CPSC 340: Machine Learning and Data Mining

Non-Linear Regression

Admin

- Assignment 1 grades are out.
- Assignment 2 is due Sunday.
  - Extra office hours added on Saturday 12-2pm (see office hours calendar)
- Assignment 3 will be out by early next week.
  - Will be due before the break
- Midterm is after the break (March 1 in class)
- Tutorial next week: practice problems for hw3

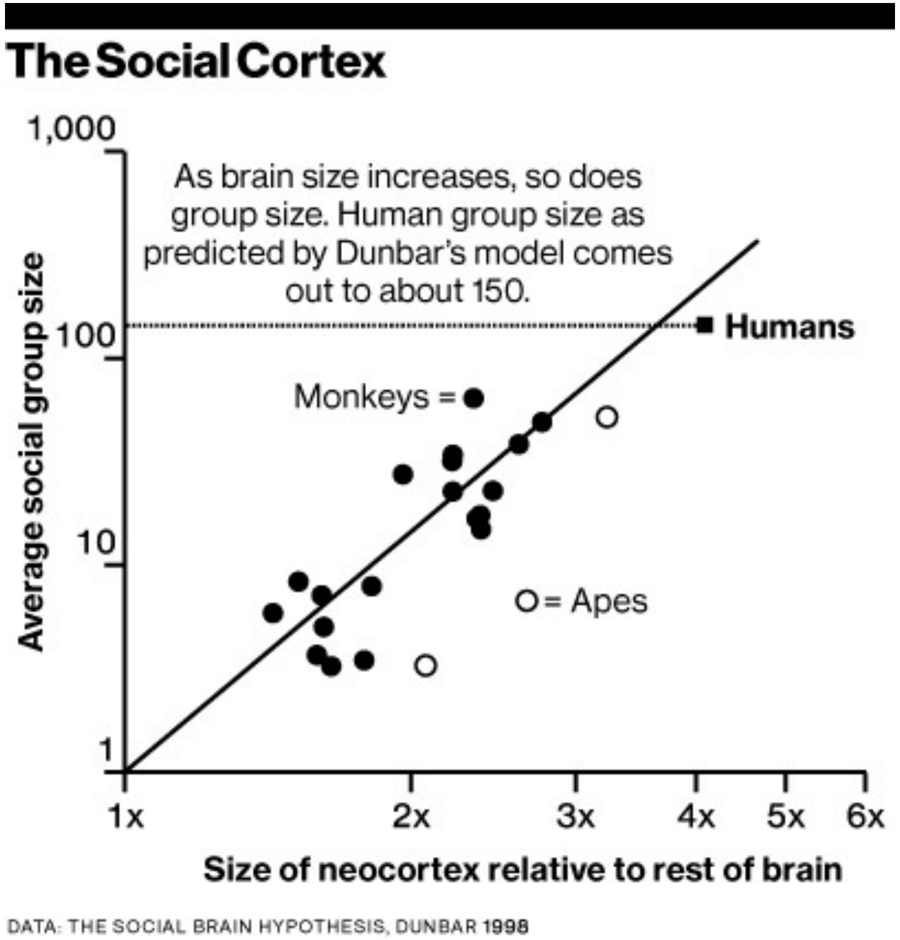
Last Time: Linear Regression

- We discussed linear models:

$$y_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$$
$$= \sum_{j=1}^{d} w_j x_{ij} = w^T x_i$$

- "Multiply feature x_{ij} by weight w_j, add them to get y_i".
- We discussed squared error function:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n} (\underbrace{w^T x_i}_{\text{Predicted value}} - \underbrace{y_i}_{\text{True value}})^2$$



To predict on test case $\hat{x}_i$ use $\hat{y}_i = w^T \hat{x}_i$

http://www.bloomberg.com/news/articles/2013-01-10/the-dunbar-number-from-the-guru-of-social-networks

Last Time: Supervised Learning Notation

- We're treating 'w', 'y', and each x_i as column-vectors:

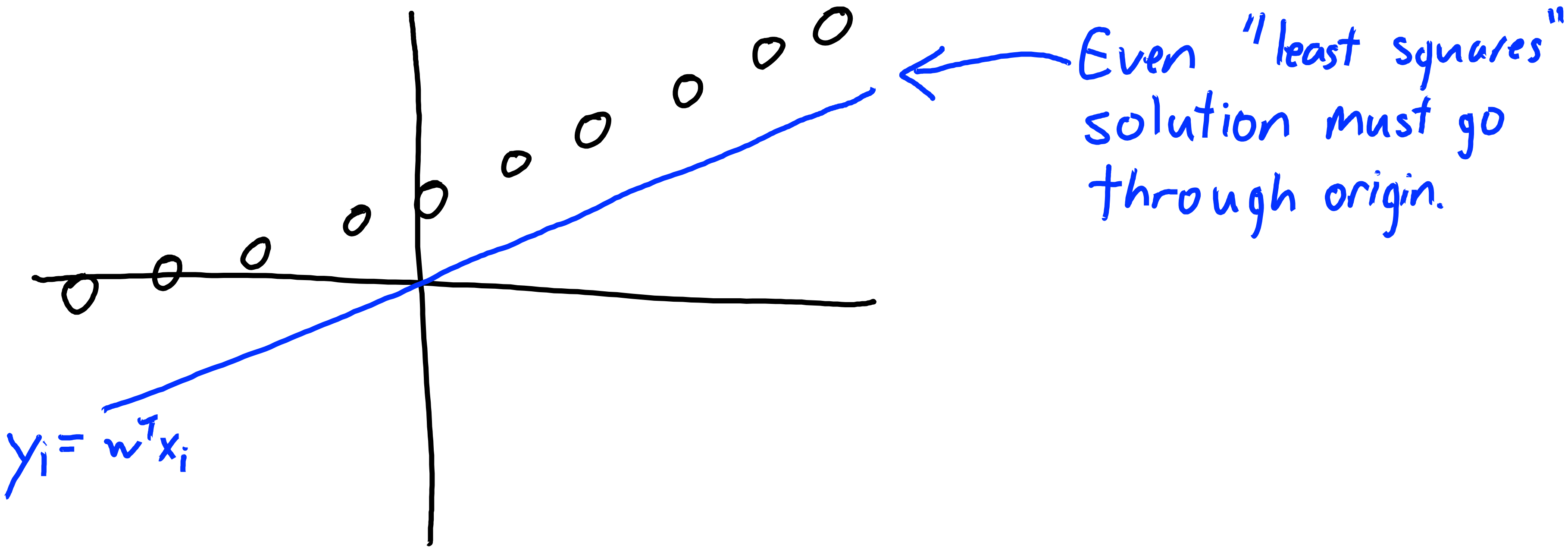
$$w = \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}}_{d \times 1} \qquad y = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{n \times 1} \qquad x_i = \underbrace{\begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix}}_{d \times 1}$$

- So feature matrix 'X' actually has x_i transposed as rows:

$$X = \begin{bmatrix} \text{---} & x_1^T & \text{---} \\ \text{---} & x_2^T & \text{---} \\ & \vdots & \\ \text{---} & x_n^T & \text{---} \end{bmatrix}$$

Why don't we have a y-intercept?

- Last time: Linear models with no y-intercept.
  - Linear model is $y_i = w^T x_i$ instead of $y_i = w^T x_i + w_0$ with y-intercept w_0.
  - So if $x_i = 0$ then we must predict $y_i = 0$.



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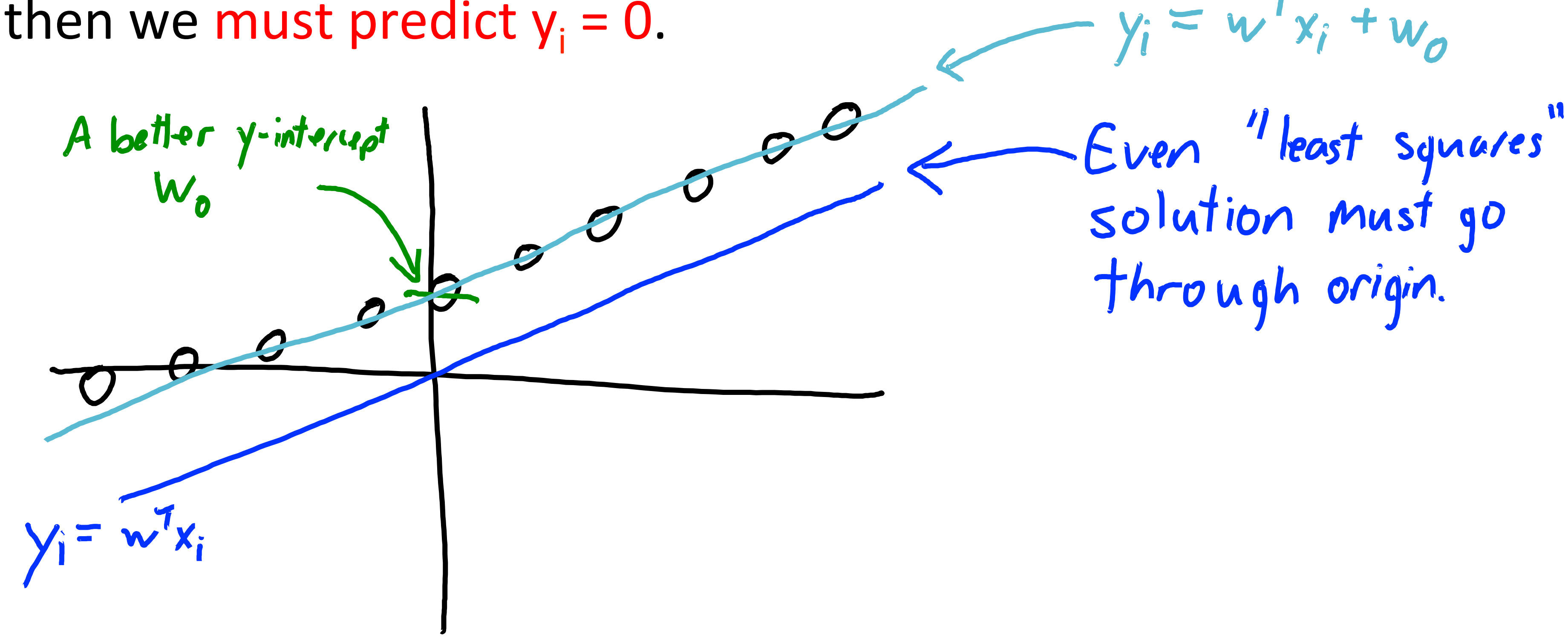
Adding y-intercept fixes this.



Adding a Bias Variable

- Simple trick to add a y-intercept ("bias") variable:
  - Make a new matrix "Z" with an extra feature that is always "1".

$$X = \begin{bmatrix} 0.1 & 0.3 \\ 0.5 & -0.6 \\ 0.2 & 0.4 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0.1 & 0.3 \\ 1 & 0.5 & -0.6 \\ 1 & 0.2 & 0.4 \end{bmatrix}$$

$$Z = \begin{bmatrix} 1 & \underbrace{\begin{matrix} 0.1 & 0.3 \\ 0.5 & -0.6 \\ 0.2 & 0.4 \end{matrix}}_{X} \end{bmatrix}$$

- Now use "Z" as features to get a model with a non-zero y-intercept:

$$y_i = w_0 \underbrace{z_{i0}}_{\text{"1"}} + w_1 \underbrace{z_{i1}}_{x_{i1}} + w_2 \underbrace{z_{i2}}_{x_{i2}}$$

$$= w_0 + w_1 x_{i1} + w_2 x_{i2}$$

- So we can have a non-zero y-intercept by changing features.

Linear Least Squares

Prediction:

$$\underbrace{y = X * w}_{\text{Why?}}$$

$$y_i = w^T x_i \quad \text{so} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} w^T x_1 \\ w^T x_2 \\ \vdots \\ w^T x_n \end{bmatrix} = \begin{bmatrix} x_1^T w \\ x_2^T w \\ \vdots \\ x_n^T w \end{bmatrix} = \underbrace{\begin{bmatrix} — x_1^T — \\ — x_2^T — \\ \vdots \\ — x_n^T — \end{bmatrix}}_{X} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix} = Xw$$

Linear Least Squares

- We can rewrite the objective function as a norm

Want 'w' that minimizes

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(\underbrace{w^T x_i - y_i}_{r_i})^2 = \frac{1}{2}\sum_{i=1}^{n} r_i^2 = \frac{1}{2} r^T r = \frac{1}{2}\|r\|_2^2 = \boxed{\frac{1}{2}\|Xw - y\|^2}$$

Define "residual" r_i as signed error on example 'i':

$$r_i = w^T x_i - y_i$$

$$r = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{bmatrix} = \begin{bmatrix} w^T x_1 - y_1 \\ w^T x_2 - y_2 \\ \vdots \\ w^T x_n - y_n \end{bmatrix} = \underbrace{\begin{bmatrix} w^T x_1 \\ w^T x_2 \\ \vdots \\ w^T x_n \end{bmatrix}}_{Xw} - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = Xw - y$$

Linear Least Squares

Want 'w' that minimizes

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \underbrace{\boxed{\frac{1}{2}\|Xw - y\|^2}}_{\text{Let's expand then compute gradient.}} = \frac{1}{2}(Xw-y)^T(Xw-y)$$

$$= \frac{1}{2}((Xw)^T - y^T)(Xw-y)$$

$$= \frac{1}{2}(w^T X^T - y^T)(Xw - y)$$

$$= \frac{1}{2}(w^T X^T(Xw-y) - y^T(Xw-y))$$

$$= \frac{1}{2}(w^T X^T X w - w^T X^T y - y^T X w + y^T y)$$

$$= \frac{1}{2}w^T X^T X w - w^T X^T y + \frac{1}{2}y^T y$$

A good way to check your step: make sure that dimensions all make sense.

Linear Least Squares

See notes on linear and quadratic derivatives for details.

Training: `w = solve(X.T @ X, X.T @ y)`

Why?

Want 'w' that minimizes

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \frac{1}{2}\|Xw - y\|_2^2 = \underbrace{\frac{1}{2}w^TX^TXw - w^TX^Ty + \frac{1}{2}y^Ty}_{\text{What are the gradients of these terms?}}$$

} a quadratic function (in matrix notation)

$$\nabla f(w) = X^TXw - X^Ty + 0$$

So at a minimizer where $\nabla f(w) = 0$ we have: $\boxed{\underbrace{X^TX}_{\text{Some matrix}}w = \underbrace{X^Ty}_{\text{Some vector}}}$ "normal equations"

This is a linear system $Aw = b$ for some matrix 'A' and vector 'b'

Cheat sheet:

$$\nabla_w[c] = 0$$

$$\nabla_w[w^Tb] = b$$

This is like saying $\frac{d}{dw}[\alpha w] = \alpha$

$$\nabla_w\left[\frac{1}{2}w^TAw\right] = Aw \text{ for symmetric } A.$$

The Punch Line

$$\min_w \frac{1}{2}||Xw - y||_2^2$$

```
w = solve(X.T @ X,  x.T @ y)
```

Note that
$f(w)$ is a "convex" function
so solving $\nabla f(w) = 0$ gives minimizer

Incorrect Solutions to Least Squares Problem

The least squares objective is $f(w) = \frac{1}{2}\|Xw - y\|^2$

The minimizers of this objective are solutions to the linear system:

$$X^T X w = X^T y$$

The following are not the solutions to the least squares problem:

$w = (X^T X)^{-1}(X^T y)$ (only true if $X^T X$ is invertible)

$w X^T X = X^T y$ (matrix multiplication is not commutative, dimensions don't even match)

$w = \frac{X^T y}{X^T X}$ (you cannot divide by a matrix)

Least Squares Issues

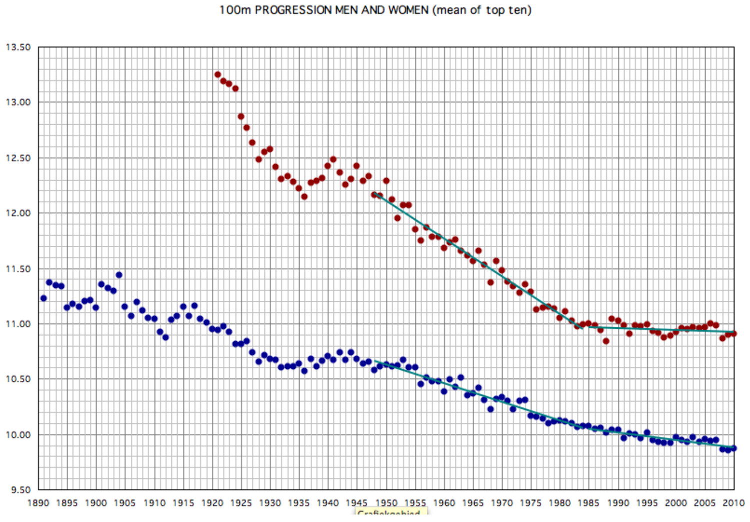
- Issues with least squares model:
  - Solution might not be unique.
  - It is sensitive to outliers.
  - It always uses all features.
  - Data can might so big we can't store X^TX.
  - It might predict outside range of y_i values.
  - It assumes a linear relationship between x_i and y_i.

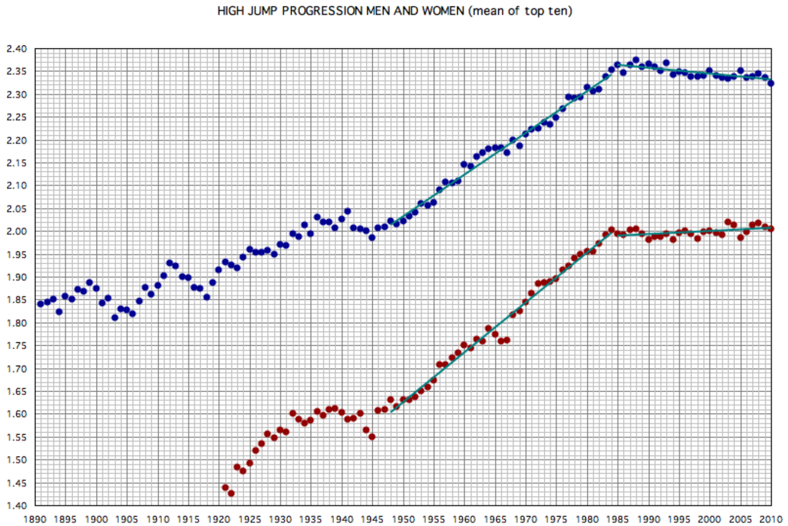
X is $n \times d$
so X^T is $d \times n$
and X^TX is $d \times d$.

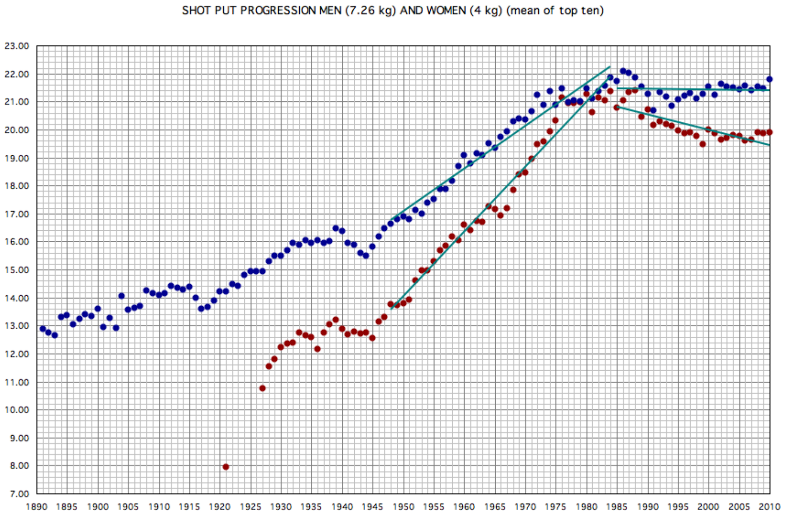
Costs $O(nd^2)$ to calculate:
- Each of the $O(d^2)$ elements is an inner product between length 'n' vectors.

Example: Non-Linear Progressions in Athletics

- Are top athletes going faster, higher, and farther?







http://www.at-a-lanta.nl/weia/Progressie.html
https://en.wikipedia.org/wiki/Usain_Bolt
http://www.britannica.com/biography/Florence-Griffith-Joyner

Adapting Counting/Distance-Based Methods

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Adapting Counting/Distance-Based Methods

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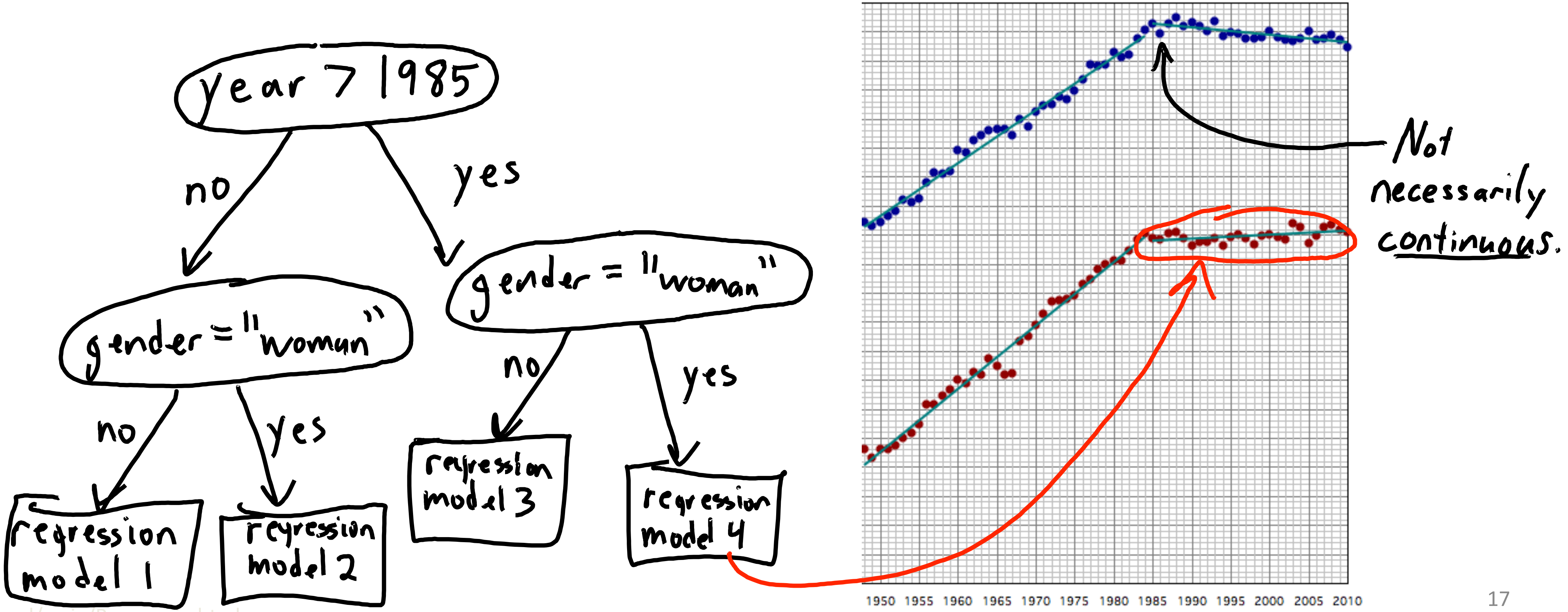
  - Regression tree: tree with mean value or linear regression at leaves.



http://www.at-a-lanta.nl/weia/Progressie.html

Adapting Counting/Distance-Based Methods

- We can adapt our classification methods to perform regression:
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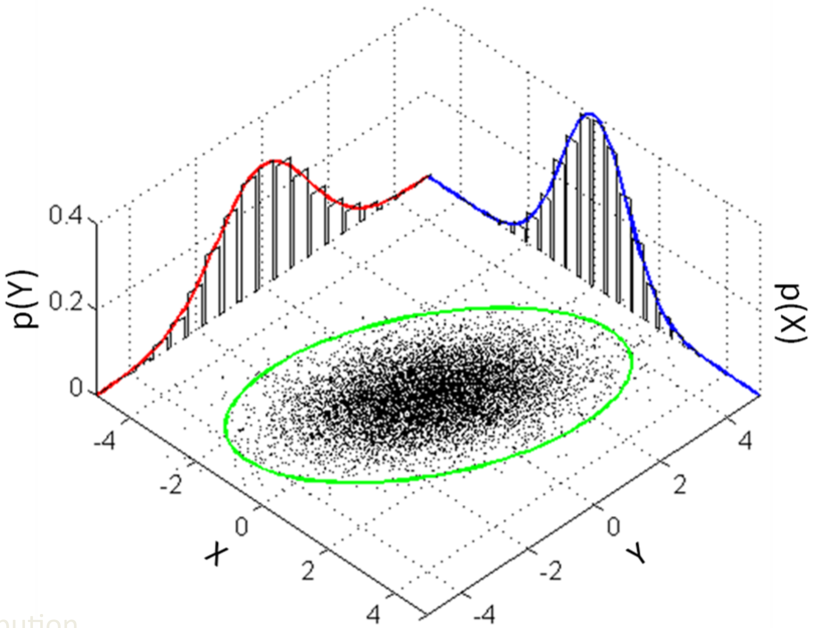
  - Generative models: fit $p(x_i \mid y_i)$ and $p(y_i)$ with Gaussian or other model.



https://en.wikipedia.org/wiki/Multivariate_normal_distribution

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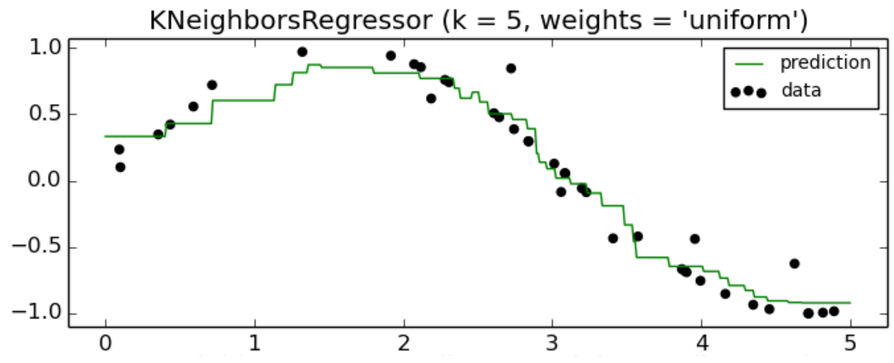

http://scikit-learn.org/stable/modules/neighbors.html

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  - Non-parametric models:
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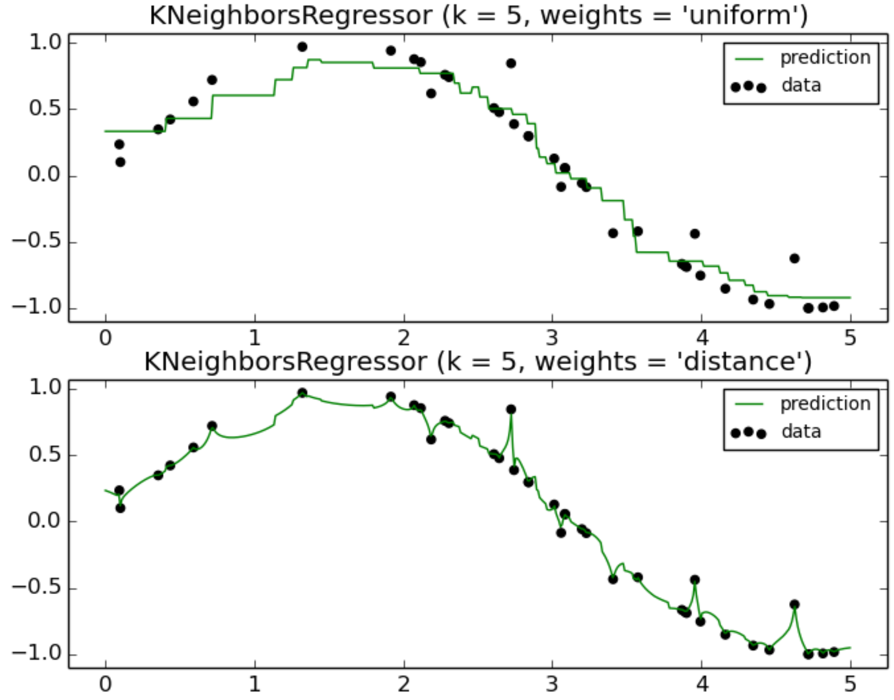
    - Could be weighted by distance.
      - Close points 'j' get more "weight" w_{ij}.



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  - Non-parametric models:
    - Mean y_i among k-nearest neighbours.
    - Could be weighted by distance.
  - Ensemble methods:
    - Can improve performance by averaging across regression models.

http://www.itl.nist.gov/div898/handbook/pmd/section4/pmd423.htm

Linear Least Squares for Quadratic Models

- Can we use linear least squares to fit a quadratic model?

$$y_i = w_0 + w_1 x_i + w_2 x_i^2$$

- You can do this by changing the features (change of basis):

$$X = \begin{bmatrix} 0.2 \\ -0.5 \\ 1 \\ 4 \end{bmatrix} \qquad Z = \begin{array}{ccc} & & \\ \left[\begin{matrix} 1 & 0.2 & (0.2)^2 \\ 1 & -0.5 & (-0.5)^2 \\ 1 & 1 & (1)^2 \\ 1 & 4 & (4)^2 \end{matrix}\right] \\ \text{y-int} \quad\;\; x \quad\;\; x^2 \end{array}$$

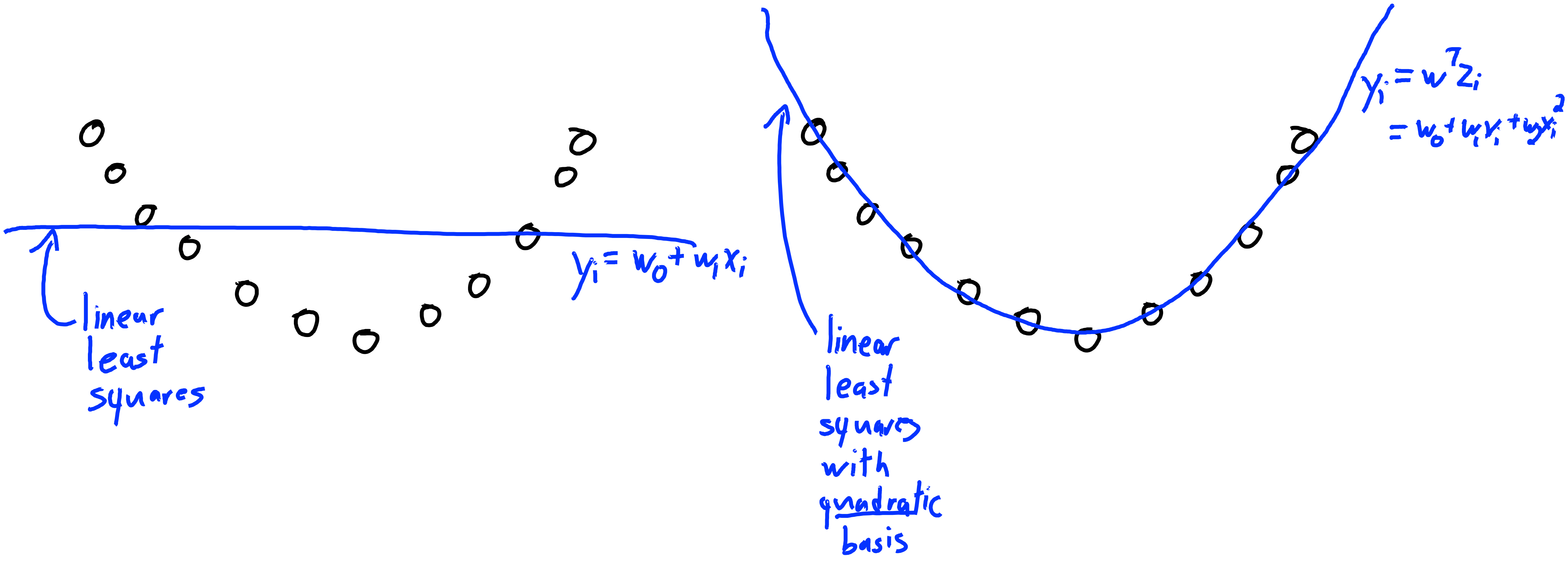
$$\begin{aligned} y_i &= w^T z_i \\ &= w_0 z_{i0} + w_1 z_{i1} + w_2 z_{i2} \\ &= w_0 + w_1 x_i + w_2 x_i^2 \end{aligned}$$

"solve linear system"

- Fitting with least squares: $w = (Z^T Z) \backslash (Z^T y)$
- It's a linear function of w, but a quadratic function of x_i.

To predict on new data $\hat{X}$, form $\hat{Z}$ from $\hat{X}$ and take $y = \hat{Z}w$

Linear Least Squares for Quadratic Models



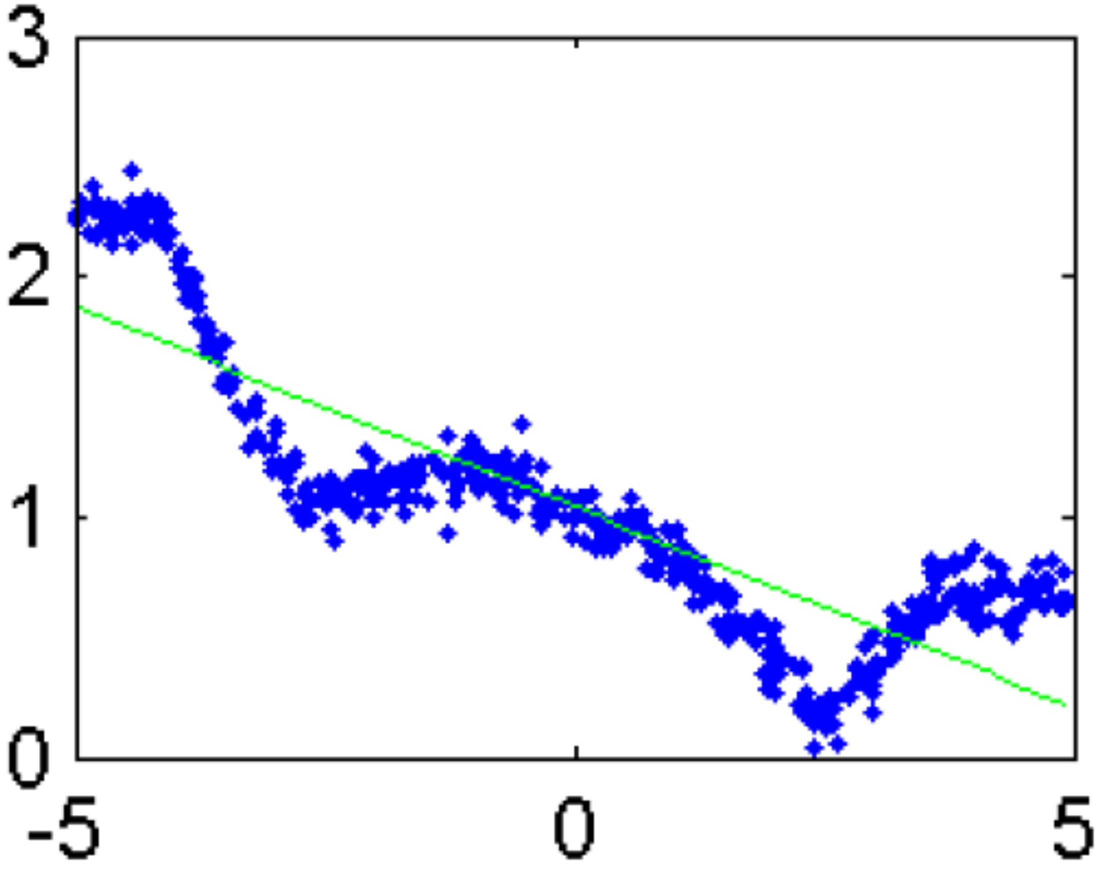
General Polynomial Basis

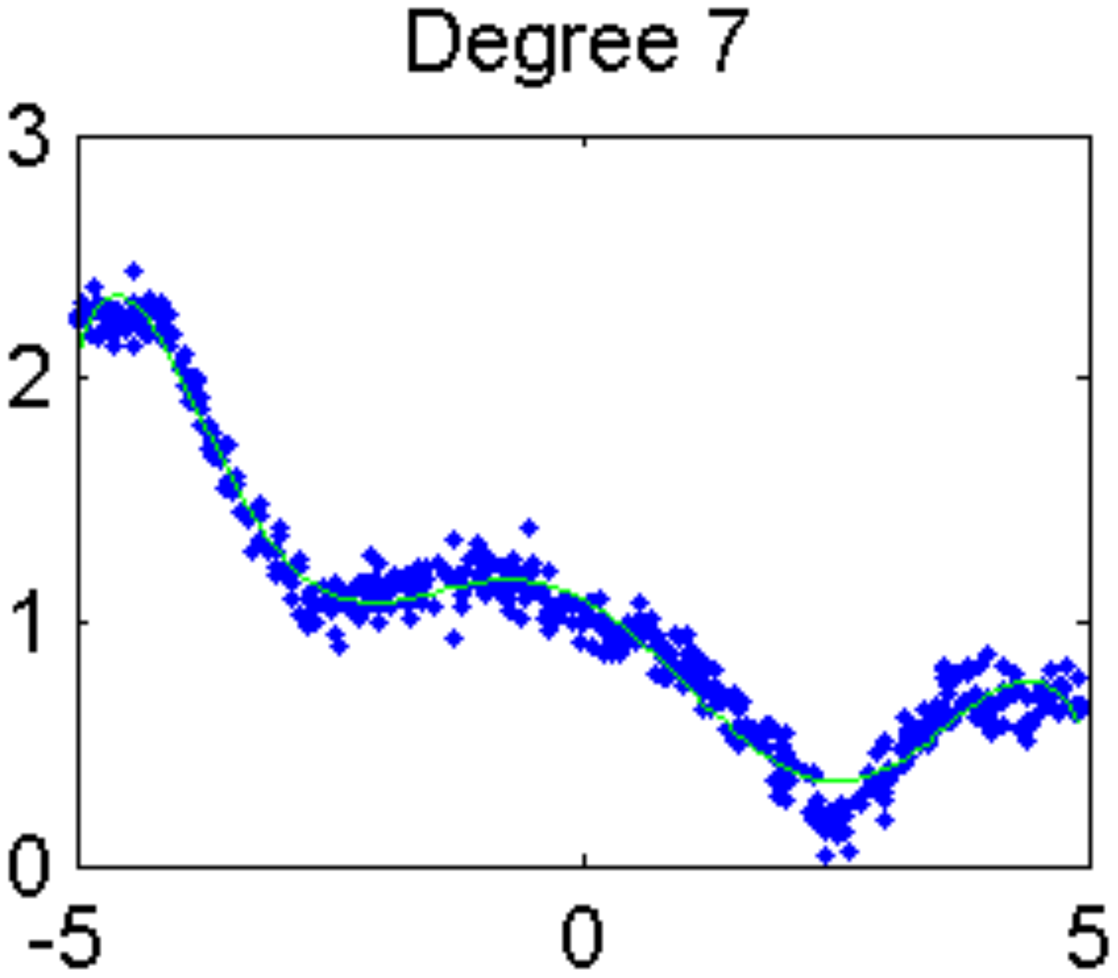
- We can have a polynomial of degree 'p' by using a basis:

$$Z = \begin{bmatrix} 1 & x_1 & (x_1)^2 & \cdots & (x_1)^p \\ 1 & x_2 & (x_2)^2 & \cdots & (x_2)^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & (x_n)^2 & \cdots & (x_n)^p \end{bmatrix}$$

- There are polynomial basis functions that are numerically nicer:
  - E.g., Lagrange polynomials (see CPSC 303)

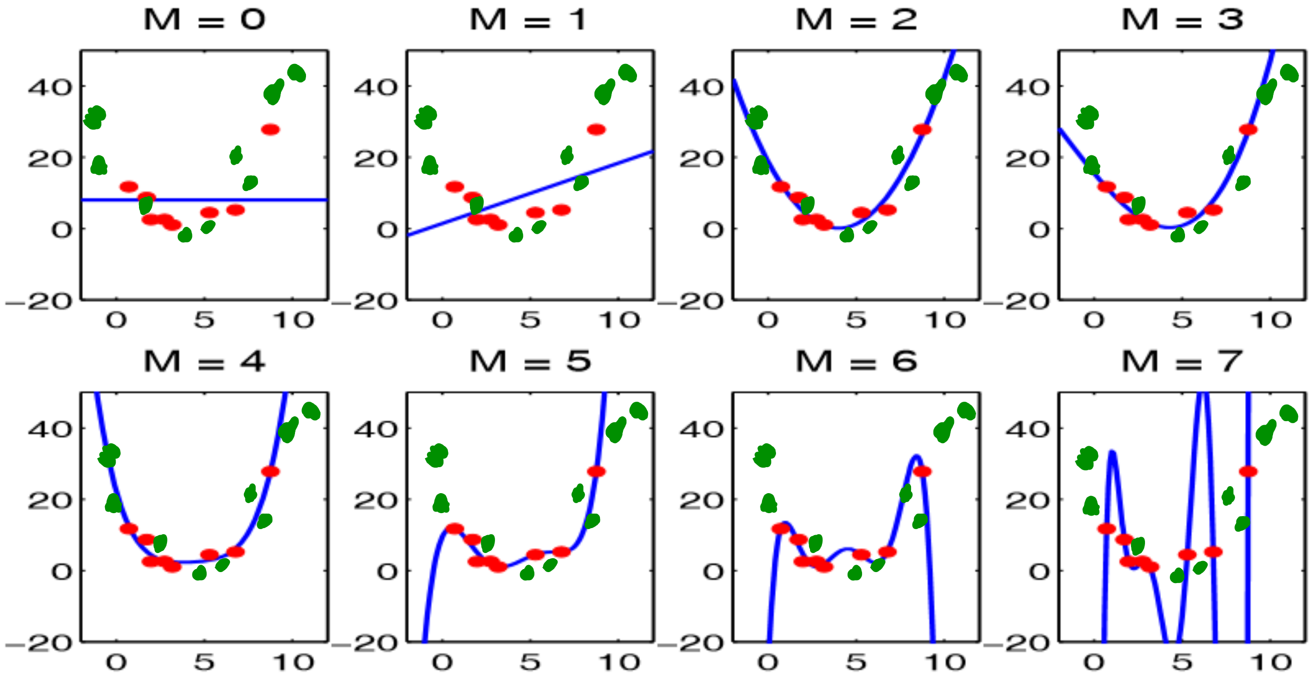
General Polynomial Basis





Degree of Polynomial and Fundamental Trade-Off

- As the polynomial degree increases, the training error goes down.



- But training error becomes worse approximation test error.
- Usual approach to selecting degree: validation or cross-validation.

http://www.cs.ubc.ca/~arnaud/stat535/slides5_revised.pdf

Summary

- Y-intercept can be modeled by using a column of 1s.
- Linear least squares solution is given by normal equations:
  - Solve $(X^TX)w = X^Ty$.
- Tree/generative/non-parametric/ensemble methods for regression.
- Change of basis allows linear models to model non-linear data

- Next time:
  - A general method for avoiding overfitting.