Polynomial, Logistic Regression

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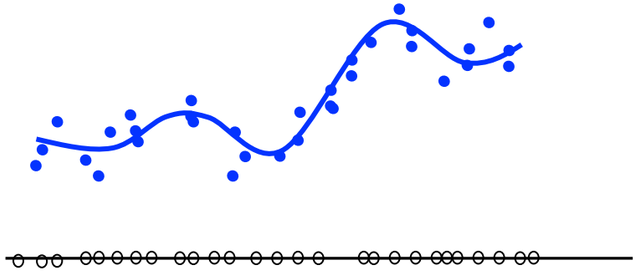
Machine Learning 10-701

Beyond Linear Regression

Polynomial regression
Regression with nonlinear features



Kernelized Ridge Regression (later in course)

Local Kernel Regression (later in course)

Polynomial Regression

degree m

Univariate (1-dim) case:

$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_m X^m = \mathbf{X}\beta$$

where $\mathbf{X} = [1 \;\; X \;\; X^2 \ldots X^m], \beta = [\beta_1 \ldots \beta_m]^T$

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \text{ or } (\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n(X) = \mathbf{X}\widehat{\beta}$$

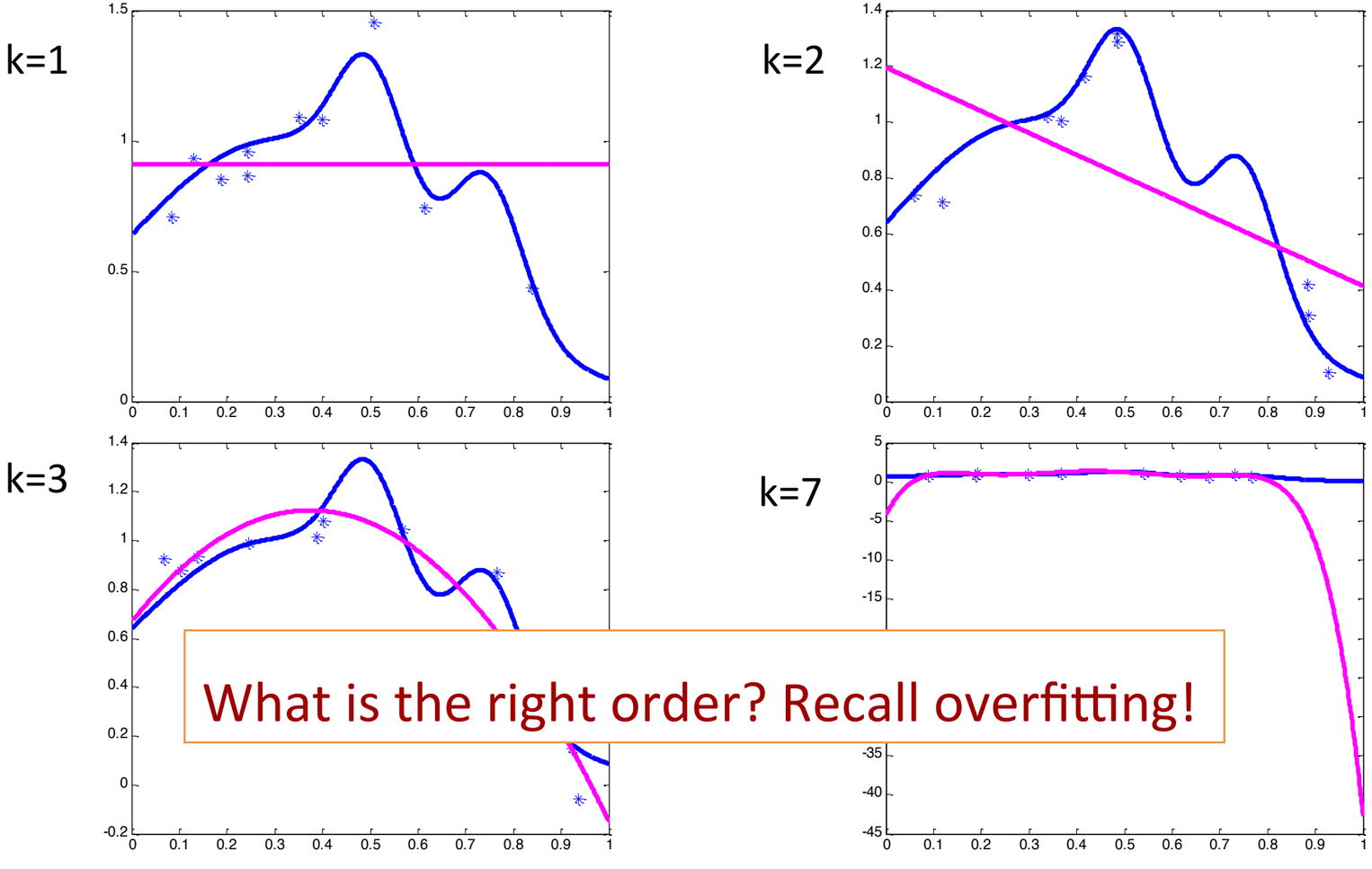
where $\mathbf{A} = \begin{bmatrix} 1 & X_1 & X_1^2 & \ldots & X_1^m \\ \vdots & & & \ddots & \vdots \\ 1 & X_n & X_n^2 & \ldots & X_n^m \end{bmatrix}$

Multivariate (p-dim) case:

$$\begin{aligned} f(X) \;=\; & \beta_0 + \beta_1 X^{(1)} + \beta_2 X^{(2)} + \cdots + \beta_p X^{(p)} \\ & + \sum_{i=1}^{p}\sum_{j=1}^{p} \beta_{ij} X^{(i)} X^{(j)} + \sum_{i=1}^{p}\sum_{j=1}^{p}\sum_{k=1}^{p} X^{(i)} X^{(j)} X^{(k)} \\ & + \ldots \text{terms up to degree m} \end{aligned}$$

Polynomial Regression

Polynomial of order k, equivalently of degree up to k-1

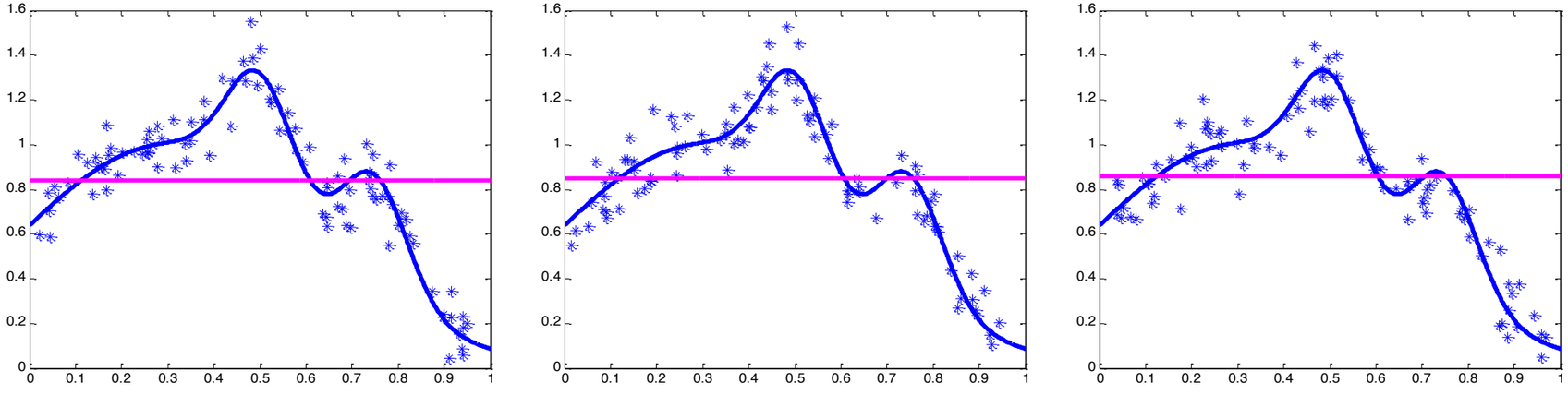


What is the right order? Recall overfitting!

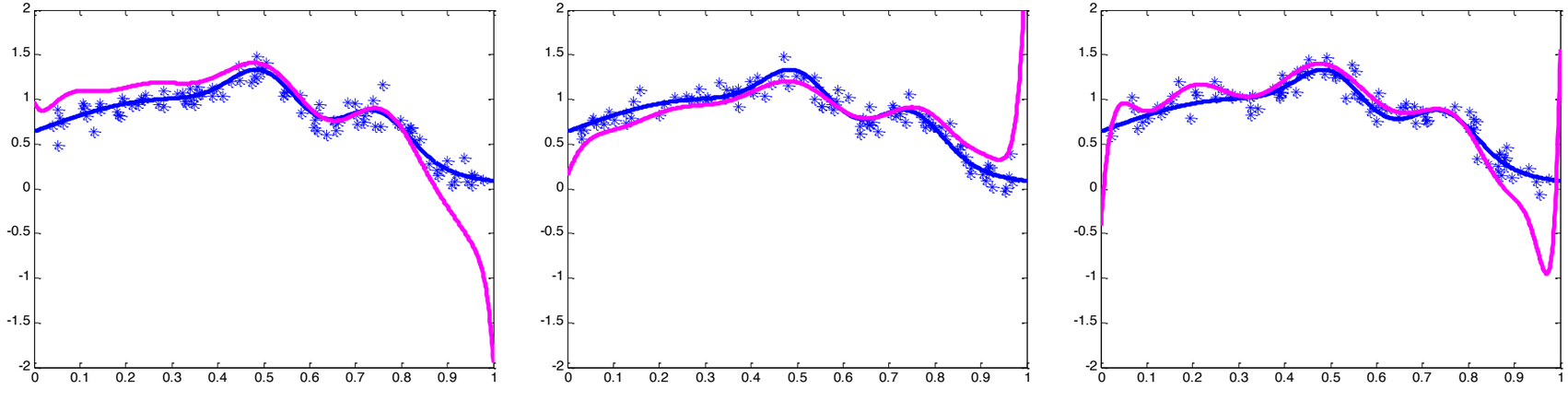
Bias – Variance Tradeoff

3 Independent training datasets

Large bias, Small variance – poor approximation but robust/stable



Small bias, Large variance – good approximation but unstable



Bias – Variance Decomposition

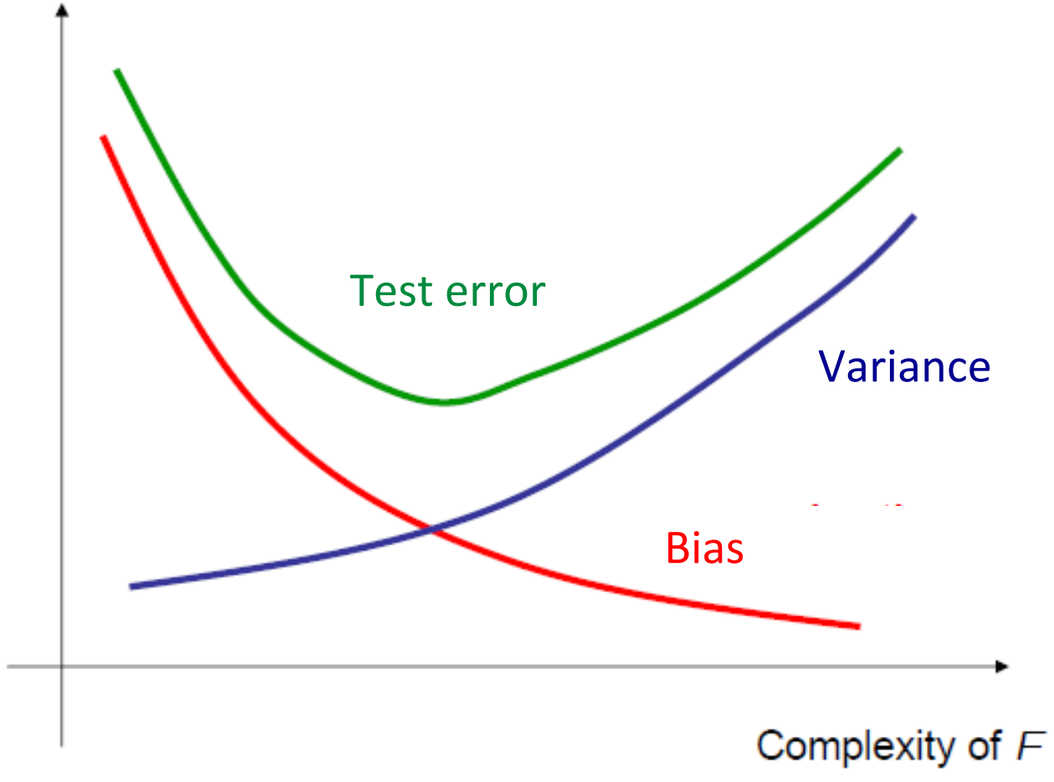
Later in the course, we will show that

$E[(f(X) - f^*(X))^2] = Bias^2 + Variance$

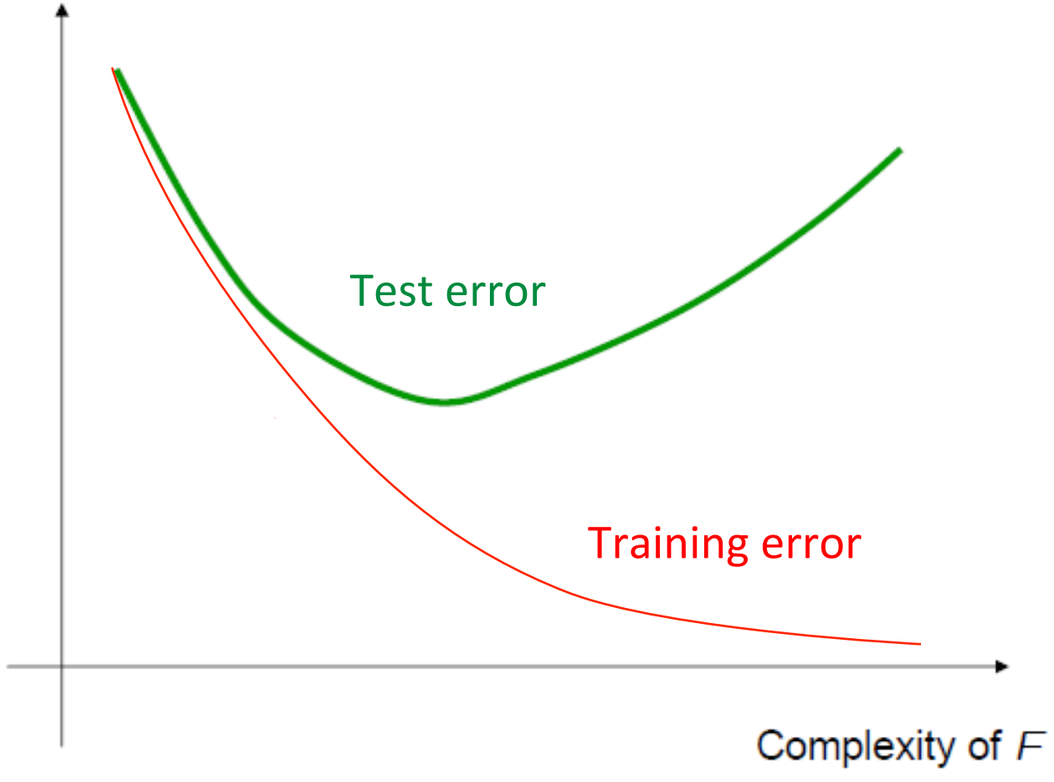
$Bias = E[f(X)] - f^*(X)$ How far is the model from best model

$Variance = E[(f(X) - E[f(X)])^2]$ How variable is the model

Effect of Model Complexity



Effect of Model Complexity



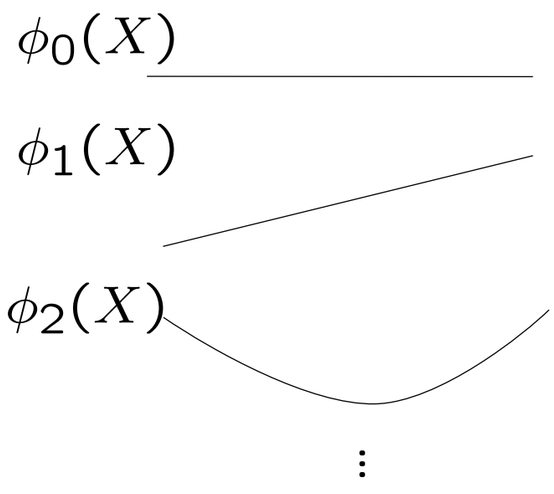
Regression with basis functions

$$f(X) = \sum_{j=0}^{m} \beta_j \phi_j(X)$$

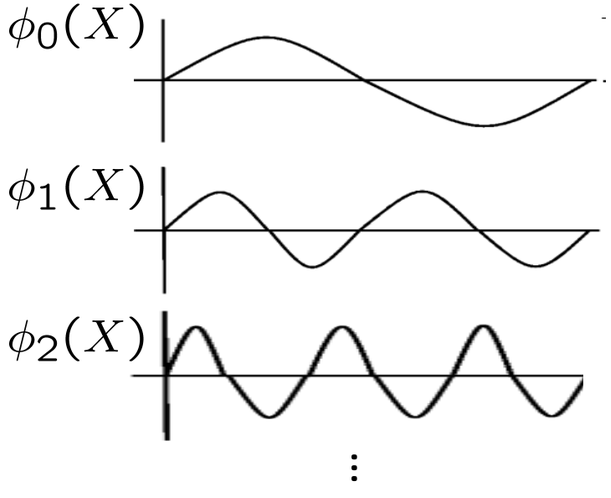
Basis coefficients

Basis functions (Linear combinations yield meaningful spaces)

Polynomial Basis

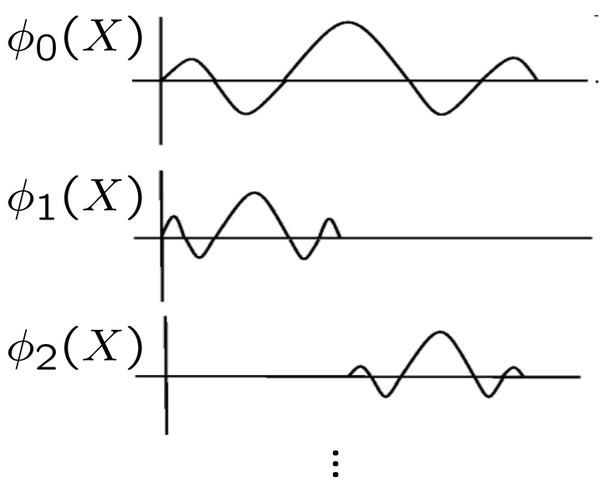


Fourier Basis



Good representation for periodic functions

Wavelet Basis



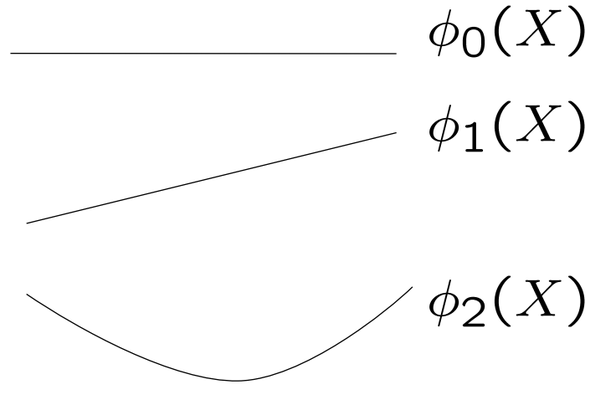
Good representation for local functions

Regression with nonlinear features

$$f(X) = \sum_{j=0}^{m} \beta_j X^j = \sum_{j=0}^{m} \beta_j \phi_j(X)$$

Weight of each feature

Nonlinear features



In general, use any nonlinear features

e.g. e^X, log X, 1/X, sin(X), …

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y}$$

or

$$(\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{Y}$$

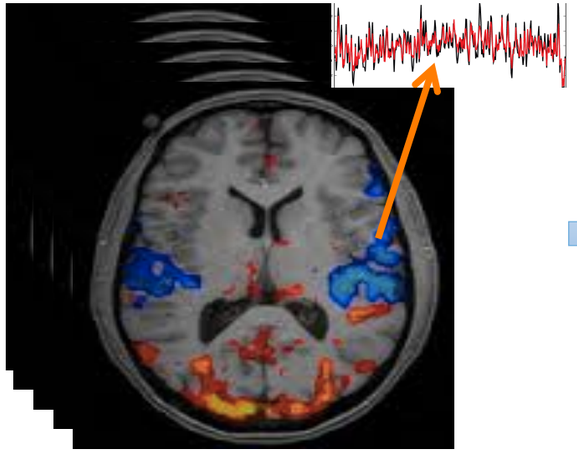
$$\mathbf{A} = \begin{bmatrix} \phi_0(X_1) & \phi_1(X_1) & \dots & \phi_m(X_1) \\ \vdots & & \ddots & \vdots \\ \phi_0(X_n) & \phi_1(X_n) & \dots & \phi_m(X_n) \end{bmatrix}$$

$$\widehat{f}_n(X) = \mathbf{X}\widehat{\beta}$$

$$\mathbf{X} = [\phi_0(X) \;\; \phi_1(X) \;\; \dots \;\; \phi_m(X)]$$

Regression to Classification

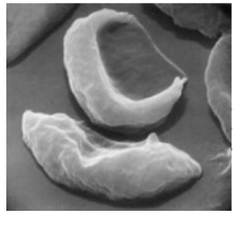
Regression

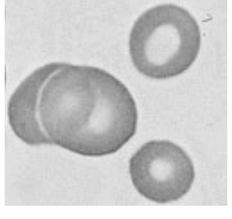


X = Brain Scan

Y = Age of a subject

Classification





X = Cell Image

Anemic cell
Healthy cell

Y = Diagnosis

Can we predict the "probability" of class label being Anemic or Healthy – a real number – using regression methods?

But output (probability) needs to be in [0,1]

Logistic Regression

Not really regression

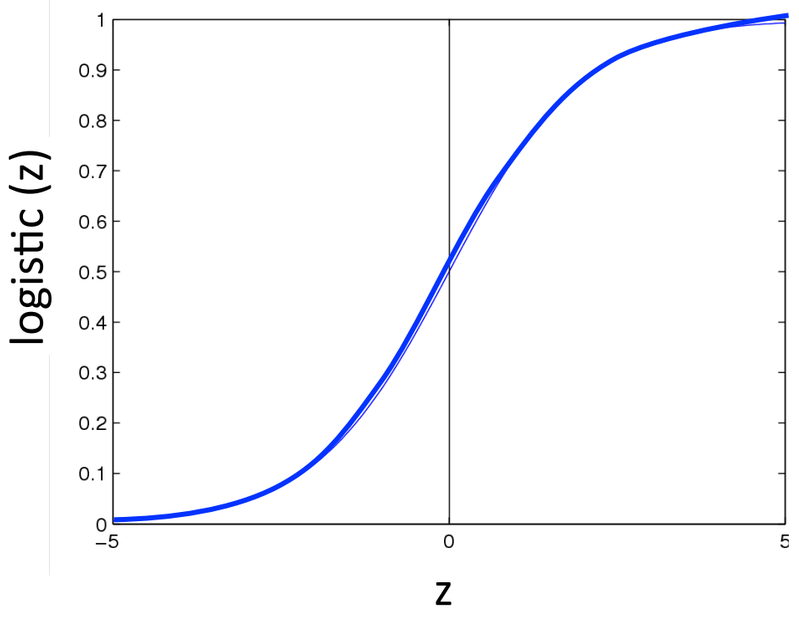
Assumes the following functional form for P(Y|X):

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

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):

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

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

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

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

Logistic Regression is a Linear Classifier!

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

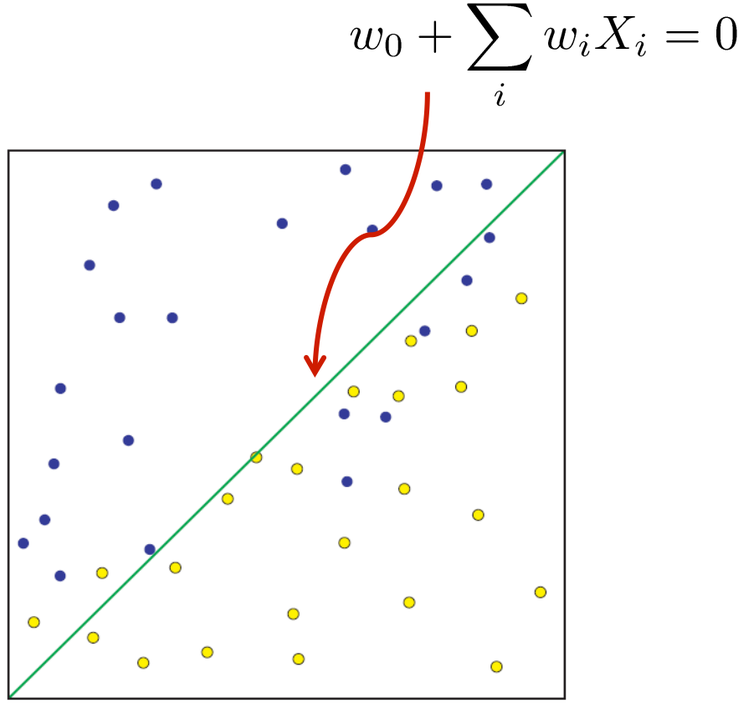
$$P(Y=0|X) = \frac{1}{1+\exp(w_0 + \sum_i w_i X_i)}$$

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)



Training Logistic Regression

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

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

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 $w_0, w_1, \ldots w_d$? (d features)

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

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

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

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

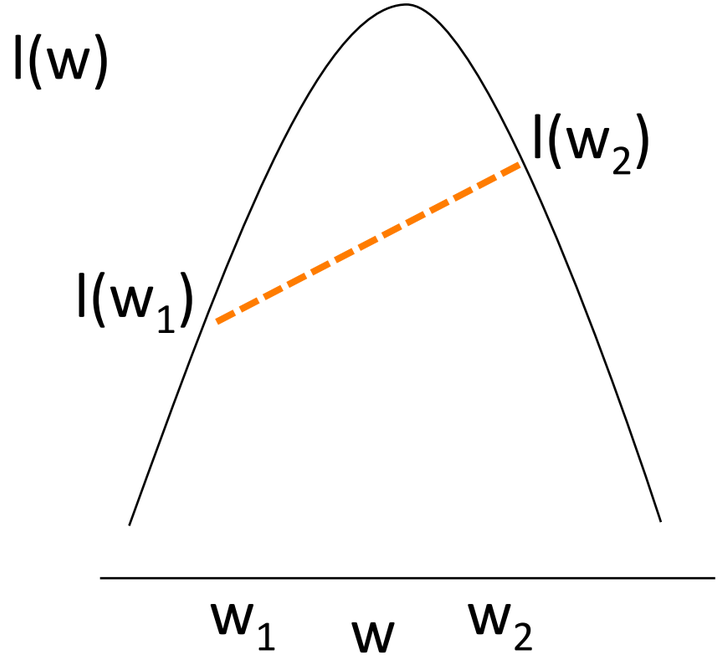
$$\begin{aligned} l(\mathbf{w}) &\equiv \ln \prod_j P(y^j|\mathbf{x}^j, \mathbf{w}) \\ &= \sum_j \left[y^j (w_0 + \sum_i^d w_i x_i^j) - \ln(1 + exp(w_0 + \sum_i^d w_i x_i^j)) \right] \end{aligned}$$

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

Good news: *l*(**w**) is concave function of **w**

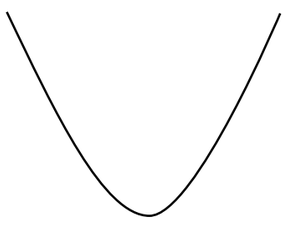
concave functions easy to maximize

Concave function

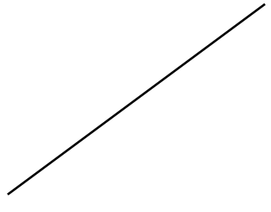


A function l(w) is called **concave** if the line joining two points $l(w_1), l(w_2)$ on the function does not go above the function on the interval $[w_1, w_2]$

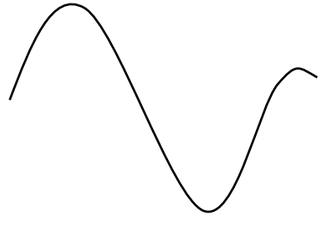
(Strictly) Concave functions have a unique maximum!



Convex



Both Concave & Convex

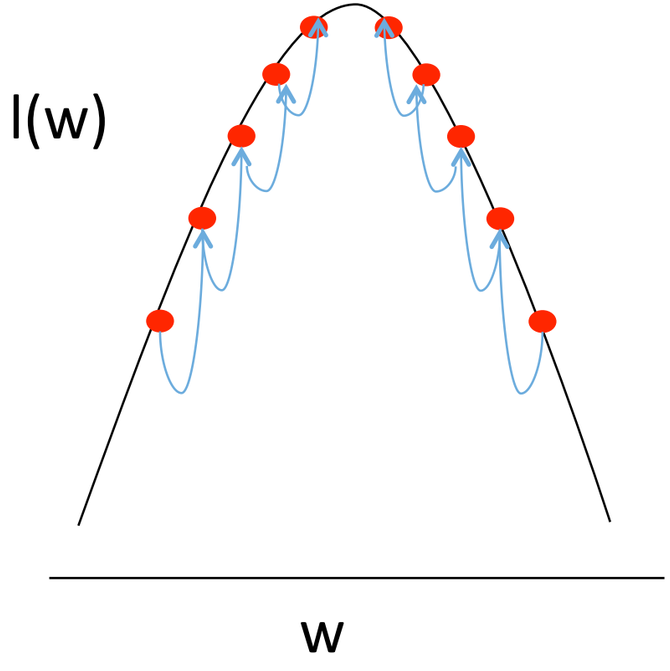


Neither

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:

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

Learning rate, η>0

Update rule:

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

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

Gradient Ascent for Logistic Regression

Gradient ascent rule for w_0:

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

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

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

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

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,

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

repeat

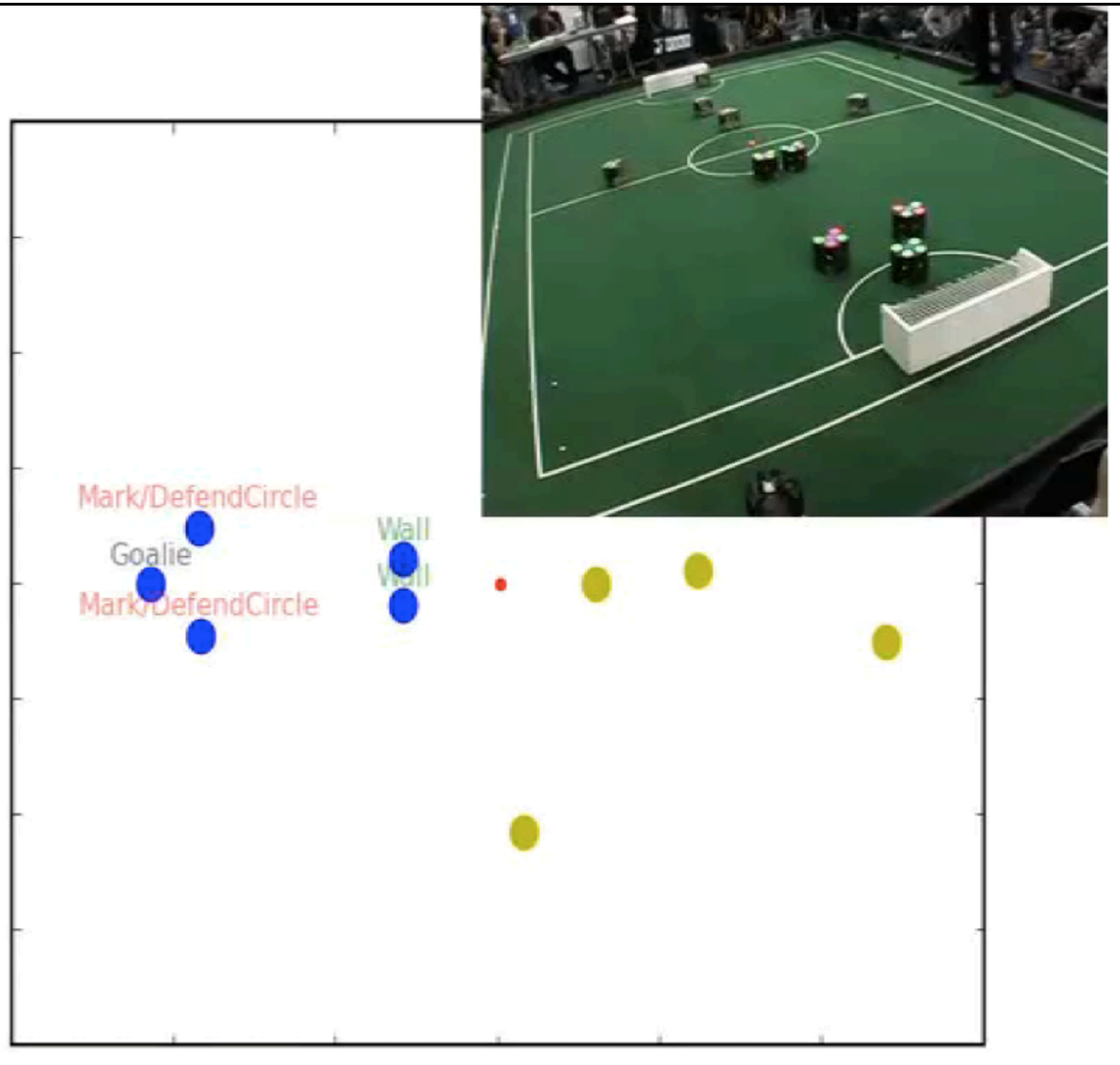
Predict what current weight thinks label Y should be

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

Classification

- Multiple classes
- Choice of features
- Many algorithms
- Efficient computation
- ….

Multiclass Classification – Opponent Strategy



That's all 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

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

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

Penalizes large weights

Still concave objective!

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

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

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

Extra term Penalizes large weights

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

- Maximum conditional likelihood estimate

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

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

- Maximum conditional a posteriori estimate

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

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

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?