "Pushes" parameters towards zero
- Corresponds to ***Regularization***
  - Helps avoid very large weights and overfitting
  - More on this later in the semester
- M(C)AP estimate

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

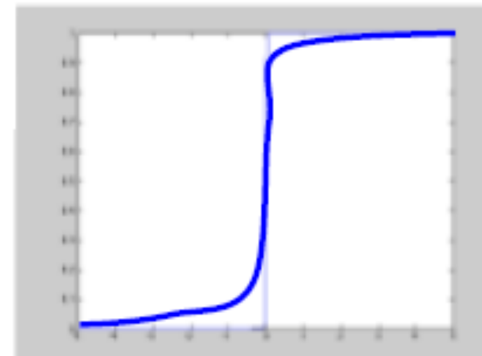
Large weights → Overfitting



$$\frac{1}{1+e^{-x}}$$

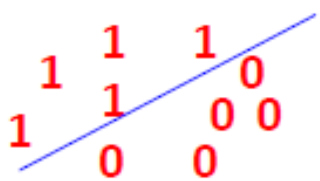


$$\frac{1}{1+e^{-2x}}$$



$$\frac{1}{1+e^{-100x}}$$

- Large weights lead to overfitting:



- Penalizing high weights can prevent overfitting...
  - again, more on this later in the semester

M(C)AP – Regularization

- Regularization

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

Zero-mean Gaussian prior

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

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

Calculate Partial Derivative – A Beautiful Result

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

$$\frac{\partial l(w)}{\partial w_i} = \sum_j x_i^j \left(y^j - P\left(y^j = 1 \middle| x^j, w\right)\right) - \frac{w_i}{k^2}$$

Gradient Ascent for 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,

$$w_i^{(t+1)} \leftarrow w_i^{(t)} + \eta \sum_j x_i^j [y^j - \underbrace{\hat{P}(Y^j = 1 \mid \mathbf{x}^j, \mathbf{w}^{(t)})]}_{\text{Predict what current weight thinks label Y should be}} \quad -\eta \frac{w_i}{k^2}$$

repeat

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