CSE 158 – Lecture 2

Web Mining and Recommender Systems

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

$$X\theta = y$$

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

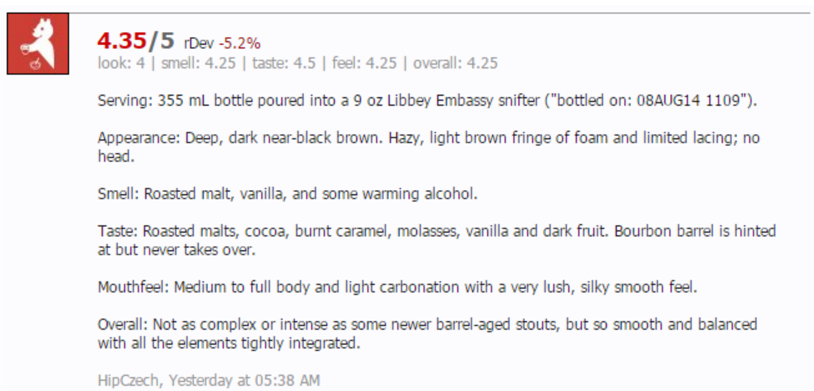
A: $\theta = (X^T X)^{-1} X^T y$

Example 1

Beeradvocate

Beers:

Ratings/reviews:



User profiles:

Example 1

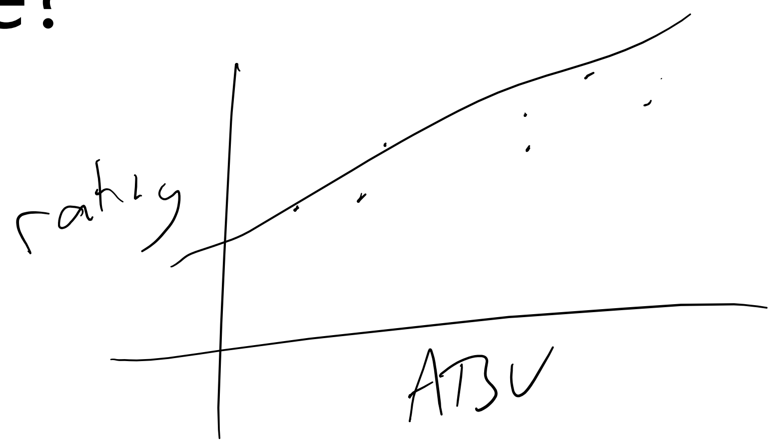
50,000 reviews are available on
http://jmcauley.ucsd.edu/cse158/data/beer/beer_50000.json
(see course webpage)

See also – non-alcoholic beers:
http://jmcauley.ucsd.edu/cse158/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/cse158/code/week1.py)

Example 1.5: Polynomial functions

What about something like ABV^2?

$$\text{rating} = \theta_0 + \theta_1 \times \text{ABV} + \theta_2 \times \text{ABV}^2 + \theta_3 \times \text{ABV}^3$$

- Note that this is perfectly straightforward: the model still takes the form

$$\text{weight} = \theta \cdot x$$

- We just need to use the feature vector

```
x = [1, ABV, ABV^2, ABV^3]
```

Fitting complex functions

Note that we can use the same approach to fit arbitrary functions of the features! E.g.:

$$\text{Rating} = \theta_0 + \theta_1 \times \text{ABV} + \theta_2 \times \text{ABV}^2 + \theta_3 \exp(\text{ABV}) + \theta_4 \sin(\text{ABV})$$

- We can perform arbitrary combinations of the **features** and the model will still be linear in the **parameters** (theta):

$$\text{Rating} = \theta \cdot x$$

Fitting complex functions

The same approach would **not** work if we wanted to transform the parameters:

$$\text{Rating} = \theta_0 + \theta_1 \times \text{ABV} + \theta_2^2 \times \text{ABV} + \sigma(\theta_3) \times \text{ABV}$$

- The **linear** models we've seen so far do not support these types of transformations (i.e., they need to be linear in their parameters)
- There *are* alternative models that support non-linear transformations of parameters, e.g. neural networks

Example 2

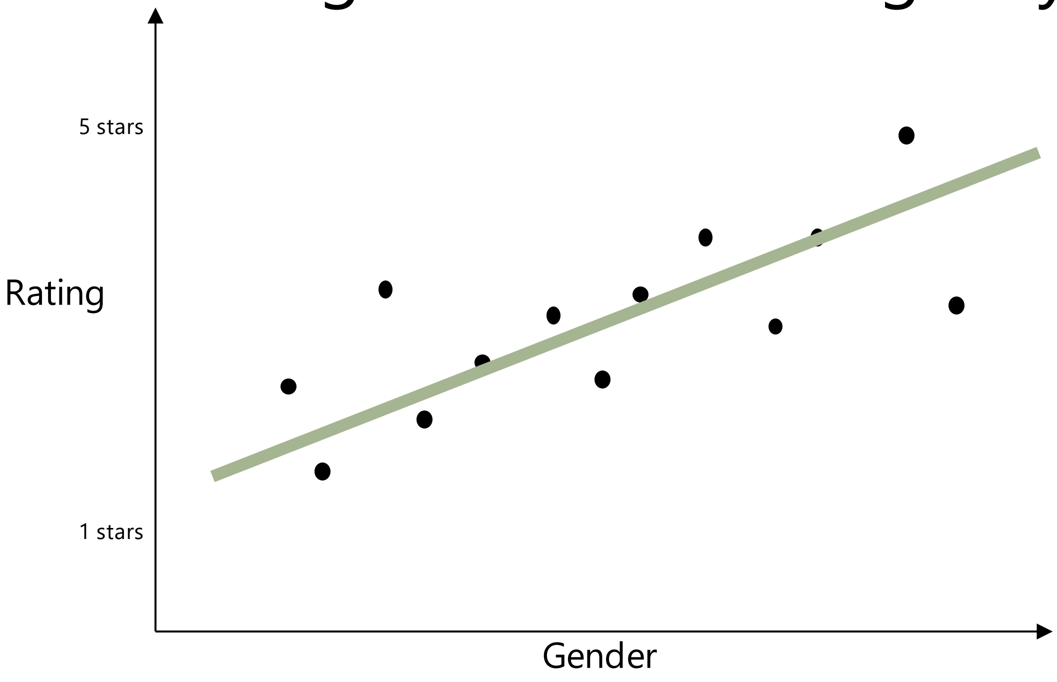
Categorical features

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

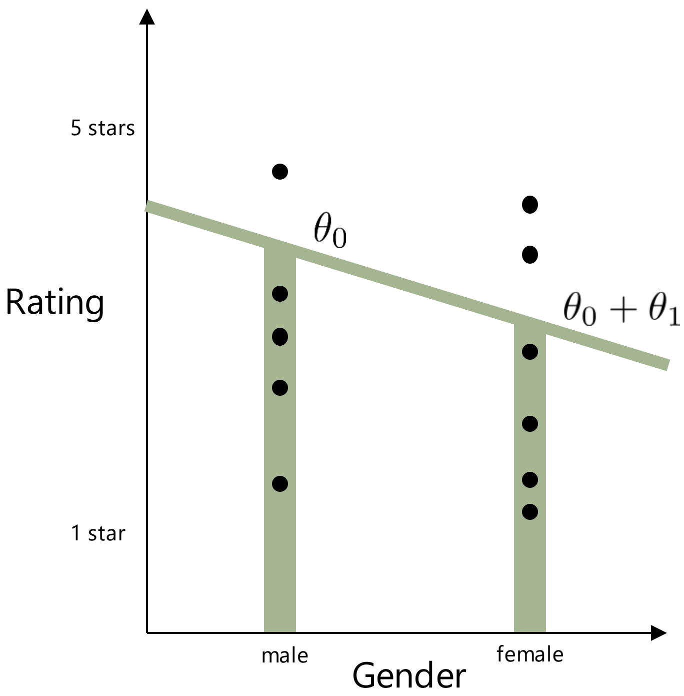
(code for all examples is on http://jmcauley.ucsd.edu/cse158/code/week1.py)

Example 2

E.g. How does rating vary with **gender?**



Example 2



θ_0 is the (predicted/average) rating for males

θ_1 is the **how much higher** females rate than males (in this case a negative number)

We're really still fitting a line though!

$$\text{rating} = \theta_0 + \theta_1 [\text{if female}]$$

$$= \theta \cdot x$$

$$x = [1, 0] \text{ if male}$$

$$[1, 1] \text{ if female}$$

Motivating examples

What if we had more than two values?
(e.g {“male”, “female”, “other”, “not specified”})

Could we apply the same approach?

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

gender = **0 if “male”, 1 if “female”, 2 if “other”, 3 if “not specified”**

$$\text{Rating} = \theta_0$$ **if male**

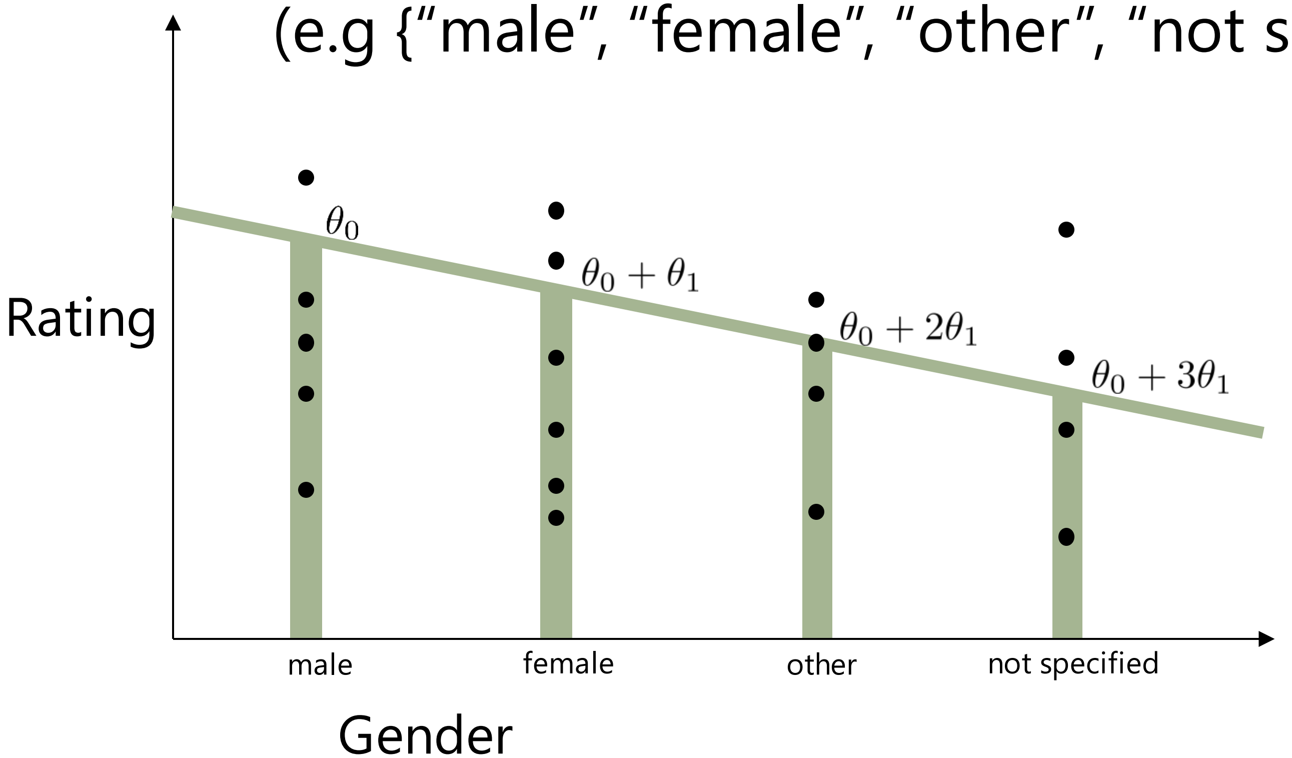
$$\text{Rating} = \theta_0 + \theta_1$$ **if female**

$$\text{Rating} = \theta_0 + 2\theta_1$$ **if other**

$$\text{Rating} = \theta_0 + 3\theta_1$$ **if not specified**

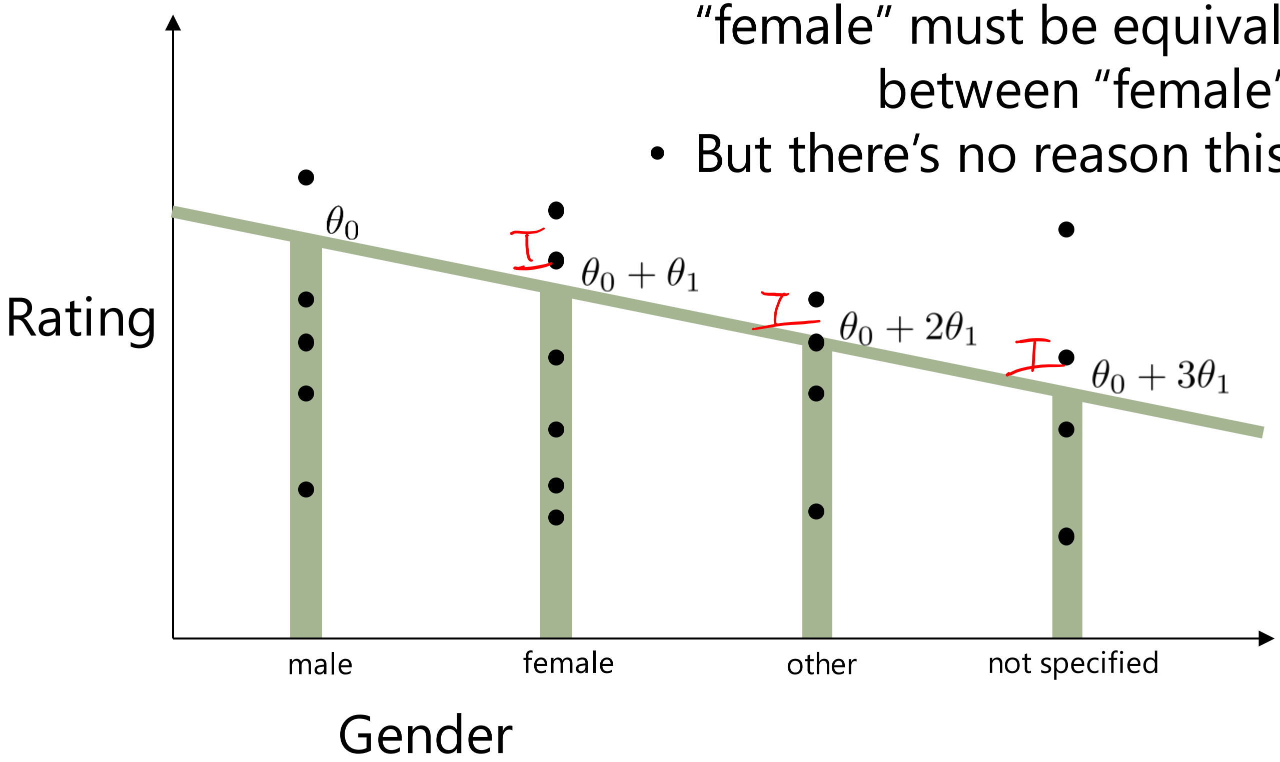
Motivating examples

What if we had more than two values?
(e.g {“male”, “female”, “other”, “not specified”})



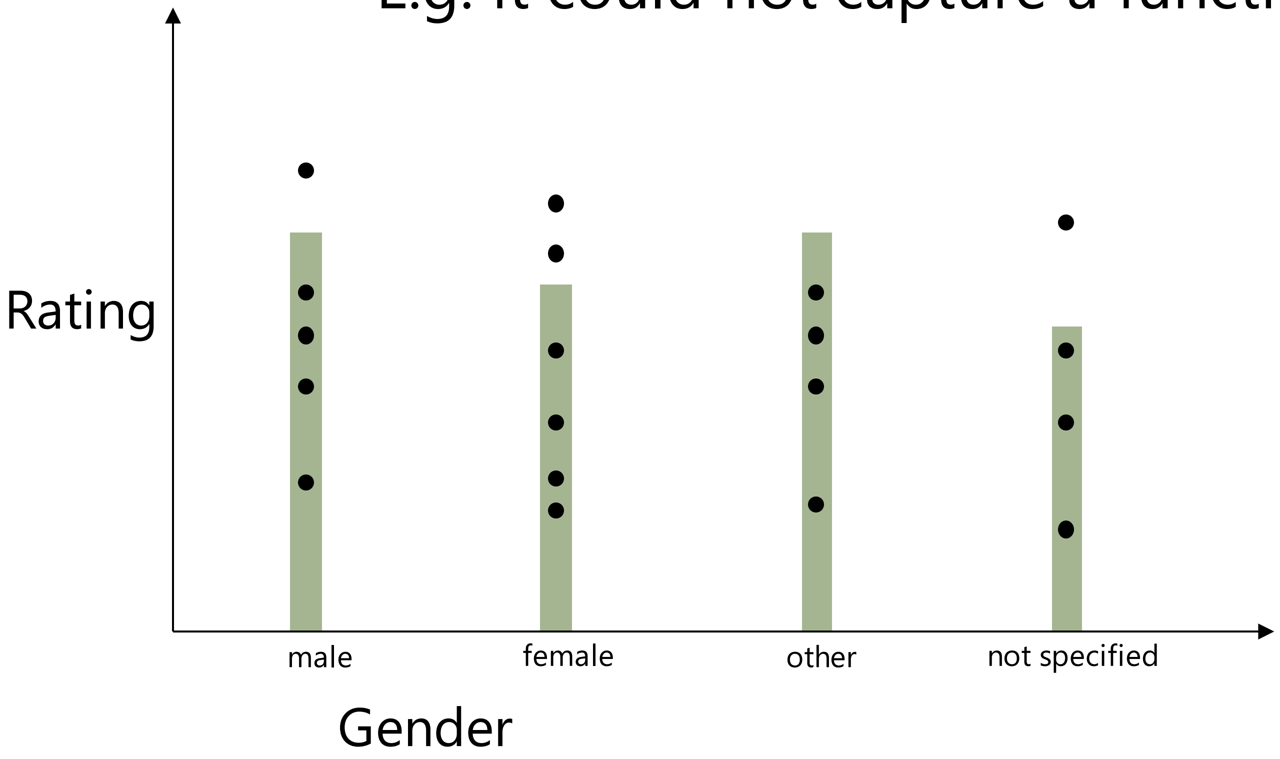
Motivating examples

- This model is **valid,** but won't be very **effective**
- It assumes that the difference between "male" and "female" must be equivalent to the difference between "female" and "other"
- But there's no reason this should be the case!



Motivating examples

E.g. it could not capture a function like:



Motivating examples

Instead we need something like:

$$\text{Rating} = \theta_0$$ **if male**

$$\text{Rating} = \theta_0 + \theta_1$$ **if female**

$$\text{Rating} = \theta_0 + \theta_2$$ **if other**

$$\text{Rating} = \theta_0 + \theta_3$$ **if not specified**

Motivating examples

This is equivalent to:

$$(\theta_0, \theta_1, \theta_2, \theta_3) \cdot (1; \text{feature})$$

where feature = [1, 0, 0] for "female"
feature = [0, 1, 0] for "other"
feature = [0, 0, 1] for "not specified"

Concept: One-hot encodings

feature = [1, 0, 0] for “female”
feature = [0, 1, 0] for “other”
feature = [0, 0, 1] for “not specified”

- This type of encoding is called a **one-hot encoding** (because we have a feature vector with only a single “1” entry)
- Note that to capture 4 possible categories, we only need three dimensions (a dimension for “male” would be redundant)
- This approach can be used to capture a variety of categorical feature types, as well as objects that belong to multiple categories

Linearly dependent features

$$\text{rating} = \theta_0 + \theta_1 \times [\text{is Male}] + \theta_2 \times [\text{is Female}]$$

$$X = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

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

$$X^T X = \begin{bmatrix} 5 & 2 & 3 \\ 2 & 2 & 0 \\ 3 & 0 & 3 \end{bmatrix} \begin{matrix} a+b \\ b \\ a \end{matrix}$$

Linearly dependent features

$$\text{rating} = 2 + 2[\text{if } M] + \sout{3[\text{if } F]}$$

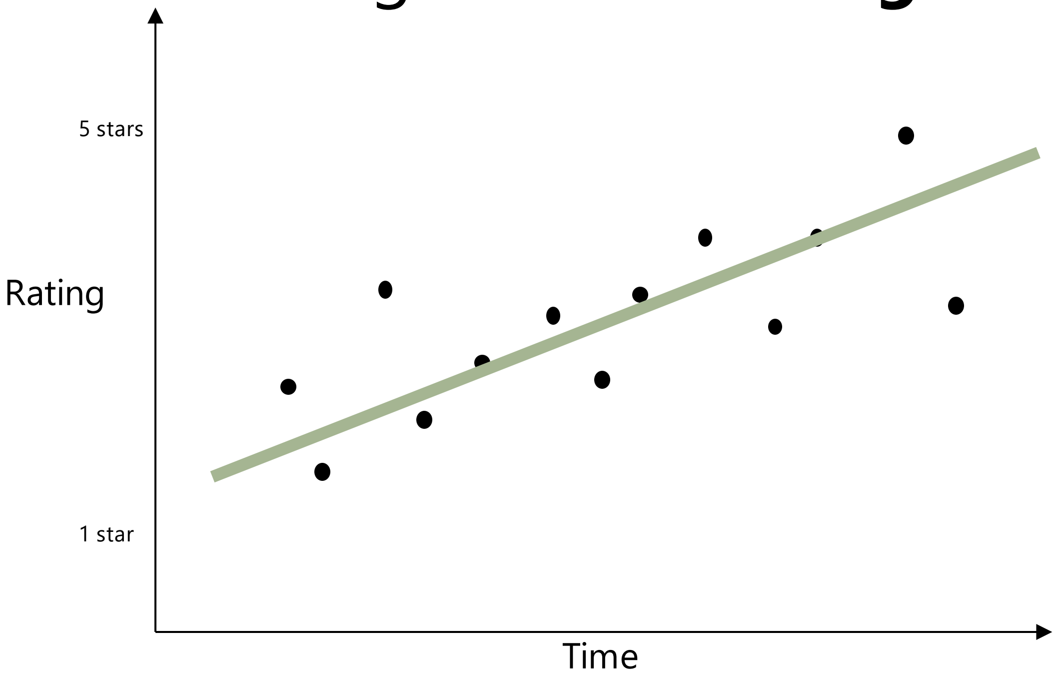
$$\text{rating} = 1000 - 996[\text{if } M] - 995[\text{if } F]$$

Example 3

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

Motivating examples

E.g. How do **ratings** vary with **time**?



Motivating examples

E.g. How do **ratings** vary with **time**?

- In principle this picture looks okay (compared our previous example on categorical features) – we're predicting a **real valued** quantity from **real valued** data (assuming we convert the date string to a number)
- So, what would happen if (e.g. we tried to train a predictor based on the month of the year)?

Motivating examples

E.g. How do **ratings** vary with **time**?

- Let's start with a simple feature representation, e.g. map the month name to a month number:

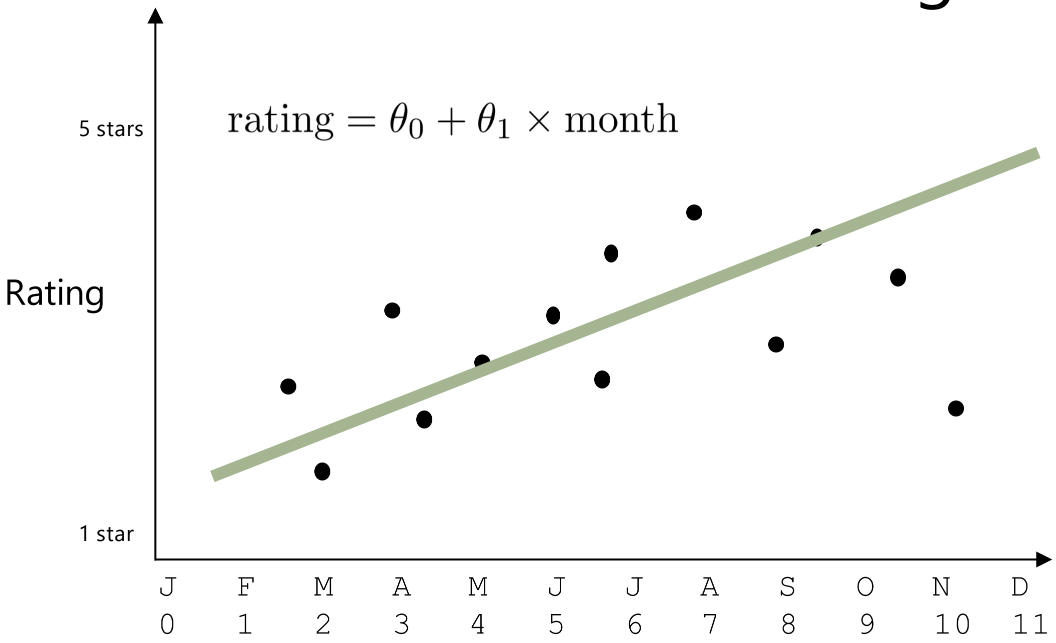
$$\text{rating} = \theta_0 + \theta_1 \times \text{month}$$

where

```
Jan = [0]
Feb = [1]
Mar = [2]
etc.
```

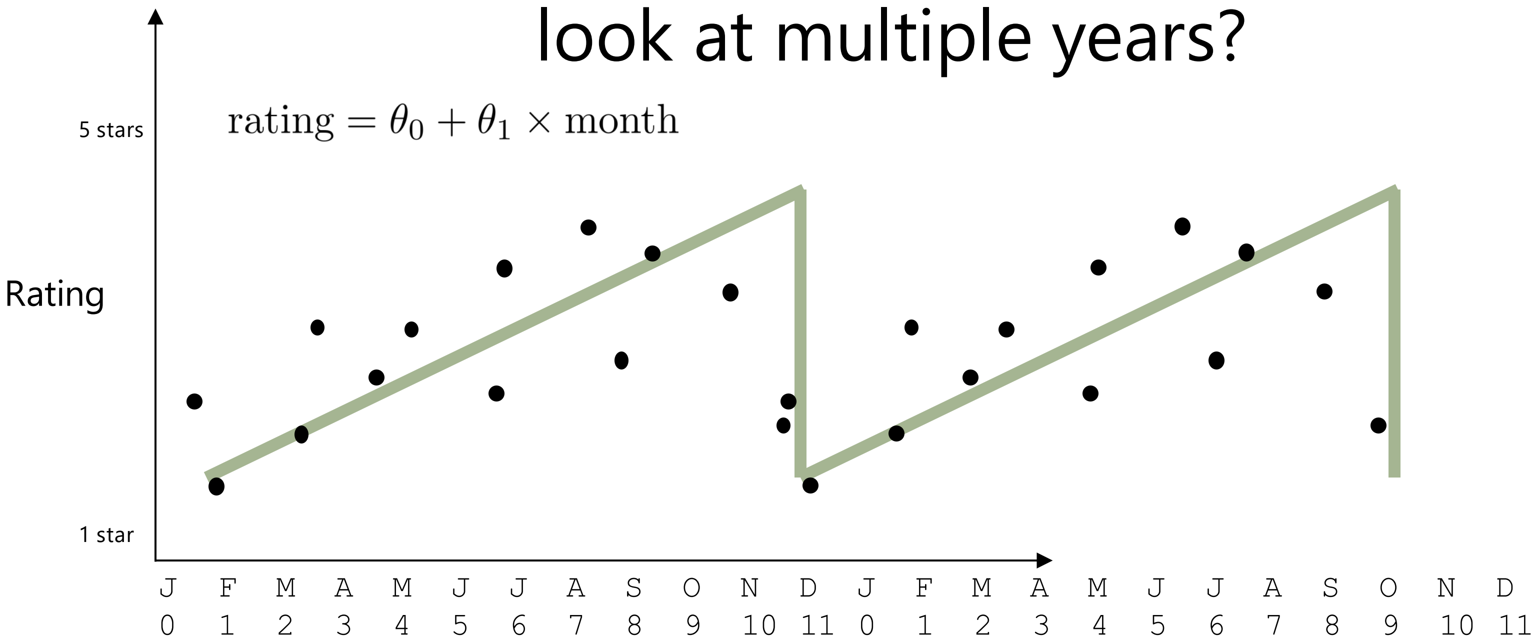
Motivating examples

The model we'd learn might look something like:



Motivating examples

This seems fine, but what happens if we look at multiple years?



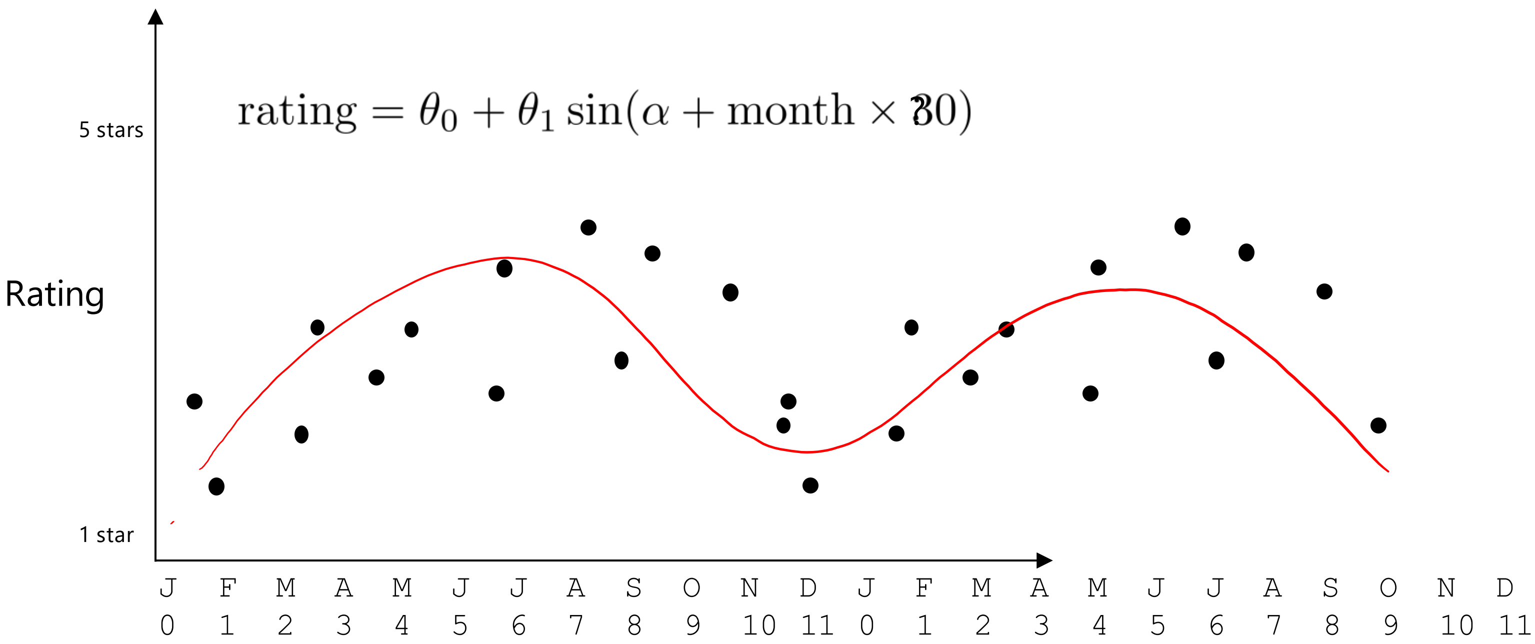
Modeling temporal data

This seems fine, but what happens if we look at multiple years?

- This representation implies that the model would "wrap around" on December 31 to its January 1st value.
- This type of "sawtooth" pattern probably isn't very realistic

Modeling temporal data

What might be a more realistic shape?



Modeling temporal data

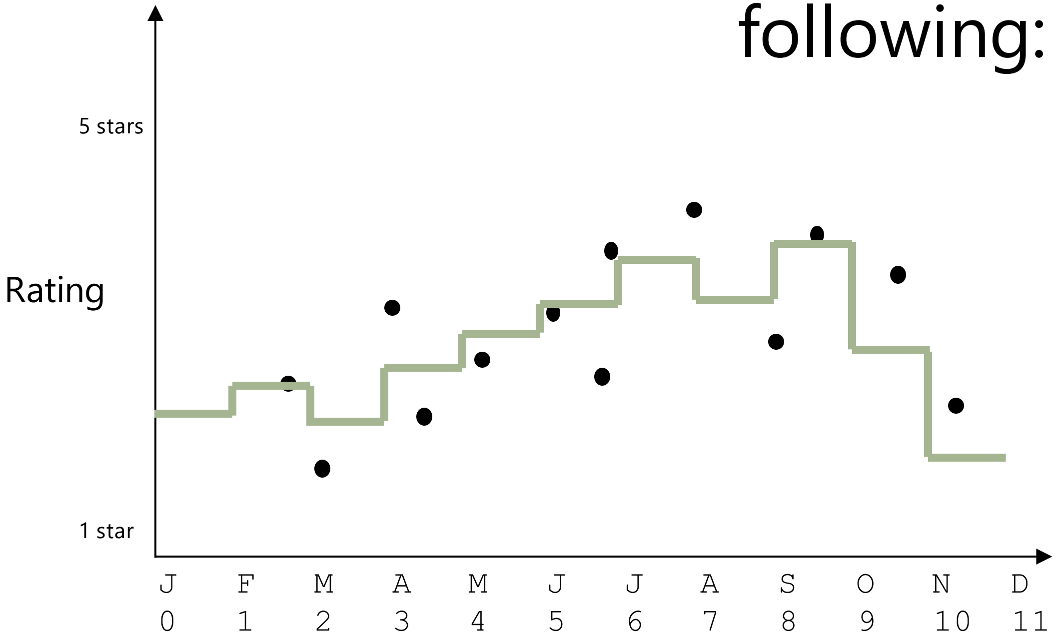
Fitting some periodic function like a sin wave would be a valid solution, but is difficult to get right, and fairly inflexible

- Also, it's not a **linear model**

- **Q:** What's a class of functions that we can use to capture a more flexible variety of shapes?
- **A:** Piecewise functions!

Concept: Fitting piecewise functions

We'd like to fit a function like the following:



Fitting piecewise functions

In fact this is very easy, even for a linear model! This function looks like:

rating = Θ_0[Jan] + $\Theta_1 \times$ [Feb] ...

$$\text{rating} = \theta_0 + \theta_1 \times \delta(\text{is Feb}) + \theta_2 \times \delta(\text{is Mar}) + \theta_3 \times \delta(\text{is Apr}) \cdots$$

1 if it's Feb, 0 otherwise

- Note that we don't need a feature for January
- i.e., theta_0 captures the January value, theta_~~0~~ 1 captures the *difference* between February and January, etc.

Fitting piecewise functions

Or equivalently we'd have features as follows:

$\text{rating} = \theta \cdot x$ where

```
x = [1,1,0,0,0,0,0,0,0,0,0,0] if February
    [1,0,1,0,0,0,0,0,0,0,0,0] if March
    [1,0,0,1,0,0,0,0,0,0,0,0] if April
    ...
    [1,0,0,0,0,0,0,0,0,0,0,1] if December
```

Fitting piecewise functions

Note that this is still a form of **one-hot** encoding, just like we saw in the "categorical features" example

- This type of feature is very flexible, as it can handle complex shapes, periodicity, etc.
- We could easily increase (or decrease) the resolution to a week, or an entire season, rather than a month, depending on how fine-grained our data was

Concept: Combining one-hot encodings

We can also extend this by combining several one-hot encodings together:

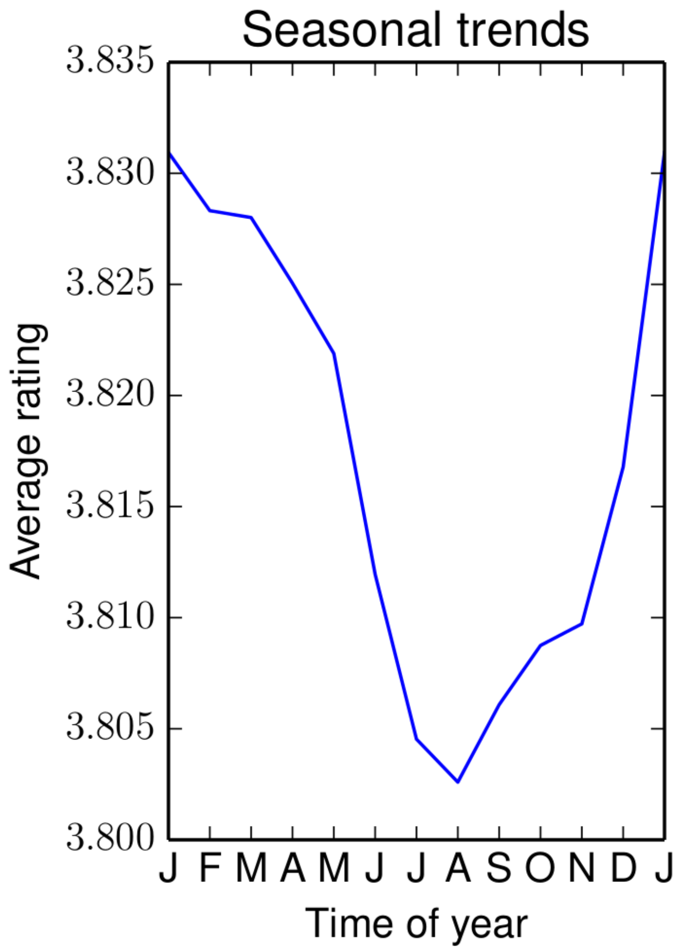
$$\text{rating} = \theta \cdot x = \theta \cdot [x_1; x_2]$$ where

```
x1 = [1,1,0,0,0,0,0,0,0,0,0,0] if February
     [1,0,1,0,0,0,0,0,0,0,0,0] if March
     [1,0,0,1,0,0,0,0,0,0,0,0] if April
     ...
     [1,0,0,0,0,0,0,0,0,0,0,1] if December
```

```
x2 = [1,0,0,0,0,0] if Tuesday
     [0,1,0,0,0,0] if Wednesday
     [0,0,1,0,0,0] if Thursday
     ...
```

What does the data actually look like?

Season vs. rating (overall)



CSE 158 – Lecture 2

Web Mining and Recommender Systems

Regression Diagnostics

Today: Regression diagnostics

Mean-squared error (MSE)

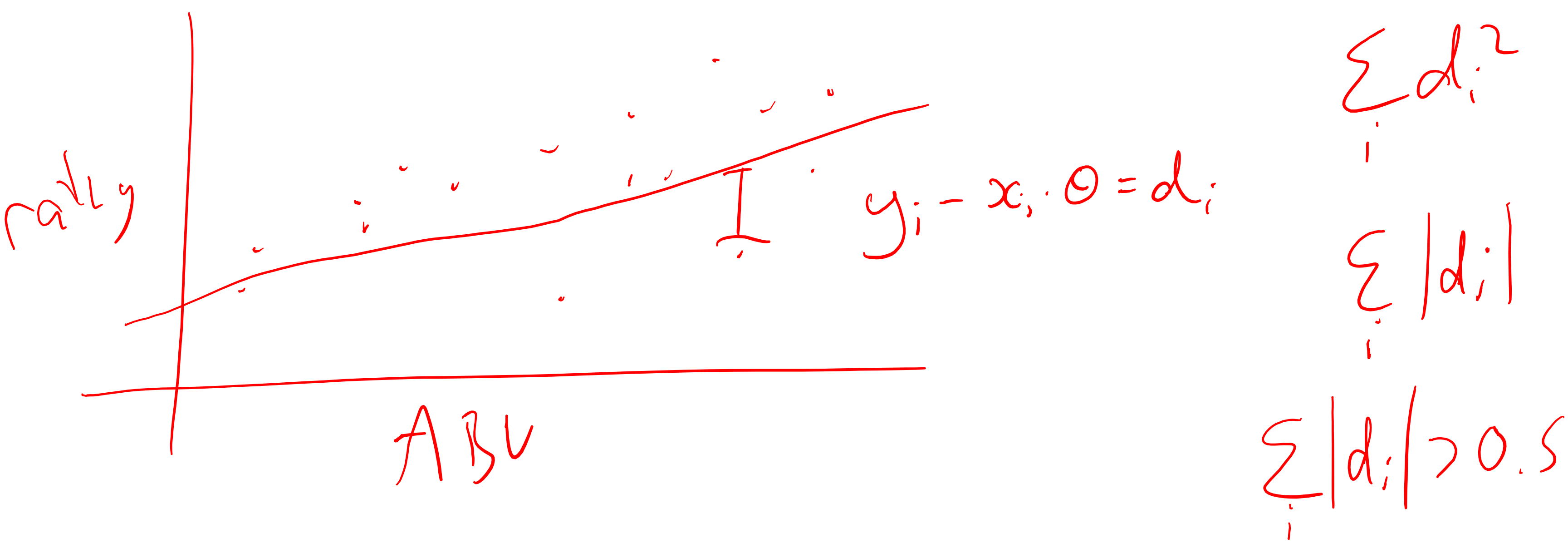
$$\frac{1}{N}\|y - X\theta\|_2^2$$

$$\|\theta\|_2^2 = \sum_i \theta_i^2$$

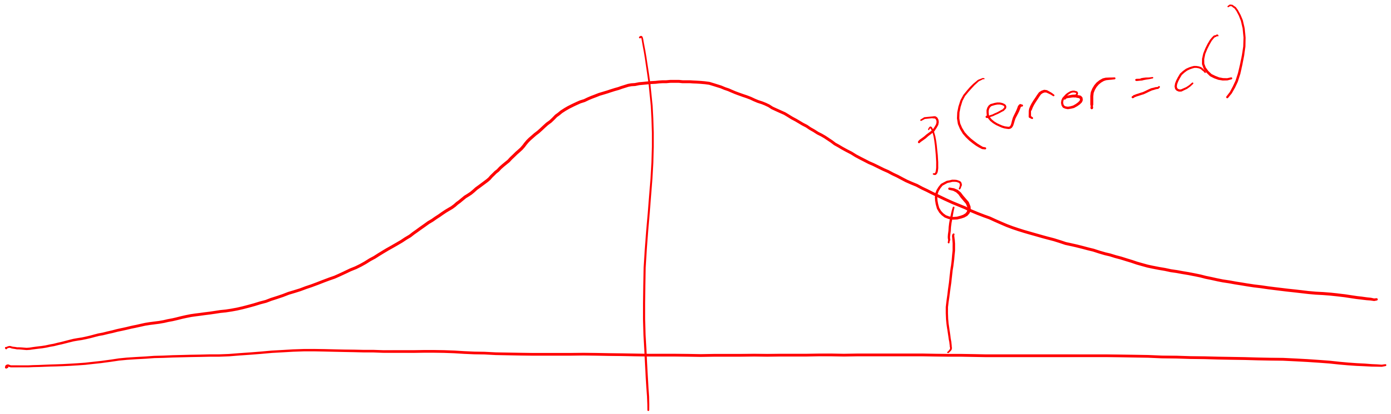
$$= \frac{1}{N}\sum_{i=1}^{N}(y_i - X_i \cdot \theta)^2$$

Regression diagnostics

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



Regression diagnostics



$$d = y_i - x_i \cdot \theta$$

$$y_i = x_i \cdot \theta + \text{error}$$
$$= x_i \cdot \theta + \mathcal{N}(0, \sigma^2)$$

Regression diagnostics

$$p_\theta(y|X) = \prod_i \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - X_i \cdot \theta)^2}{2\sigma^2}}$$

$$\max_\theta p_\theta(y|X) = \prod_i e^{-(y_i - X_i \cdot \theta)^2}$$

$$\min_\theta p_\theta = \sum_i (y_i - X_i \cdot \theta)^2$$

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

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

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

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**

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

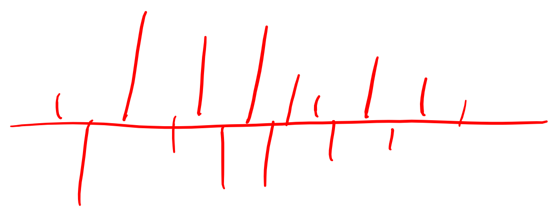
$$X\theta = y$$

"hypothesis"

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

Occam's razor

$$\text{rating} = \theta_0 + \theta_1 \text{ABV} + \theta_2 \text{ABV}^2 \ldots$$

$\theta =$  "complex"

$\theta =$  "simple"

$\theta =$  "simple"

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

$\sum_i |\theta_i|$

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 → $||\theta||_2$ is small

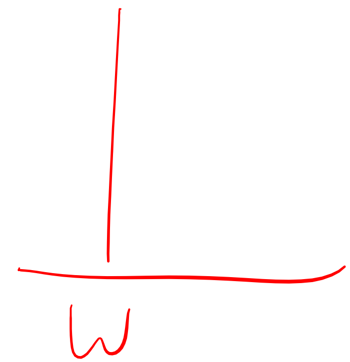
$\sum_i \theta_i^2$

"Proof"

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

$\theta_a =$

θ_b



$$\|\theta_a\|_1 = \|\theta_b\|_1 \qquad \|\theta_a\|_2 < \|\theta_b\|_2$$

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

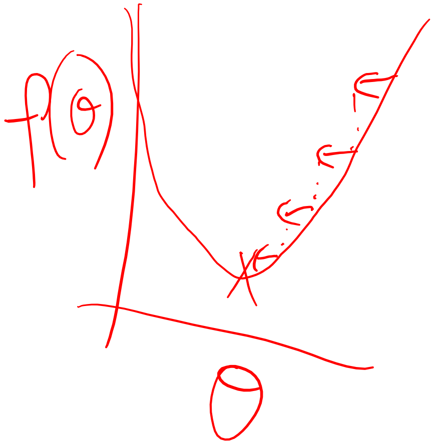
Regularization is the process of penalizing model complexity during training

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

How much should we trade-off accuracy versus complexity?

Optimizing the (regularized) model

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



- Could look for a closed form solution as we did before
- Or, we can try to solve using **gradient descent**

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

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

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

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

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

Optimizing the (regularized) model

Gradient descent in scipy:

(code for all examples is on http://jmcauley.ucsd.edu/cse158/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

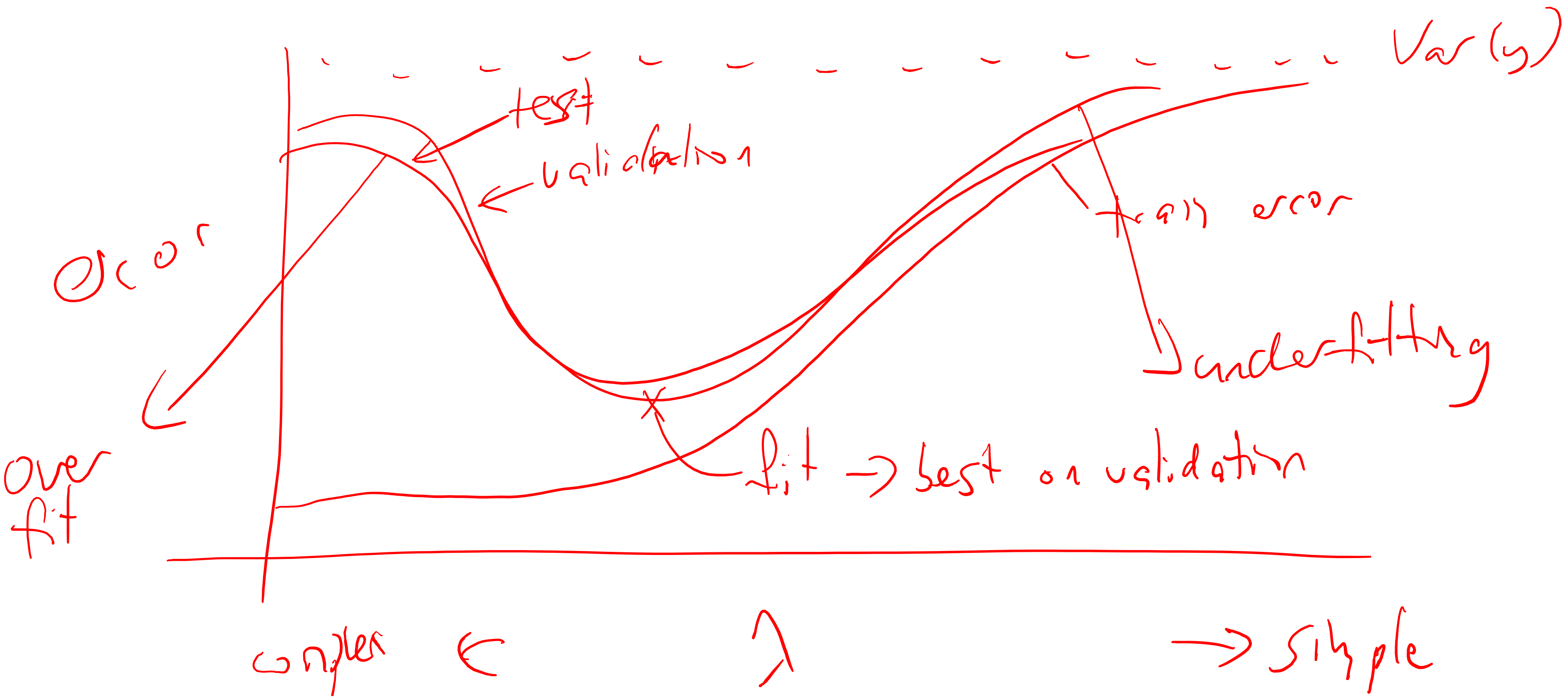
- Training set: used to **optimize the model's parameters**
- Test set: used to report how well we expect the model to perform on **unseen data** → Only once!
- Validation set: used to **tune** any model parameters that are not directly optimized

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

Homework

Homework is **available** on the course webpage
http://cseweb.ucsd.edu/classes/fa19/cse158-a/files/homework1.pdf

Please submit it at the beginning of the **week 3** lecture (Oct 14)

All submissions should be made as **pdf files on gradescope**

Questions?