CSE 255 – Lecture 2

Data Mining and Predictive Analytics

Supervised learning – Regression

Supervised versus unsupervised learning

Learning approaches attempt to **model data** in order to solve a problem

Unsupervised learning approaches find patterns/relationships/structure in data, but **are not** optimized to solve a particular predictive task

Supervised learning aims to directly model the relationship between input and output variables, so that the output variables can be predicted accurately given the input

Regression

Regression is one of the simplest supervised learning approaches to learn relationships between input variables (features) and output variables (predictions)

Linear regression

Linear regression assumes a predictor of the form

$x_i \cdot \theta = y_i$

$$X\theta = y$$

matrix of features (data)

unknowns (which features are relevant)

vector of outputs (labels)

(or $Ax = b$ if you prefer)

Linear regression

Linear regression assumes a predictor of the form

$$X\theta = y$$

Q: Solve for theta

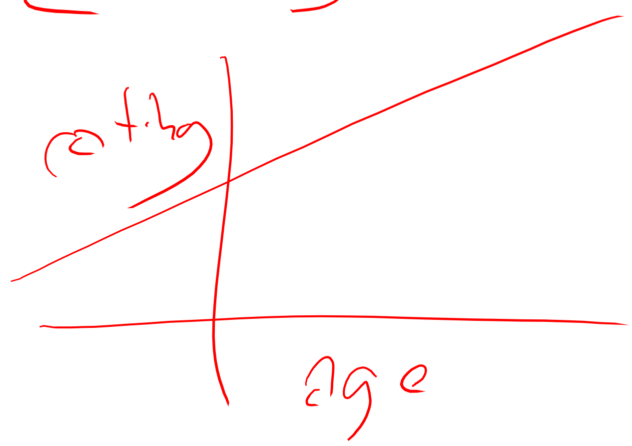
A: $\theta = (X^T X)^{-1} X^T y$

Example 1

How do preferences toward certain beers vary with age?

$$\text{rating} = \theta_0 + \theta_1 \, \text{age}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} 1 & \text{age}_1 \\ 1 & \text{age}_2 \\ \vdots & \vdots \\ 1 & \text{age}_N \end{bmatrix} \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix}$$



Example 1

Beeradvocate

Beers:

Displayed for educational use only; do not reuse.

BA SCORE	THE BROS	
100	95	Ratings: 9,587
world-class	world-class	Reviews: 2,537
		rAvg: 4.59
		pDev: 9.59%
		Wants: 2,109
9,587 Ratings	(view ratings)	Gots: 4,563 | FT: 472

Brewed by:
Goose Island Beer Co.
Illinois, United States

Style | ABV
American Double / Imperial Stout | 13.80% ABV

Availability: Winter

Notes/Commercial Description:
60 IBU

(Beer added by: drewbage on 06-26-2003)

Ratings/reviews:

4.35/5 rDev -5.2%
look: 4 | smell: 4.25 | taste: 4.5 | feel: 4.25 | overall: 4.25

Serving: 355 mL bottle poured into a 9 oz Libbey Embassy snifter ("bottled on: 08AUG14 1109").

Appearance: Deep, dark near-black brown. Hazy, light brown fringe of foam and limited lacing; no head.

Smell: Roasted malt, vanilla, and some warming alcohol.

Taste: Roasted malts, cocoa, burnt caramel, molasses, vanilla and dark fruit. Bourbon barrel is hinted at but never takes over.

Mouthfeel: Medium to full body and light carbonation with a very lush, silky smooth feel.

Overall: Not as complex or intense as some newer barrel-aged stouts, but so smooth and balanced with all the elements tightly integrated.

HipCzech, Yesterday at 05:38 AM

User profiles:

HipCzech
Aficionado
Male, from Texas
Profile Page

Member Since:	Jul 12, 2014	HipCzech was last seen:
Points:	175	Today at 12:19 AM
Beers:	108	
Places:	6	
Posts:	0	
Likes Received:	0	
Trading:	0% | 0	

Example 1

50,000 reviews are available on
http://jmcauley.ucsd.edu/cse255/data/beer/beer_50000.json
(see course webpage)

See also – non-alcoholic beers:
http://jmcauley.ucsd.edu/cse255/data/beer/non-alcoholic-beer.json

Example 1

Real-valued features

How do preferences toward certain beers vary with age?
How about **ABV**?

(code for all examples is on http://jmcauley.ucsd.edu/cse255/code/week1.py)

Example 1

Preferences vs **ABV**

$$\theta_0 + \theta_1 \times ABV + \theta_2 \times ABV^2 + \theta_3 \times ABV^3$$

Example 1

Real-valued features

What is the interpretation of:

$$\theta = (3.4, 10e^{-7})$$

3.4 + $10e^{-7}$ × sign.ln seconds

Example 2

Categorical features

How do beer preferences vary as a function of **gender**?

$$r = \theta_0 + \theta_1 \times \text{gender}$$

female = [1] male = [0]

male = θ_0 , female = $\theta_0 + \theta_1$

(code for all examples is on http://jmcauley.ucsd.edu/cse255/code/week1.py)

Linearly dependent features

Male = [0, 1]   female = [1, 0]

male = $\theta_0 + \theta_2$ female = $\theta_0 + \theta_1$

$$X = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \qquad X^T X = \begin{bmatrix} 7 & 4 & 3 \\ 4 & 4 & 0 \\ 3 & 0 & 3 \end{bmatrix} \begin{array}{l} A \\ B \\ A - B \end{array}$$

$$(X^T X)^{-1} X y$$

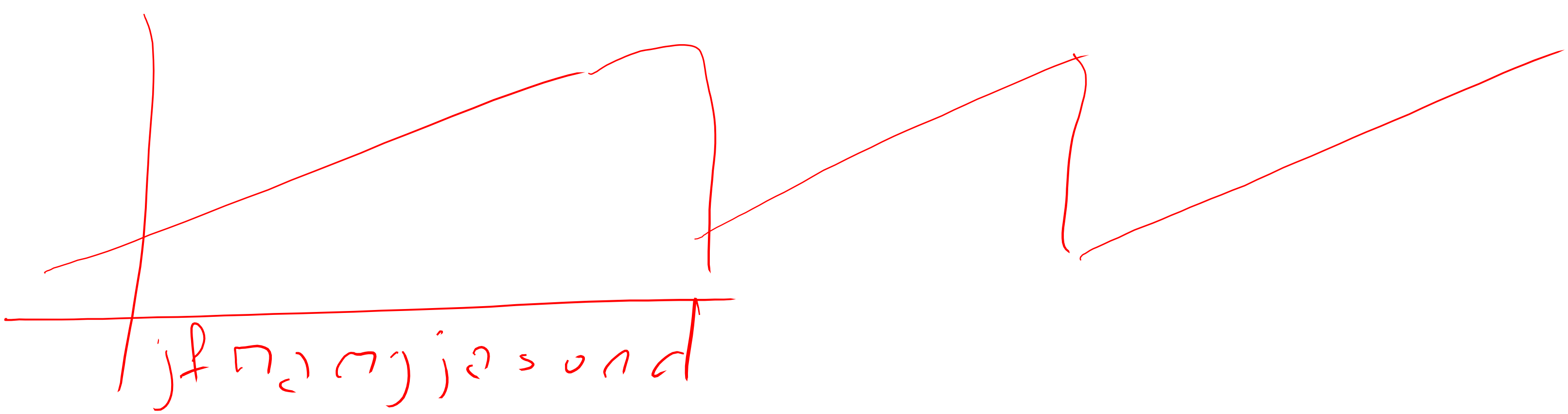
$$r = 2 + 3[m] + 4[f]$$

$$r = 1 + 4[m] + 5[f]$$

Exercise

How would you build a feature to represent the **month**, and the impact it has on people's rating behavior?

jan = [1] feb : [2] . . . .



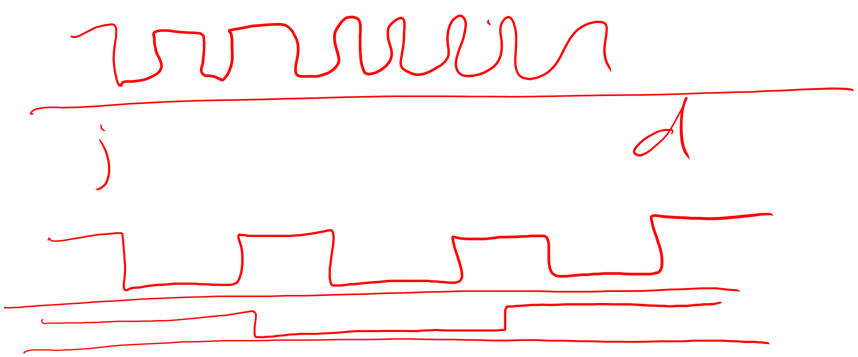
Exercise

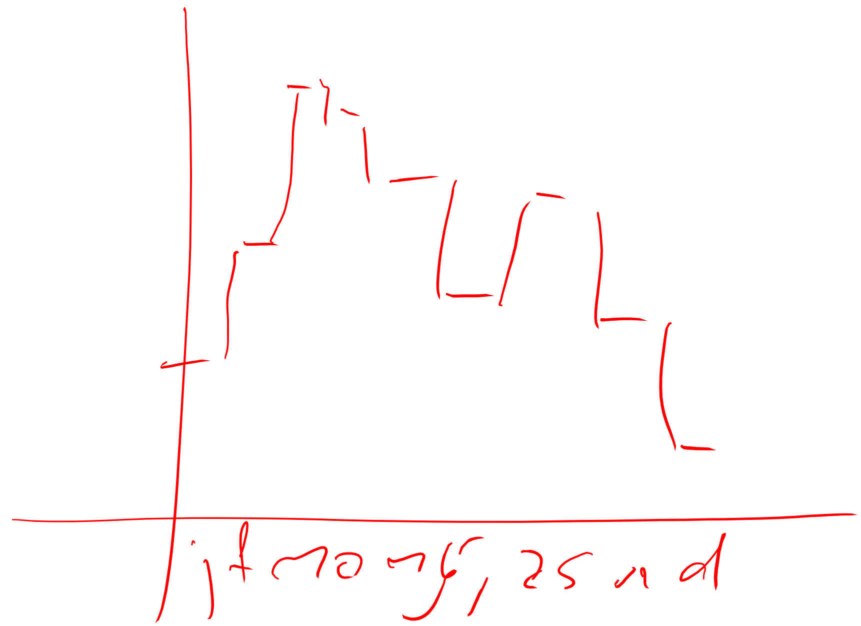
jan [1 0 0 0 0 0 0 0 0 0 0 0]

feb [0 1 0 0 0 . . . .]

jan = [0 0 0 1]

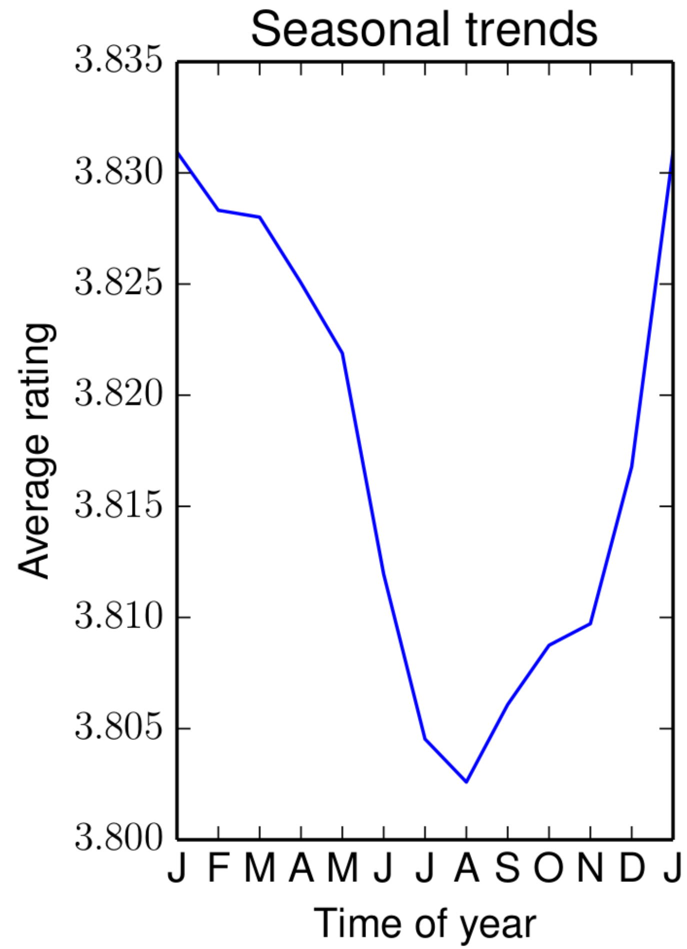
feb = [0 0 1 0]





What does the data actually look like?

Season vs. rating (overall)



Example 3

Random features

What happens as we add more and more **random** features?

(code for all examples is on http://jmcauley.ucsd.edu/cse255/code/week1.py)

CSE 255 – Lecture 2

Data Mining and Predictive Analytics

Regression Diagnostics

Today: Regression diagnostics

Mean-squared error (MSE)

$$\frac{1}{N}\|y - X\theta\|_2^2$$

$$= \frac{1}{N}\sum_{i=1}^{N}(y_i - X_i \cdot \theta)^2$$

$$= \frac{1}{N}\sum_i |y_i - X_i \cdot \theta|$$

Regression diagnostics

Q: Why MSE (and not mean-absolute-error or something else)

Regression diagnostics

$$y_i = x_i \cdot \theta + \mathcal{N}(0, \sigma)$$

$$y_i - x_i \cdot \theta \sim \mathcal{N}(0, \sigma)$$

$$\prod_i \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(y_i - x_i \cdot \theta)^2}{2\sigma^2}}$$

(max)

$$\sum_i (y_i - x_i \cdot \theta)^2$$

(min)

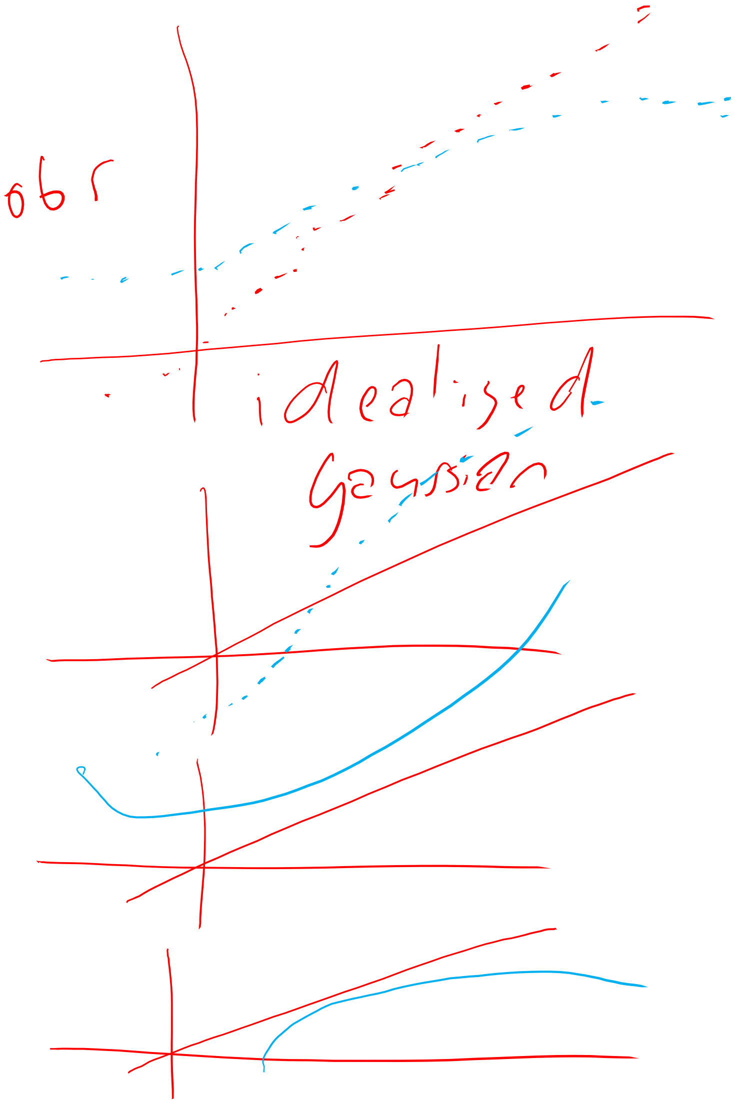
Regression diagnostics

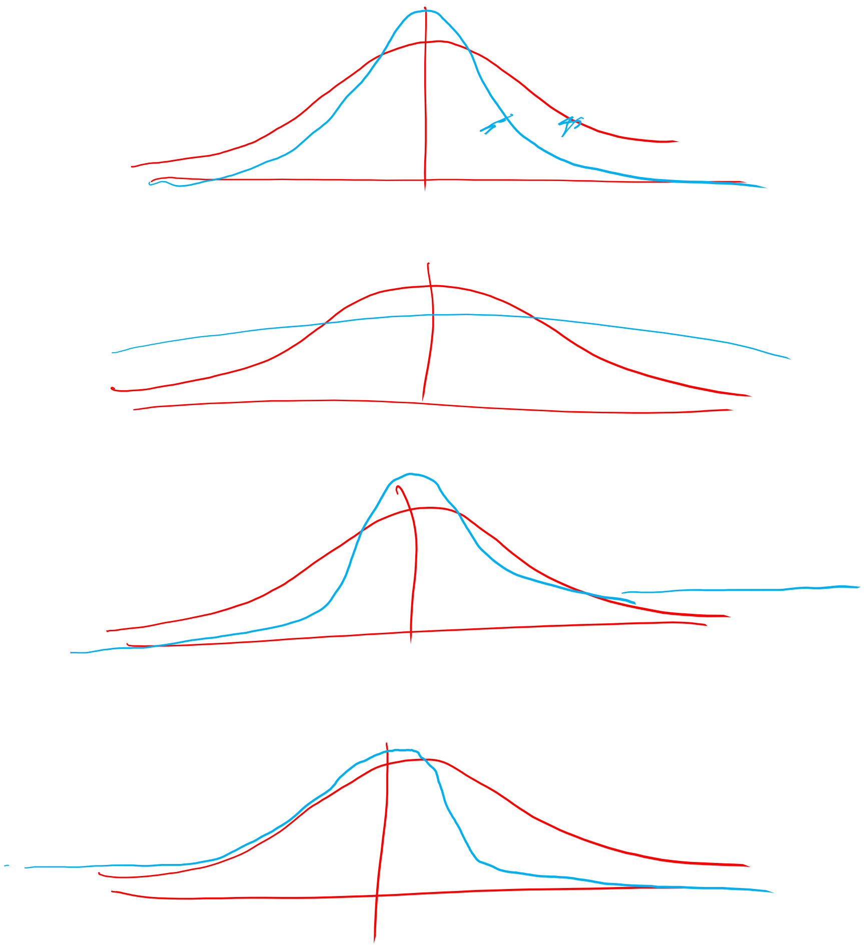
[5.5, -0.5, 3, 1, -2, 4, 0]

[-2, -0.5, 6, 1, 3, 4, 5.5]

[-6, -3, -1, 0, 1, 3, 6]

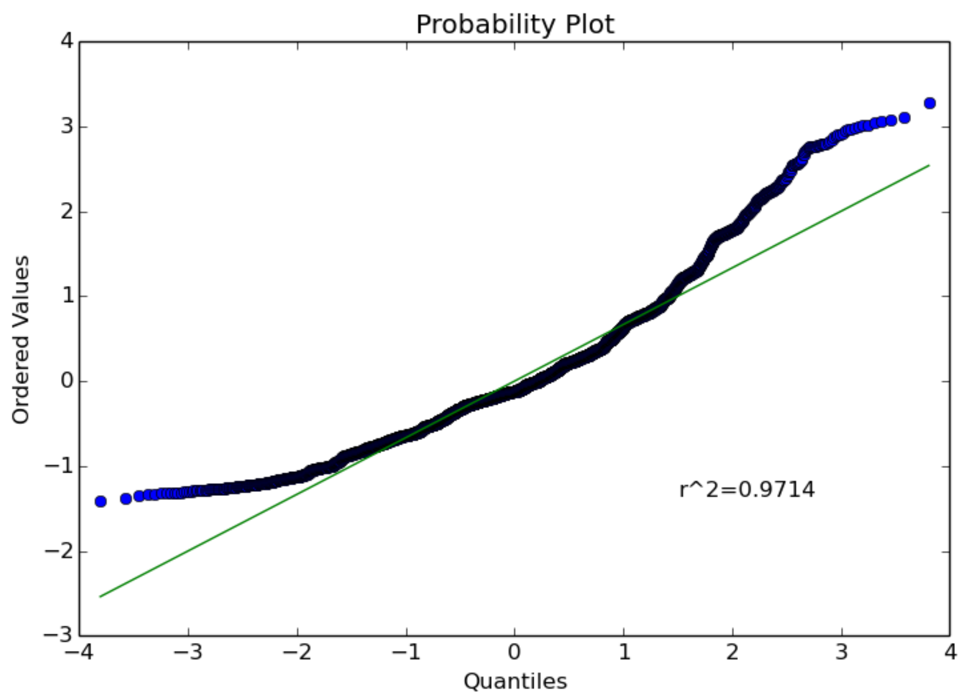
Regression diagnostics





Regression diagnostics

Quantile-Quantile (QQ)-plot



$\theta_0 + \theta_1$ VABU

Coefficient of determination

Q: How low does the MSE have to be before it's "low enough"?
A: It depends! The MSE is proportional to the **variance** of the data

Regression diagnostics

Coefficient of determination

(R^2 statistic)

Mean: $\frac{1}{N}\sum_i y_i = \bar{y}$

Variance: $\frac{1}{N}\sum_i (\bar{y} - y_i)^2$

MSE: $\frac{1}{N}\sum_i (x_i \cdot \theta - y_i)^2$

Regression diagnostics

Coefficient of determination
(R^2 statistic)

$$FVU(f) = \frac{MSE(f)}{Var(y)}$$

(FVU = fraction of variance unexplained)

$FVU(f) = 1$ → Trivial predictor
$FVU(f) = 0$ → Perfect predictor

Regression diagnostics

Coefficient of determination

(R^2 statistic)

$$R^2 = 1 - FVU(f) = 1 - \frac{MSE(f)}{Var(y)}$$

R^2 = 0 → Trivial predictor

R^2 = 1 → Perfect predictor

Overfitting

Q: But can't we get an R^2 of 1 (MSE of 0) just by throwing in enough random features?

A: Yes! This is why MSE and R^2 should always be evaluated on data that **wasn't** used to train the model

A good model is one that **generalizes to new data**

Overfitting

When a model performs well on **training** data but doesn't generalize, we are said to be **overfitting**

Q: What can be done to avoid overfitting?

Occam's razor

"Among competing hypotheses, the one with the fewest assumptions should be selected"

Occam's razor

$$X\theta = y$$

"hypothesis"

Q: What is a "complex" versus a "simple" hypothesis?

Occam's razor

A1: A "simple" model is one where theta has few non-zero parameters

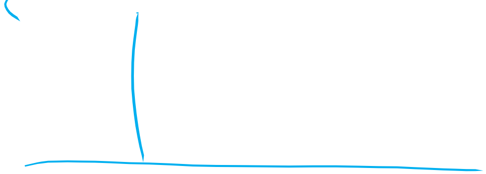
(only a few features are relevant)

A2: A "simple" model is one where theta is almost uniform

(few features are significantly more relevant than others)

Occam's razor

$\|\theta\|_k = \sqrt[k]{\sum_i \theta_i^k}$



$\sum_i |\theta_i|$

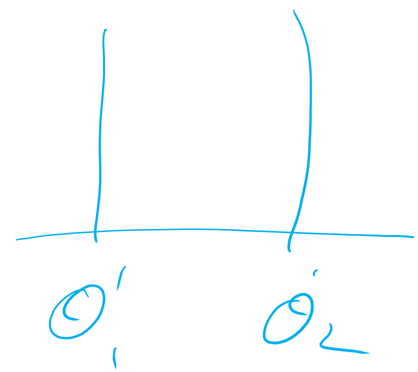
A1: A "simple" model is one where theta has few non-zero parameters → $\|\theta\|_1$ is small

A2: A "simple" model is one where theta is almost uniform → $\|\theta\|_2^2$ is small

$\sum_i \theta_i^2$

"Proof"

$$\text{height} = \theta_0 + \theta_1 \times \text{weight} + \theta_2 \times \text{shoe size}$$



$$\|\theta\|_1 = \|\theta\|_1$$

$$\|\theta\|_2 > \|\theta\|_2$$

Regularization

Regularization is the process of penalizing model complexity during training

$$\arg\min_{\theta} = \frac{1}{N}\|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

MSE

(l2) model complexity

Regularization

Regularization is the process of penalizing model complexity during training

$$\arg\min_\theta = \frac{1}{N}\|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

How much should we trade-off accuracy versus complexity?

Optimizing the (regularized) model

$$\arg\min_\theta = \underbrace{\frac{1}{N}\|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2}_{f(\theta)}$$

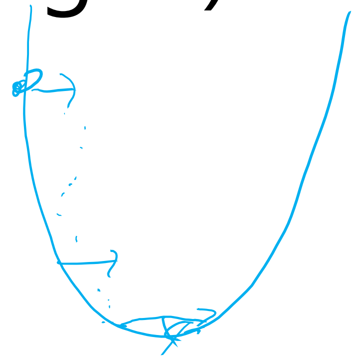
- We no longer have a convenient closed-form solution for theta
- Need to resort to some form of approximation algorithm

Optimizing the (regularized) model

Gradient descent:

1. Initialize θ at random
2. While (not converged) do

$$\theta := \theta - \alpha f'(\theta)$$



All sorts of annoying issues:

- How to initialize theta?
- How to determine when the process has converged?
- How to set the step size alpha

These aren't really the point of this class though

Optimizing the (regularized) model

$$f(\theta) = \frac{1}{N}\|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

$$\frac{\partial f}{\partial \theta_k} \; ?$$

$$f = \frac{1}{N}\sum_i (x_i \cdot \theta - y_i)^2 + \lambda \sum_k \theta_k^2$$

$$\frac{\partial f}{\partial \theta_k} = \frac{1}{N} \sum_i 2 x_{ik}(x_i \cdot \theta - y_i) + \lambda \cdot 2\theta_k$$

Optimizing the (regularized) model

Gradient descent in scipy:

(code for all examples is on http://jmcauley.ucsd.edu/cse255/code/week1.py)

(see "ridge regression" in the "sklearn" module)

Model selection

$$\arg\min_{\theta} = \frac{1}{N}\|y - X\theta\|_2^2 + \lambda\|\theta\|_2^2$$

How much should we trade-off accuracy versus complexity?

Each value of lambda generates a different model. **Q:** How do we select which one is the best?

Model selection

How to select which model is best?

A1: The one with the lowest training error?

A2: The one with the lowest test error?

We need a **third** sample of the data that is not used for training or testing

Model selection

A **validation set** is constructed to "tune" the model's parameters

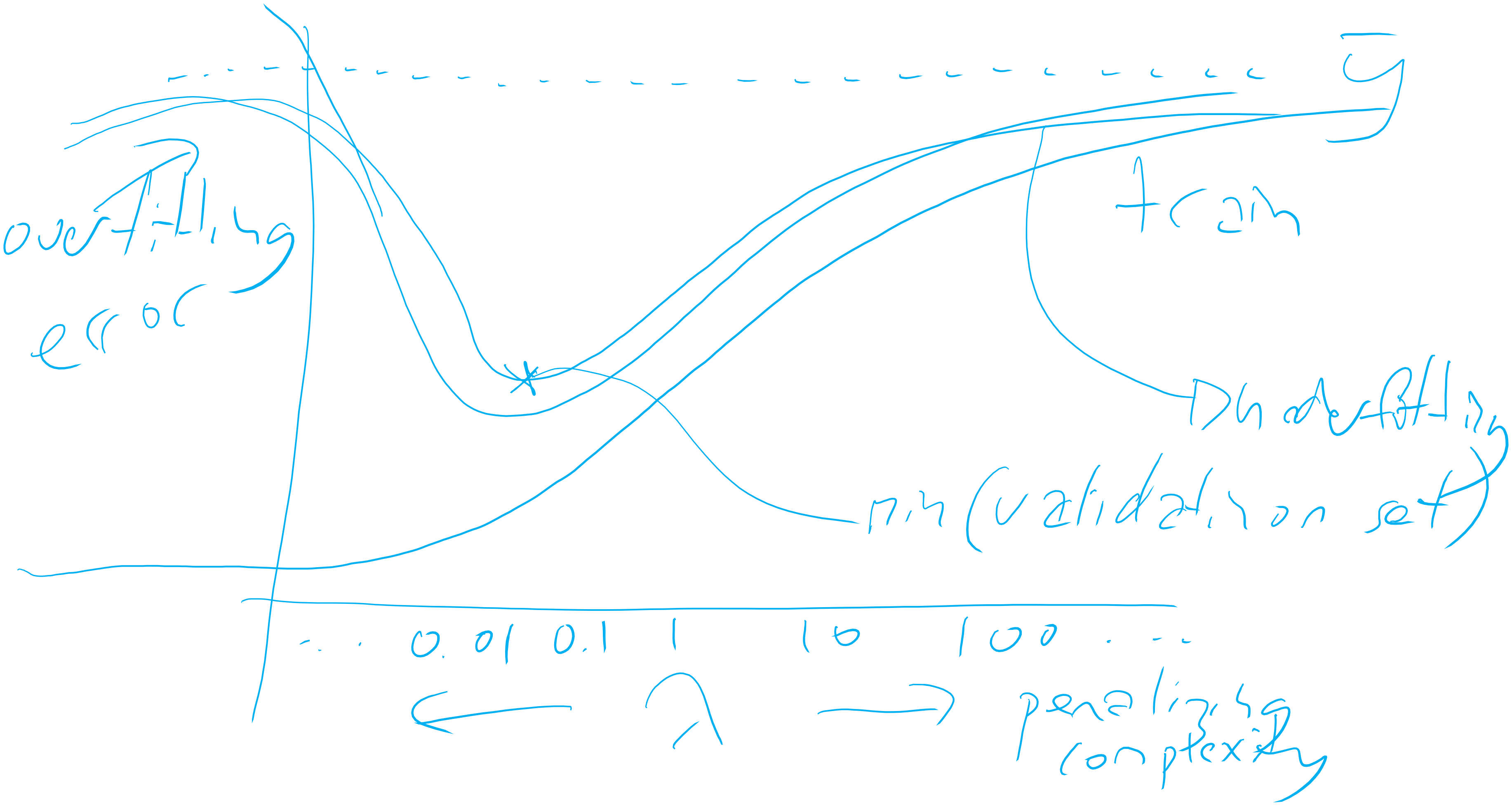
- Training set: used to **optimize the model's parameters**
- Test set: used to report how well we expect the model to perform on **unseen data**
- Validation set: used to **tune** any model parameters that are not directly optimized

Model selection

A few "theorems" about training, validation, and test sets

- The training error **increases** as lambda **increases**
- The validation and test error are at least as large as the training error (assuming infinitely large random partitions)
- The validation/test error will usually have a "sweet spot" between under- and over-fitting

Model selection



Summary of Week 1: Regression

- Linear regression and least-squares
- (a little bit of) feature design
- Overfitting and regularization
- Gradient descent
- Training, validation, and testing
- Model selection

Coming up!

An exciting case study (i.e., my own research)!

This photo recently one the Andrews award for the 'most perfect timing of a Nature photograph', I can see why.
submitted 29 days ago by SICK_OF_ to /r/pics
11 points
1 comment

NOM! (Photo by: Bohemian Waxwing)
submitted 2 months ago by ~~favoritehello~~ [deleted] to /r/PerfectTiming
1117 points
11 comments

Perfect moment bird (ex-post from r/pics)
submitted 25 days ago by 123imAwesome to /r/photoshopbattles
36 points
11 comments

A bohemian waxwing eating a berry
submitted 4 months ago by HazeySynth to /r/pics
39 points
1 comment

Bird shot at the perfect moment
submitted 25 days ago by arbili to /r/pics
2712 points
166 comments

Perfect timing.
submitted 4 months ago by animalpath to /r/pics
2555 points
71 comments

Perfect timing.
submitted 2 months ago by presaging to /r/aww
12 points
1 comment

Timing is Everything
submitted 5 months ago by Xnicko378X to /r/pics
10 points
1 comment

Homework

Homework is **available** on the course webpage
http://cseweb.ucsd.edu/classes/fa15/cse255-a/files/homework1.pdf

Please submit it at the beginning of the **week 3** lecture (Oct 12)

Questions?