Linear and Non-Linear Regression

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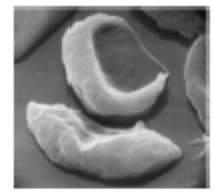
Fall, 2019

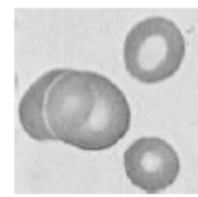
Slides Adapted from Book, CMU, Stanford Machine Learning Courses, and my presentations

Discrete to Continuous Labels

Classification

Sports
Science
News



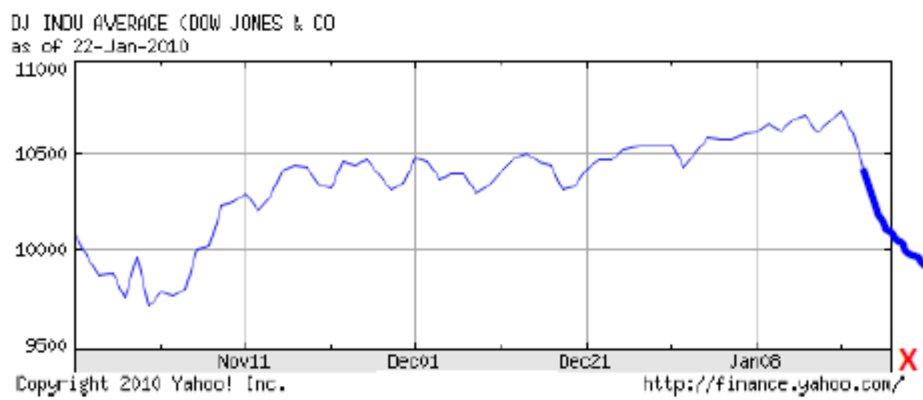


Anemic cell
Healthy cell

X = Document   Y = Topic   X = Cell Image   Y = Diagnosis

Regression

Stock Market Prediction

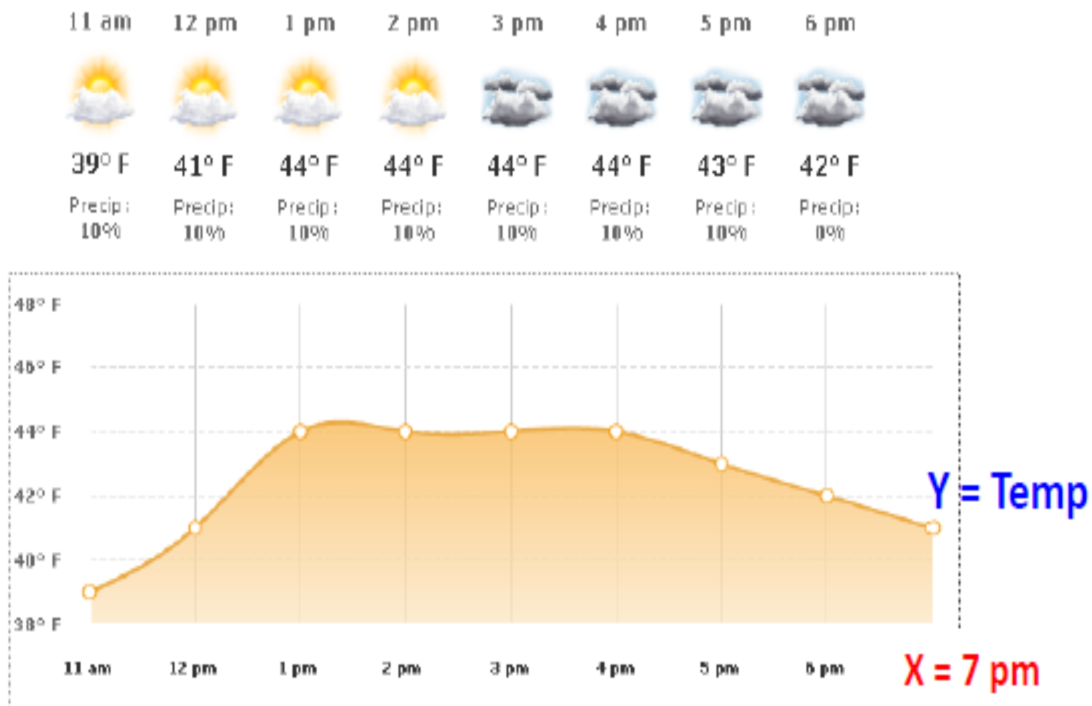


Y = ?

X = Feb01

Regression Tasks

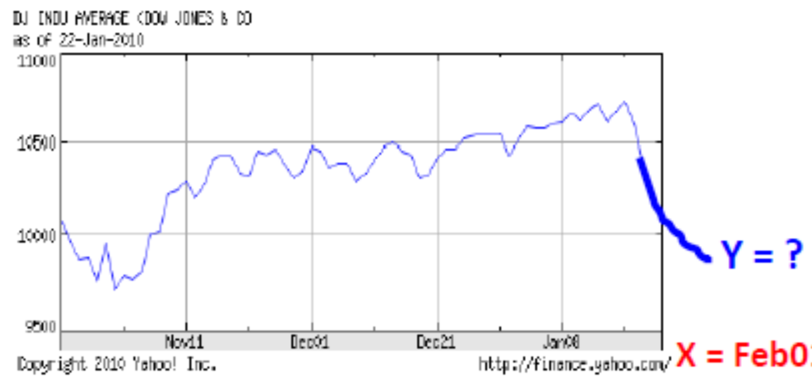
Weather Prediction



Supervised Learning

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

Sports
Science
News



Classification:

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

Probability of Error

Regression:

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

Mean Squared Error

Regression

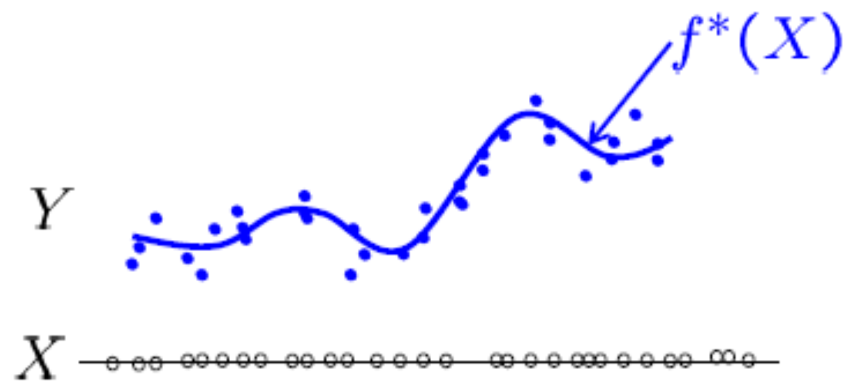
Optimal predictor:

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

$$= \mathbb{E}[Y|X] \qquad \text{(Conditional Mean)}$$

Intuition: Signal plus (zero-mean) Noise model

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



Regression

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

Proof Strategy: $R(f) \geq R(f^*)$ for any prediction rule f

$$R(f) = \mathbb{E}_{XY}[(f(X) - Y)^2] = \mathbb{E}_X[\mathbb{E}_{Y|X}[(f(X) - Y)^2|X]]$$

Dropping subscripts for notational convenience

$$= E\left[E\left[(\underbrace{f(X) - E[Y|X]} + \underbrace{E[Y|X] - Y})^2|X\right]\right]$$

$$= \begin{aligned} E[\quad & E[(f(X) - E[Y|X])^2|X] \\ & +2E\left[(f(X) - E[Y|X])(E[Y|X] - Y)|X\right] \\ & +E[(E[Y|X] - Y)^2|X]] \end{aligned}$$

$$= \begin{aligned} E[\quad & E[(f(X) - E[Y|X])^2|X] \\ & +2(f(X) - E[Y|X]) \times 0 \\ & +E[(E[Y|X] - Y)^2|X]] \end{aligned}$$

$$= \underbrace{E\left[(f(X) - E[Y|X])^2\right]}_{\geq 0} + R(f^*).$$

Regression

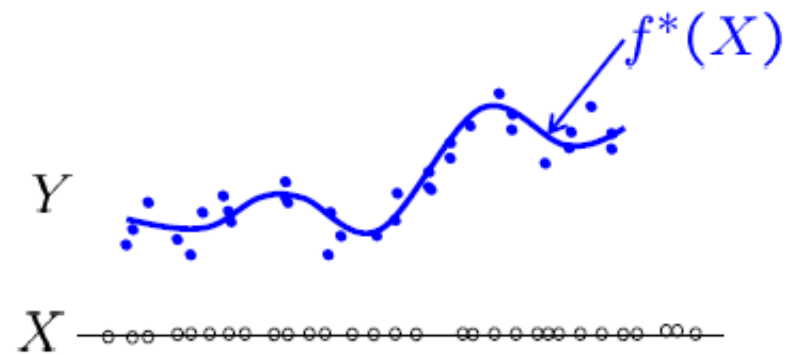
Optimal predictor:

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

$$= \mathbb{E}[Y|X] \qquad \text{(Conditional Mean)}$$

Intuition: Signal plus (zero-mean) Noise model

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



Depends on **unknown** distribution P_{XY}

Regression algorithms

Training data $\{(X_i, Y_i)\}_{i=1}^n$ → **Learning algorithm** → Prediction rule $\widehat{f}_n$

Linear Regression

Lasso, Ridge regression (Regularized Linear Regression)

Nonlinear Regression

Kernel Regression

Regression Trees, Splines, Wavelet estimators, …

Empirical Risk Minimization (ERM)

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

Empirical Risk 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 **Empirical mean**

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

ERM – you saw it before!

- Learning Distributions

  Max likelihood = Min -ve log likelihood empirical risk

$$\max_\theta P(D|\theta) = \min_\theta \frac{1}{n}\sum_{i=1}^{n} \underbrace{-\log P(X_i|\theta)}_{\text{loss}(X_i,\theta)}$$

Negative log Likelihood loss

What is the class $\mathcal{F}$?

Class of parametric distributions

Bernoulli (θ)

Gaussian (μ, σ^2)

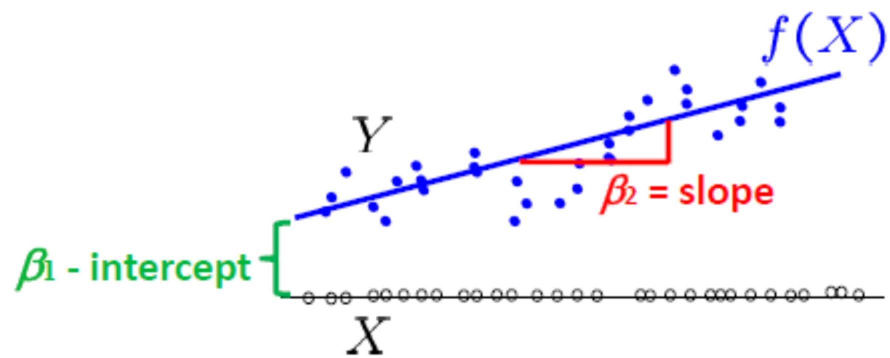
Linear Regression

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

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

Uni-variate case:

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



Multi-variate case:

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

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

Least Squares Estimator

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

$$\Downarrow$$

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

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

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

Least Squares Estimator

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

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

$$= \boldsymbol{A^T A \beta \beta^T - 2\beta^T A^T Y + Y^T Y}$$

$$\left.\frac{\partial J(\beta)}{\partial \beta}\right|_{\widehat{\beta}} = 0 \quad \boldsymbol{= 2A^T A\beta - 2A^T Y = 0}$$

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)

Revisiting Gradient Descent

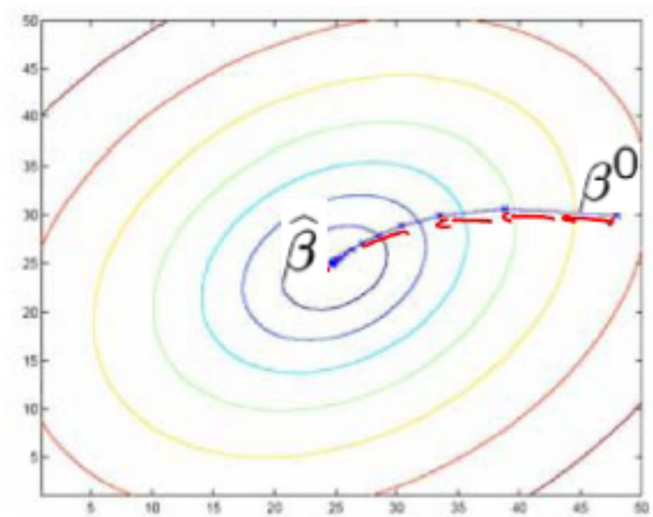
Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

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

Gradient Descent since J(β) is convex

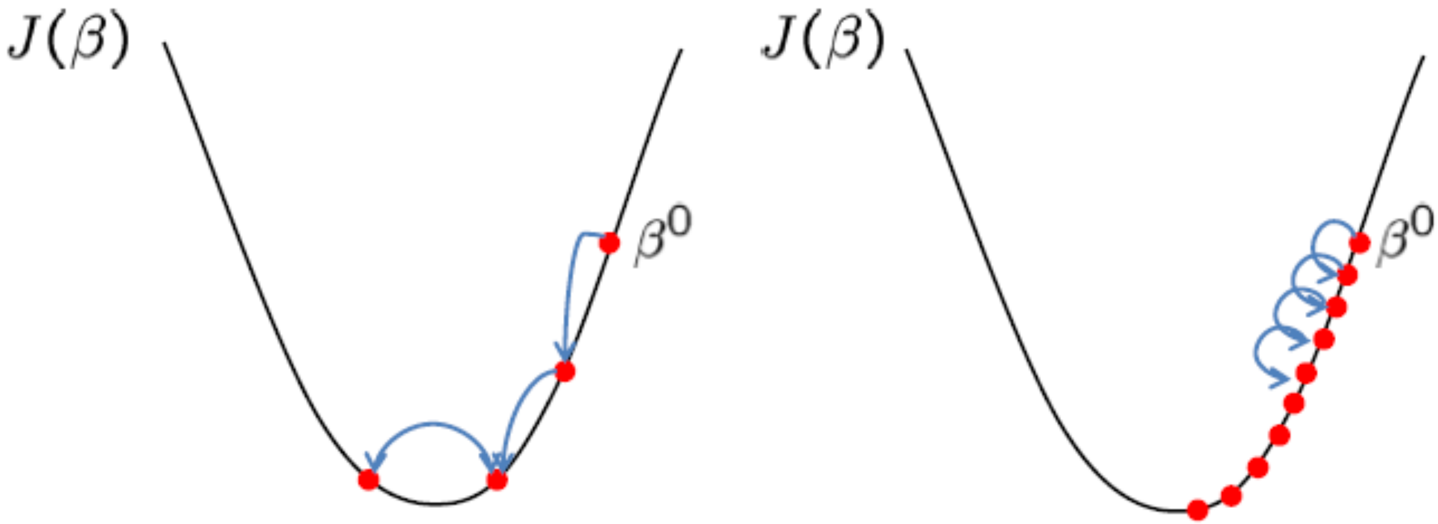
Initialize: β^0

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



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

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

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

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

$$P(Y_i|X_i) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{(Y_i - X_i\beta)^2}{-2\sigma^2}}$$

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

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

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

An early demonstration of the strength of **Gauss**'s method came when it was used to predict the future location of the newly discovered **asteroid Ceres**. On January 1, 1801, the Italian astronomer **Giuseppe Piazzi** discovered Ceres and was able to track its path for 40 days before it was lost in the glare of the sun. Based on this data, astronomers desired to **determine the location of Ceres** after it emerged from behind the sun without solving the complicated Kepler's nonlinear equations of planetary motion. The only predictions that successfully allowed Hungarian astronomer **Franz Xaver von Zach** to relocate Ceres were those performed by the **24-year-old Gauss** using **least-squares analysis**.

Source: Wikipedia

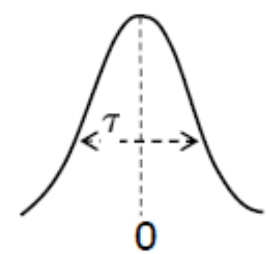
Regularized Least Squares and MAP

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

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



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

Ridge Regression

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

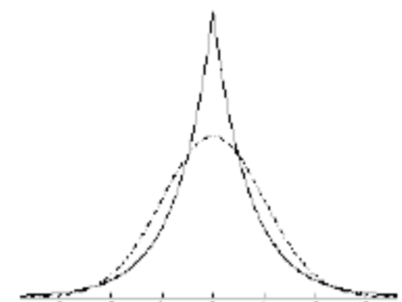
Regularized Least Squares and MAP

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

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



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

Lasso

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

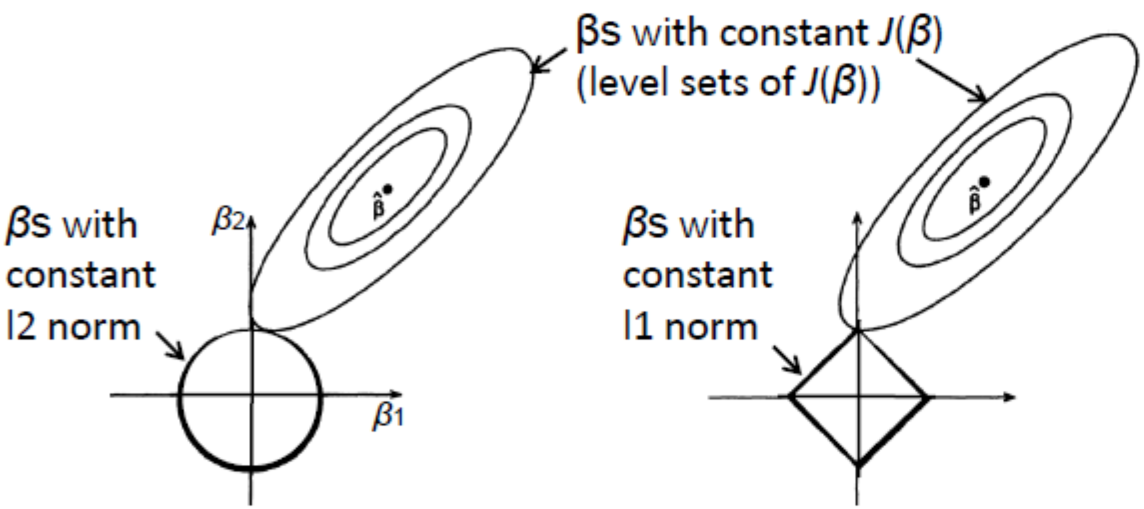
Ridge Regression vs Lasso

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

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

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

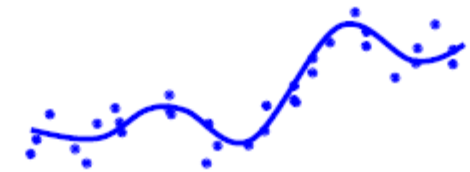
HOT!



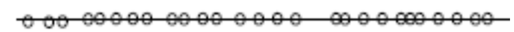
Lasso (l1 penalty) results in sparse solutions – vector with more zero coordinates
Good for high-dimensional problems – don't have to store all coordinates!

Beyond Linear Regression

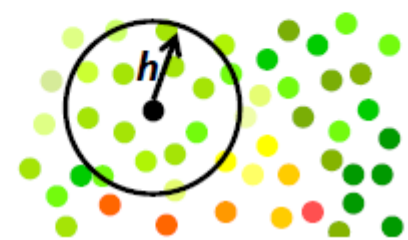
Polynomial regression



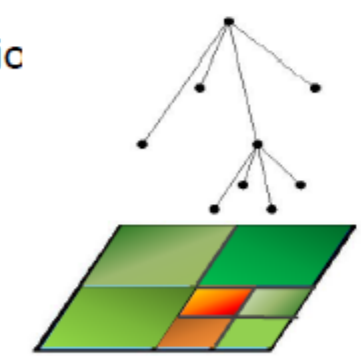
Regression with nonlinear features/basis functions



Kernel regression - Local/Weighted regression



Regression trees – Spatially adaptive regressic



Polynomial Regression

Univariate (1-d) case: $f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_m X^m = \mathbf{X}\beta$

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

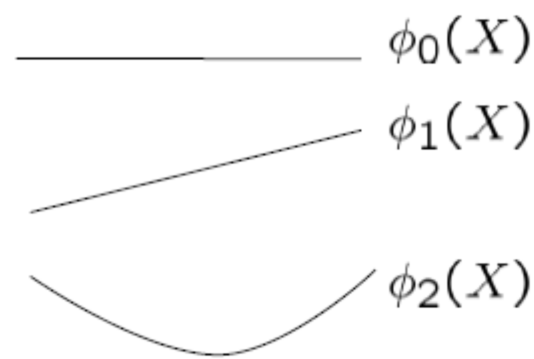
$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y}$$

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

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

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

Weight of each feature



A Regression Example

Average height and weight of American women aged 30 - 39

Height/ m	1.47	1.5	1.52	1.55	1.57	1.60	1.63	1.65	1.68	1.7	1.73	1.75	1.78	1.8	1.83
Weight/kg	52.21	53.12	54.48	55.84	57.2	58.57	59.93	61.29	63.11	64.47	66.28	68.1	69.92	72.19	74.46

Weight is not linear with height, so add a quadratic term into regression

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

$$\hat{f}(X) = X\hat{\beta}$$

$$A = \begin{bmatrix} 1 & 1.47 & 2.16 \\ 1 & 1.50 & 2.25 \\ 1 & 1.52 & 2.31 \\ 1 & 1.55 & 2.40 \\ 1 & 1.57 & 2.46 \\ 1 & 1.60 & 2.56 \\ 1 & 1.63 & 2.66 \\ 1 & 1.65 & 2.72 \\ 1 & 1.68 & 2.82 \\ 1 & 1.70 & 2.89 \\ 1 & 1.73 & 2.99 \\ 1 & 1.75 & 3.06 \\ 1 & 1.78 & 3.17 \\ 1 & 1.81 & 3.24 \\ 1 & 1.83 & 3.35 \end{bmatrix} \qquad Y = \begin{matrix} 52.21 \\ 53.12 \\ 54.48 \\ 55.84 \\ 57.2 \\ 58.57 \\ 59.93 \\ 61.29 \\ 63.11 \\ 64.47 \\ 66.28 \\ 68.1 \\ 69.92 \\ 72.19 \\ 74.46 \end{matrix}$$

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

$$\hat{\beta}_0 = ?$$

$$\hat{\beta}_1 = ?$$

$$\hat{\beta}_2 = ?$$

Source: Wikipedia

Assignment 3 – Programming 1

- Write programs in Matlab, R, C/C++, Java, Perl, or Python to implement the analytical (e.g. matrix-based) **or** iterative (e.g. gradient descent) linear regression algorithm and test it on the problem in the previous slide. Don't directly call linear regression functions in any software
- Turn in the programs and execution results

Assignment 3 – Programming 2
Due Sept. 28, 2015

Iris

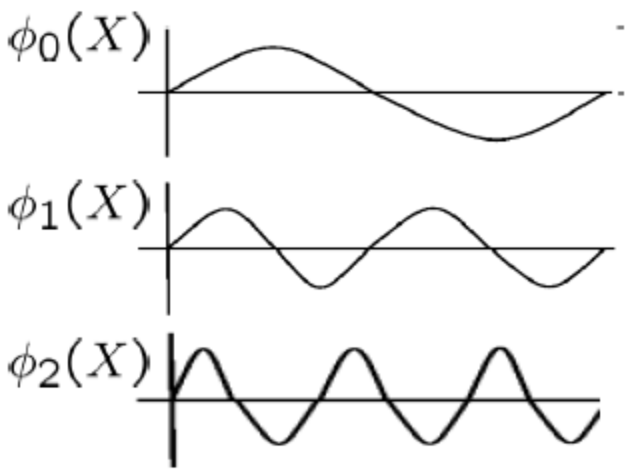
Wikipedia

- Write a program to implement the iterative (e.g. gradient ascent / descent) logistic regression algorithm for binary classification and apply it to the Iris classification data set
- Iris data set: http://archive.ics.uci.edu/ml/datasets/Iris
- Only select data points of two highlighted classes (**Iris Setosa, Iris Versicolour**, Iris Virginica)
- Submit programs and execution results

Nonlinear Regression

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

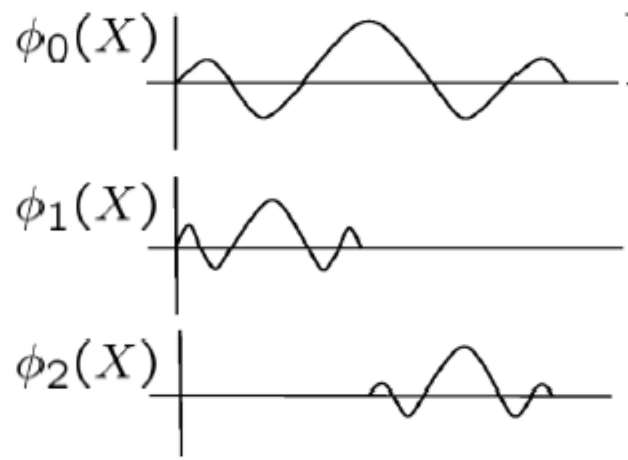
Fourier Basis



Good representation for oscillatory functions

$$\frac{1}{\sqrt{2\pi a^2}} \cdot \operatorname{sinc}\left(\frac{\omega}{2\pi a}\right)$$

Wavelet Basis



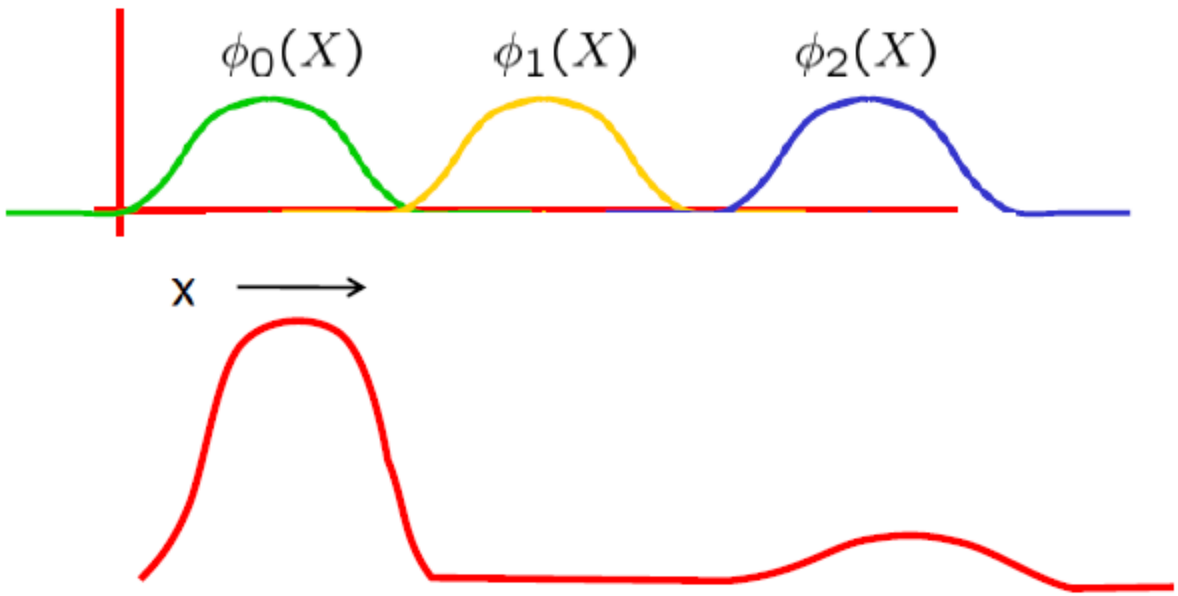
Good representation for functions localized at multiple scales

$$\psi(t) = 2\operatorname{sinc}(2t) - \operatorname{sinc}(t) = \frac{\sin(2\pi t) - \sin(\pi t)}{\pi t}$$

Local Regression

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

Basis coefficients

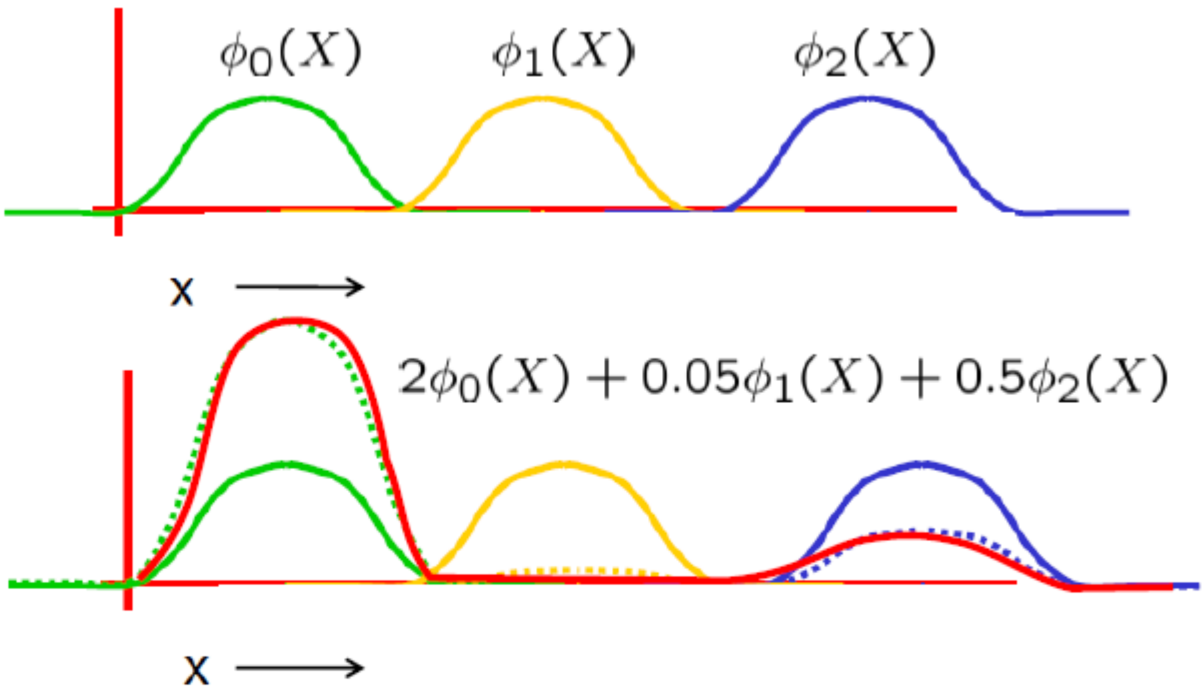


Globally supported basis functions (polynomial, fourier) will not yield a good representation

Local Regression

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

Basis coefficients



Globally supported basis functions (polynomial, fourier) will not yield a good representation

What you should know

Linear Regression

- Least Squares Estimator
- Normal Equations
- Gradient Descent

Regularized Linear Regression (connection to MAP)

- Ridge Regression, Lasso

Polynomial Regression, Basis (Fourier, Wavelet) Estimators

Next time

- Kernel Regression (Localized)
- Regression Trees