Linear Regression

Aarti Singh & Barnabas Poczos

Machine Learning 10-701/15-781
Jan 23, 2014

MACHINE LEARNING DEPARTMENT
Carnegie Mellon.
School of Computer Science

So far …

- Learning distributions
  – Maximum Likelihood Estimation (MLE)
  – Maximum A Posteriori (MAP)

- Learning classifiers
  – Naïve Bayes

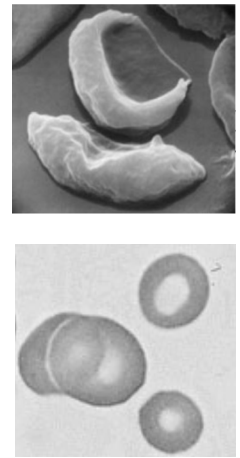
Discrete to Continuous Labels

Classification

Sports
Science
News

X = Document

Y = Topic



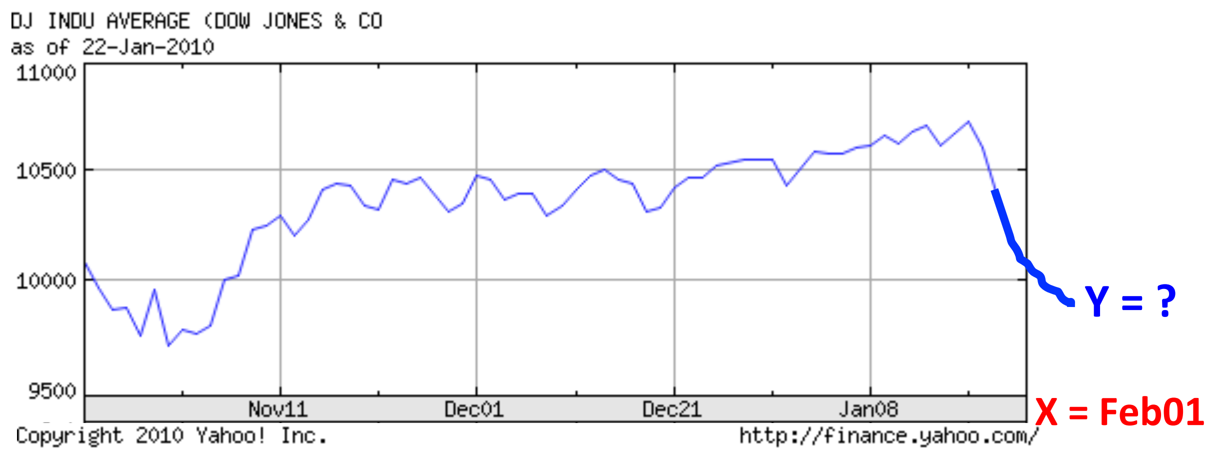
Anemic cell
Healthy cell

X = Cell Image

Y = Diagnosis

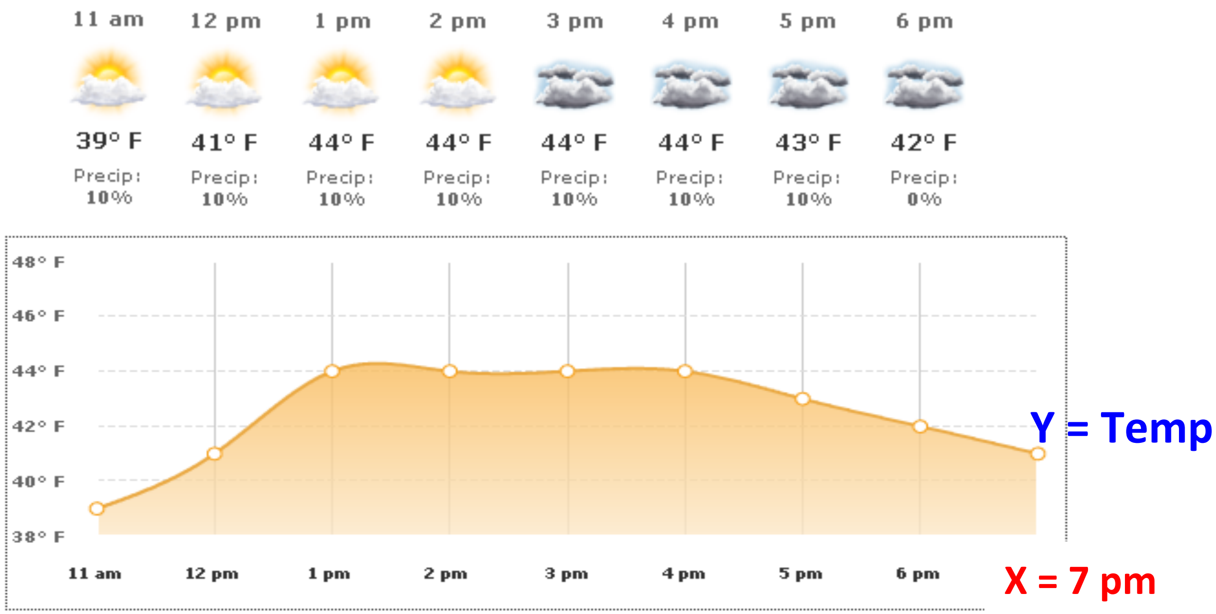
Regression

Stock Market
Prediction



Regression Tasks

Weather Prediction

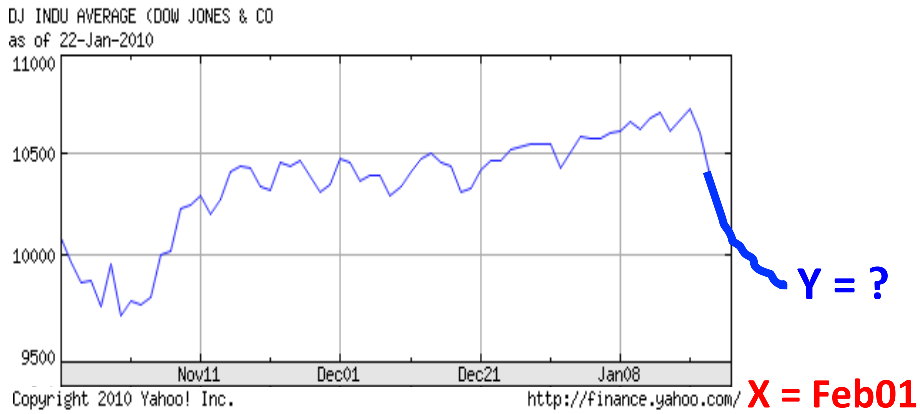


Estimating Contamination

Supervised Learning

Goal: Construct a **predictor** $f : X \to Y$ to minimize loss function (performance measure)

Sports
Science
News



Classification:

$$P(f(X) \neq Y)$$

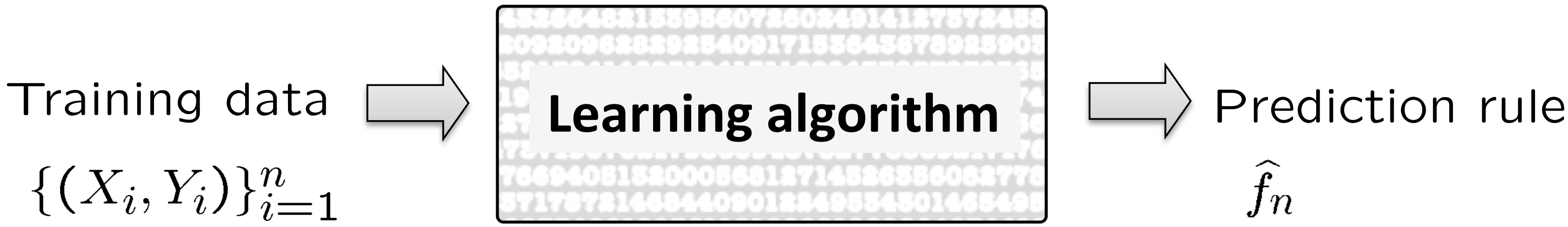
Probability of Error

Regression:

$$\mathbb{E}[(f(X) - Y)^2]$$

Mean Squared Error

Regression algorithms



Linear Regression

Regularized Linear Regression – Ridge regression, Lasso

Polynomial Regression

Kernel Regression

Regression Trees, Splines, Wavelet estimators, …

Replace Expectation with Empirical Mean

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

Empirical Minimizer: $$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n}\sum_{i=1}^{n}(f(X_i) - Y_i)^2$$

Empirical mean

Law of Large Numbers:

$$\boxed{\frac{1}{n}\sum_{i=1}^{n}[\text{loss}(Y_i, f(X_i))] \xrightarrow{n \longrightarrow \infty} \mathbb{E}_{XY}[\text{loss}(Y, f(X))]}$$

Restrict class of predictors

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

Empirical Minimizer: $$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

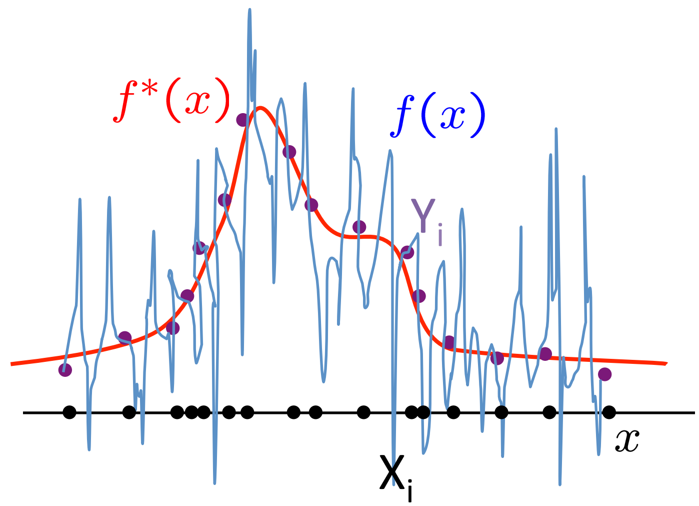
Class of predictors

Why?

Overfitting!

Empiricial loss minimized by any function of the form

$$f(x) = \begin{cases} Y_i, & x = X_i \text{ for } i = 1, \ldots, n \\ \text{any value}, & \text{otherwise} \end{cases}$$



Restrict class of predictors

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

Empirical Minimizer: $$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

Class of predictors

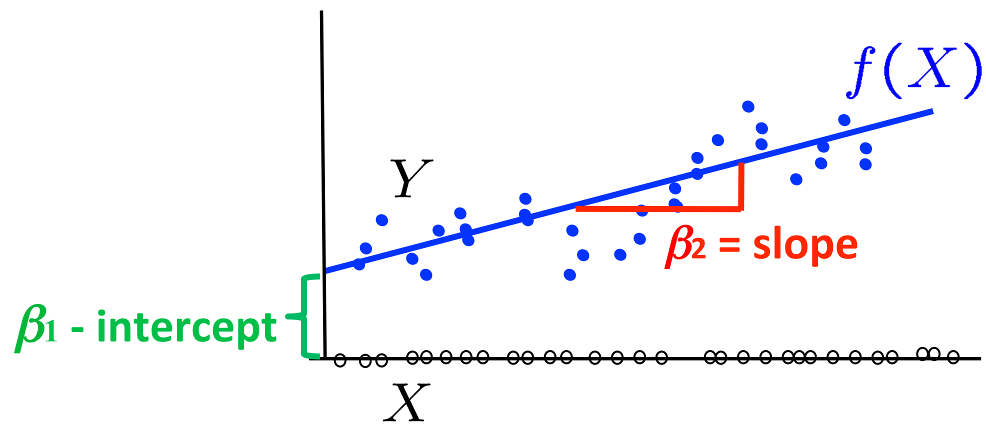
$\mathcal{F}$ - Class of Linear functions
- Class of Polynomial functions
- Class of nonlinear functions

Linear Regression

$$\widehat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

Least Squares Estimator

$\mathcal{F}_L$ - Class of Linear functions



Uni-variate case:

$$f(X) = \beta_1 + \beta_2 X$$

Multi-variate case:

$$f(X) = f(X^{(1)}, \ldots, X^{(p)}) = \beta_1 \cancelto{1}{X^{(1)}} + \beta_2 X^{(2)} + \cdots + \beta_p X^{(p)}$$

$$= X\beta \qquad \text{where} \quad X = [X^{(1)} \ldots X^{(p)}], \quad \beta = [\beta_1 \ldots \beta_p]^T$$

Least Squares Estimator

$$\widehat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2 \qquad f(X_i) = X_i \beta$$

$$\Downarrow$$

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} (X_i \beta - Y_i)^2 \qquad \widehat{f}_n^L(X) = X\widehat{\beta}$$

$$= \arg\min_{\beta} \frac{1}{n} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y})$$

$$\mathbf{A} = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} = \begin{bmatrix} X_1^{(1)} & \dots & X_1^{(p)} \\ \vdots & \ddots & \vdots \\ X_n^{(1)} & \dots & X_n^{(p)} \end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_n \end{bmatrix}$$

Least Squares Estimator

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

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

$$\left.\frac{\partial J(\beta)}{\partial \beta}\right|_{\widehat{\beta}} = 0$$

Normal Equations

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

p xp   p x1   p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

$$\boxed{\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n^L(X) = X\widehat{\beta}}$$

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?
Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$?

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?
Regularization (later)

Gradient Descent

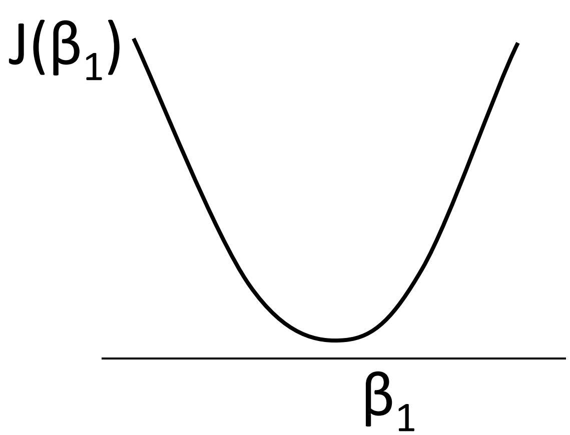
Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

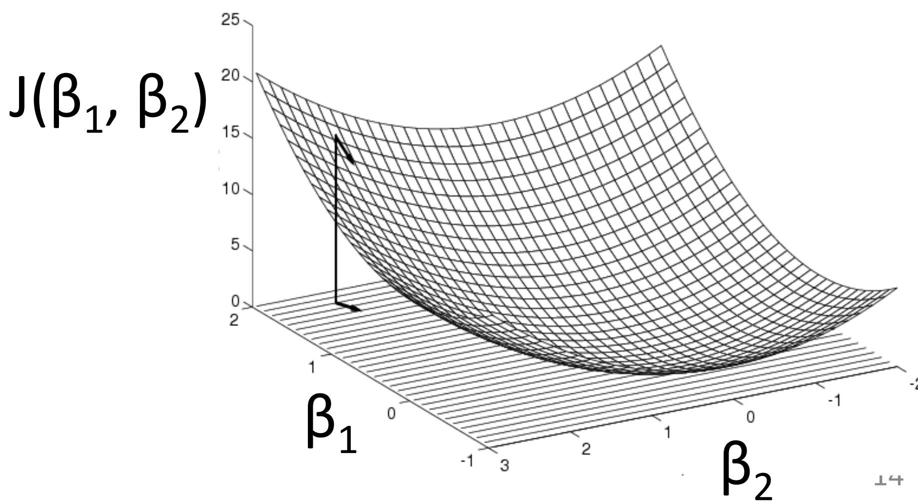
$$\widehat{\beta} \;= \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) \;= \arg\min_{\beta} J(\beta)$$

Treat as optimization problem

Observation: J(β) is convex in β.

How to find the minimizer?





Gradient Descent

Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

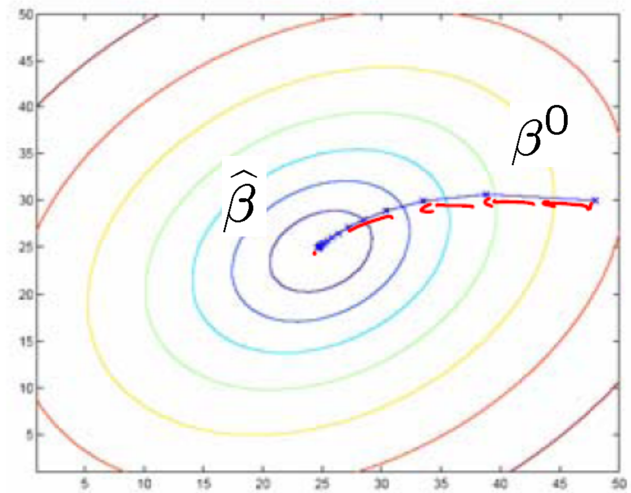
$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

Since J(β) is convex, move along negative of gradient

Initialize: β^0

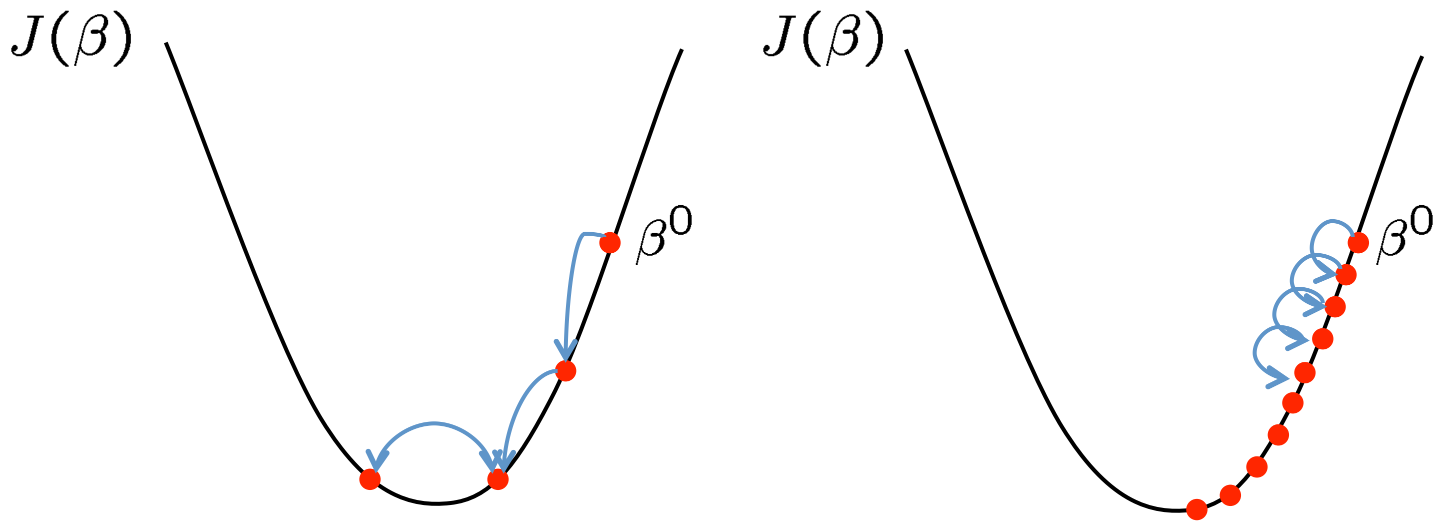
step size

Update:
$$\beta^{t+1} = \beta^t - \frac{\alpha}{2}\frac{\partial J(\beta)}{\partial \beta}\bigg|_t = \beta^t - \alpha\ \mathbf{A}^T\underbrace{(\mathbf{A}\beta^t - Y)}_{0 \text{ if } \widehat{\beta} = \beta^t}$$



Stop: when some criterion met e.g. fixed # iterations, or $\frac{\partial J(\beta)}{\partial \beta}\bigg|_{\beta^t} < \varepsilon$.

Effect of step-size α

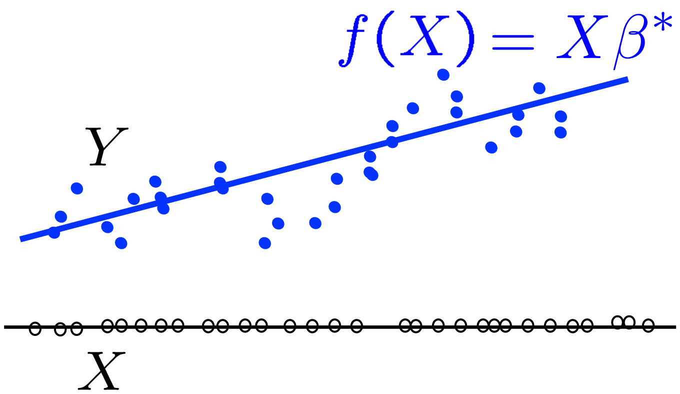


Large α => Fast convergence but larger residual error
Also possible oscillations

Small α => Slow convergence but small residual error

Least Squares and MLE

Intuition: Signal plus (zero-mean) Noise model



$$Y = f^*(X) + \epsilon = X\beta^* + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}) \quad Y \sim \mathcal{N}(X\beta^*, \sigma^2 \mathbf{I})$$

$$\widehat{\beta}_{\text{MLE}} = \arg\max_{\beta} \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}}$$

$$= \arg\min_{\beta} \sum_{i=1}^{n} (X_i\beta - Y_i)^2 = \widehat{\beta}$$

Least Square Estimate is same as Maximum Likelihood Estimate under a Gaussian model !

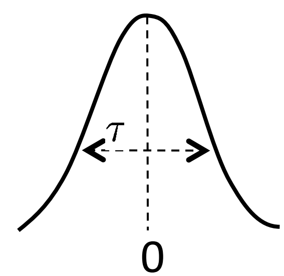
Regularized Least Squares and MAP

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

$$\widehat{\beta}_{\text{MAP}} = \arg\max_{\beta} \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

I) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2 \mathbf{I}) \qquad p(\beta) \propto e^{-\beta^T\beta/2\tau^2}$$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \underbrace{\lambda}_{\text{constant}(\sigma^2, \tau^2)} \|\beta\|_2^2$$

Ridge Regression

$$\widehat{\beta}_{\text{MAP}} = (\boldsymbol{A}^\top \boldsymbol{A} + \lambda \boldsymbol{I})^{-1} \boldsymbol{A}^\top \boldsymbol{Y}$$

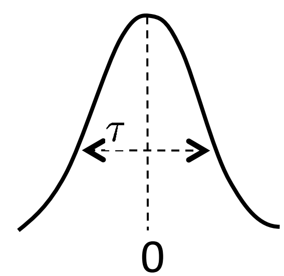
Regularized Least Squares and MAP

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

$$\widehat{\beta}_{\text{MAP}} = \arg\max_{\beta} \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

I) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2\mathbf{I}) \qquad p(\beta) \propto e^{-\beta^T\beta/2\tau^2}$$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \underbrace{\lambda}_{\text{constant}(\sigma^2, \tau^2)} \|\beta\|_2^2$$

Ridge Regression

Prior belief that β is Gaussian with zero-mean biases solution to “small” β

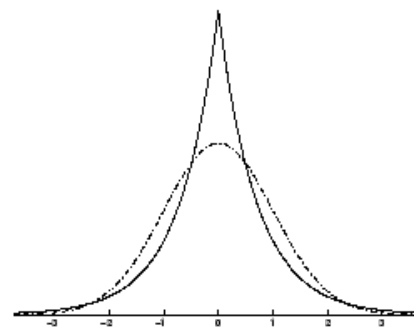
Regularized Least Squares and MAP

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

$$\widehat{\beta}_{\mathsf{MAP}} = \arg\max_\beta \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

II) Laplace Prior

$$\beta_i \overset{iid}{\sim} \text{Laplace}(0, t) \qquad\qquad p(\beta_i) \propto e^{-|\beta_i|/t}$$



$$\widehat{\beta}_{\mathsf{MAP}} = \arg\min_\beta \sum_{i=1}^n (Y_i - X_i\beta)^2 + \underset{\displaystyle\downarrow \atop \displaystyle \text{constant}(\sigma^2, t)}{\lambda}\|\beta\|_1$$

Lasso

Prior belief that β is Laplace with zero-mean biases solution to "small" β

Ridge Regression vs Lasso

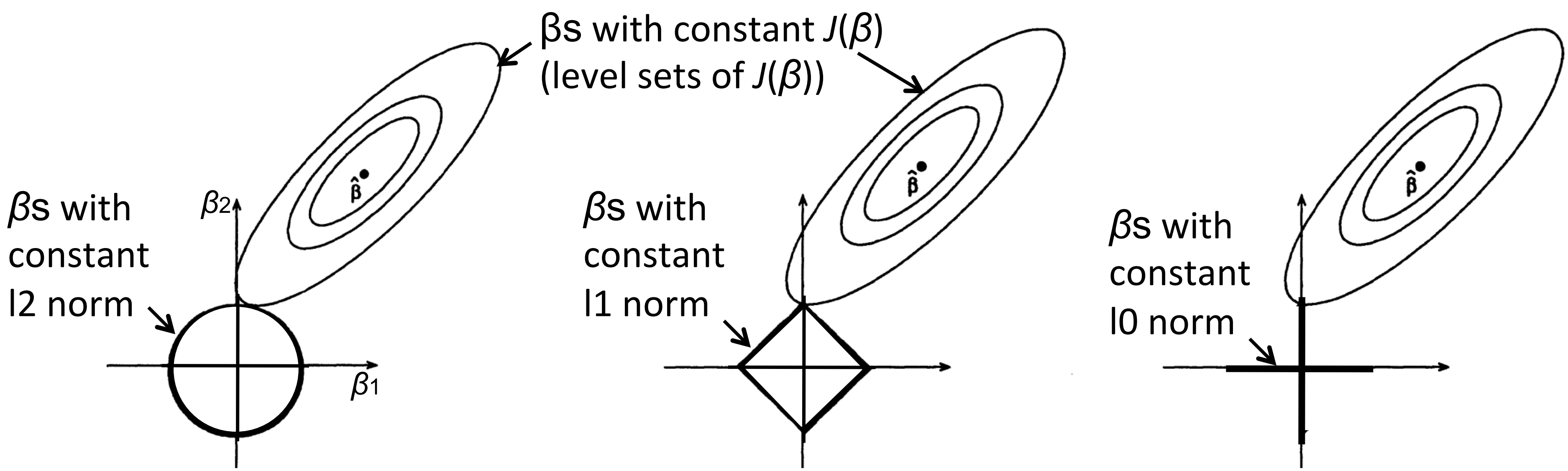
$$\min_\beta (\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) + \lambda \text{pen}(\beta) = \min_\beta J(\beta) + \lambda \text{pen}(\beta)$$

Ridge Regression:
$\text{pen}(\beta) = \|\beta\|_2^2$

Lasso:
$\text{pen}(\beta) = \|\beta\|_1$

HOT!

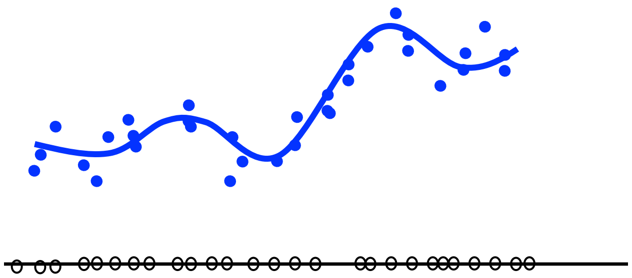
Ideally l0 penalty, but optimization becomes non-convex



Lasso (l1 penalty) results in sparse solutions – vector with more zero coordinates
Good for high-dimensional problems – don't have to store all coordinates!

Beyond Linear Regression

Polynomial regression



Regression with nonlinear features

Later …

Kernel regression - Local/Weighted regression

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

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

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

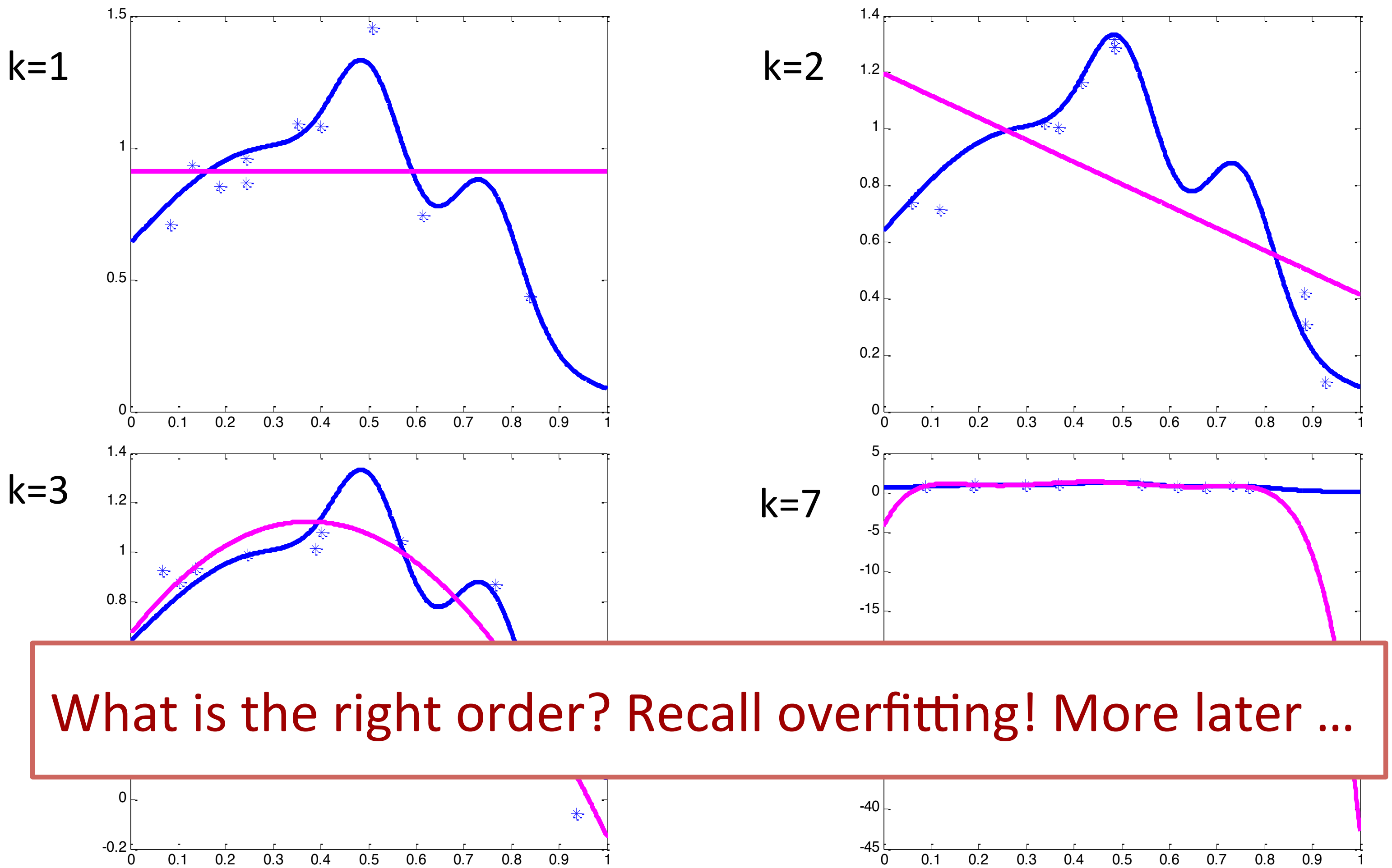
$$\widehat{f}_n(X) = \mathbf{X}\widehat{\beta}$$

Multivariate (p-dim) case:

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

Polynomial Regression

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

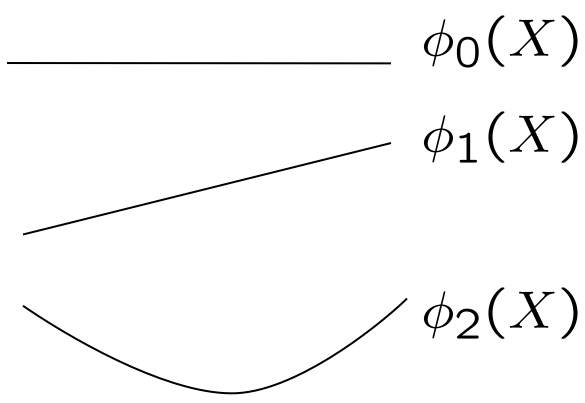


What is the right order? Recall overfitting! More later …

Regression with nonlinear features

$$f(X) = \sum_{j=0}^{m} \beta_j X^j = \sum_{j=0}^{m} \beta_j \underbrace{\phi_j(X)}_{\text{Nonlinear features}}$$

Weight of each feature



In general, use any nonlinear features

e.g. e^X, log X, 1/X, sin(X), …

What you should know

Linear Regression

- Least Squares Estimator
- Normal Equations
- Gradient Descent
- Probabilistic Interpretation (connection to MLE)

Regularized Linear Regression (connection to MAP)

- Ridge Regression, Lasso

Polynomial Regression, Regression with Non-linear features