Bias/Variance and Cross-Validation

Mark Llorente, Based on Previous Work of RH

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- Overfitting and Underfitting
- The Bias/Variance Tradeoff
- Cross-Validation
- K-fold Cross-Validation
- Subset Selection of Predictors

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We Want “Good” Models

What are “good” models? What do we expect good models to do?

How can we be sure a model works on data it hasn’t already seen?

Stepping back: One Goal of Data Science: Make Future Predictions

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One goal is to make accurate ***predictions*** on future (unseen) data.

1. Define a business goal.
   e.g. make Tesla cars the most dependable vehicles on the market

2. Collect training data.
   e.g. Tesla cars' event logs + historical record of parts replaced

3. Train a model.
   e.g. **features:** event statistics, **target:** time until failure

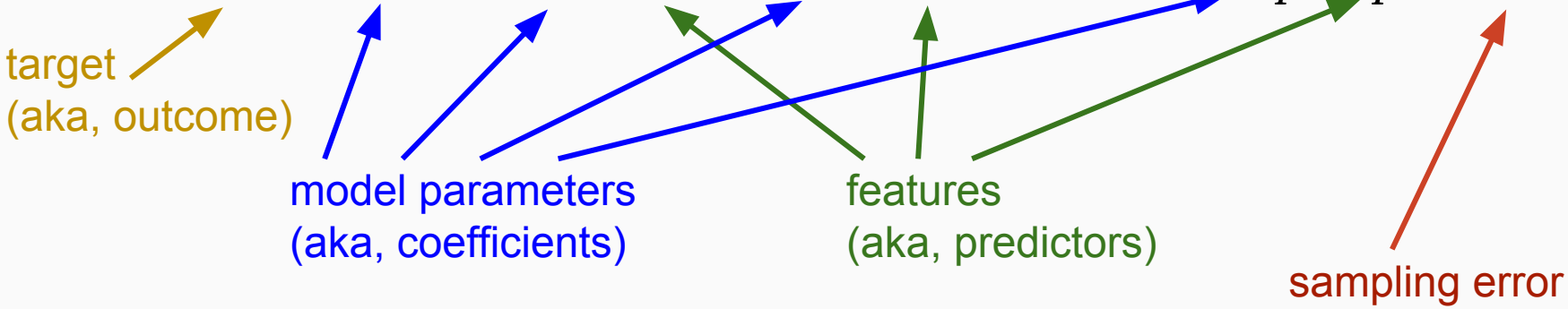
4. Deploy the model.
   e.g. monitor cars' events in real time, send mechanics to replace parts that will soon fail

Questions!

Review: Linear Regression

We assume the world is built on linear relationships. Under that assumption, we can model the relationship between *features* and a *target* like this:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$



Review: Linear Regression

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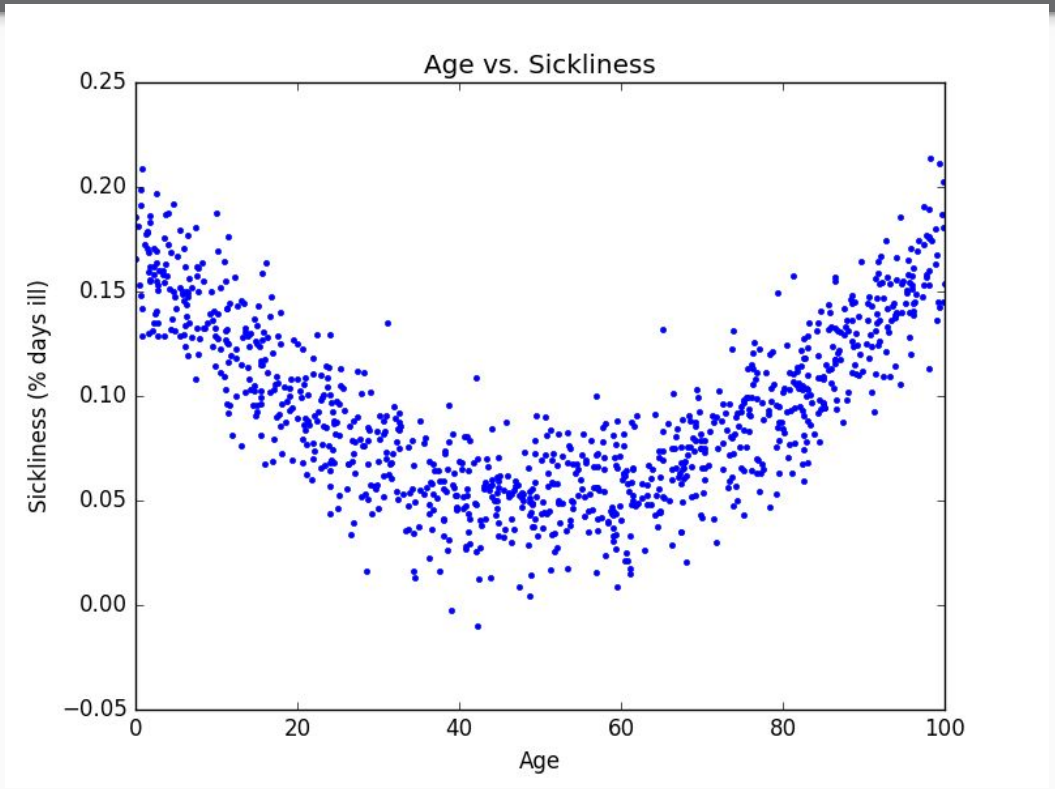
We can make linear regression non-linear by inserting extra “interaction” features or higher-order features.



Example:

$$Y = \beta_0 + \beta_1 * \text{age}$$

$$Y = \beta_0 + \beta_1 * \text{age} + \beta_2 * \text{age}^2$$

Is R^2 all that matters?

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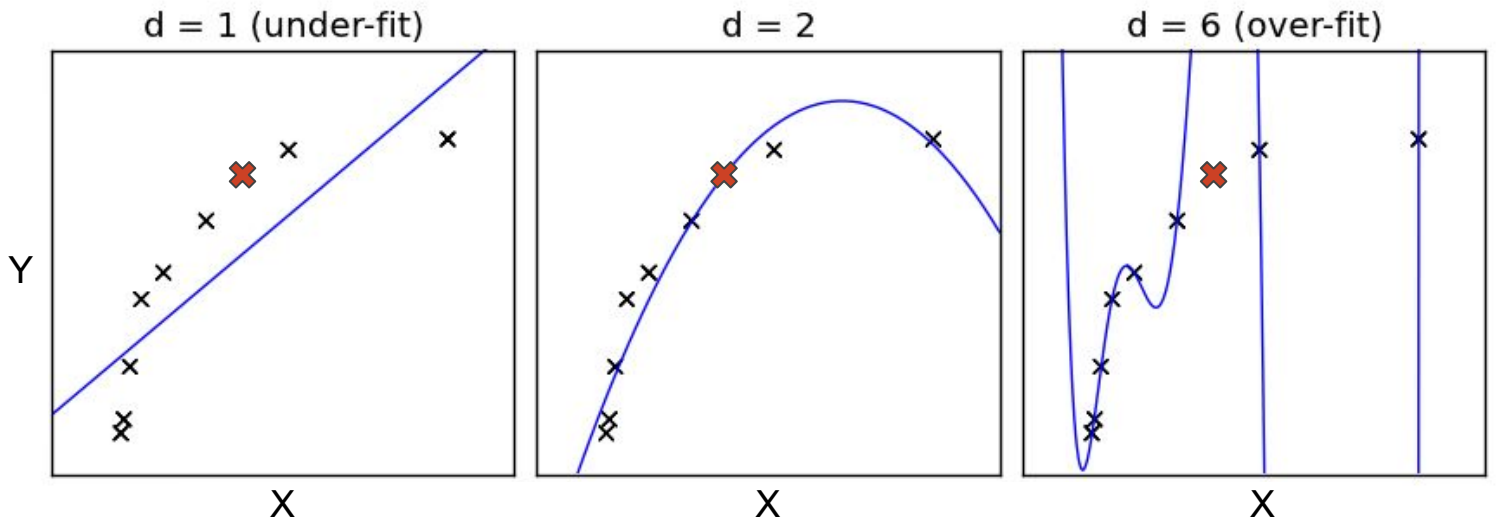
We *could* just keep inserting interaction features until $R^2 = 1$.

Boom. I solved data science. Here's my idea:

```
def train_super_awesome_perfect_model (X, y):
    while True:
        model = LinearRegression()
        model.fit(X, y)
        if calculate_r2(model, X, y) >= 0.999:
            return model
        else:
            X = insert_random_interaction_feature(X)
```

Why is this a bad idea?

Oh the woes of overfitting...



What's bad about the first model?

What's bad about the second model?

What's bad about the third model?

Underfitting and Overfitting

Underfitting: The model doesn't fully capture the relationship between predictors and the target. The model has *not* learned the data's signal.

→ What should we do if our model underfits the data? (assume using lin. reg.)

Overfitting: The model has tried to capture the sampling error. The model has learned the data's signal *and* the noise.

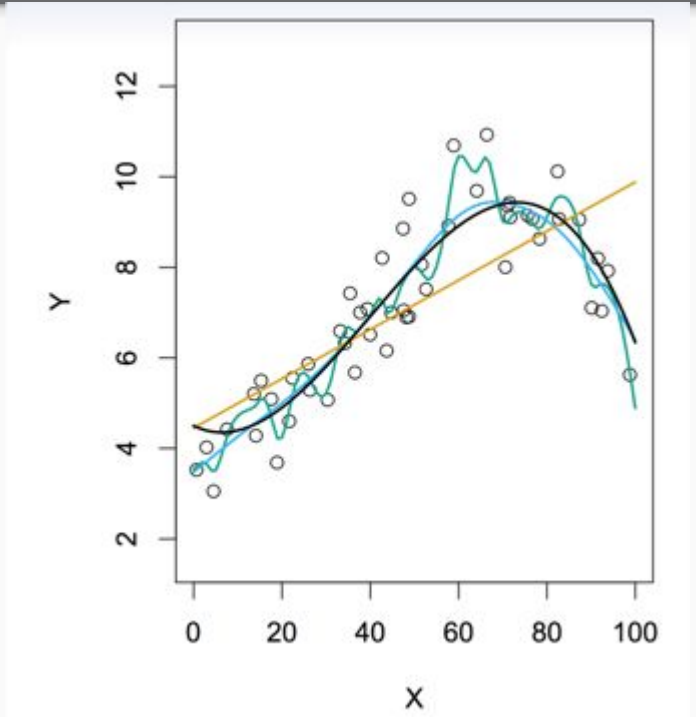
→ What should we do if our model overfits the data? (harder… any guesses?)

The Bias/Variance Tradeoff

Boardwork… build intuition...

Let's get an intuitive feel for the bias and the variance of a model… we'll see more math on the next slide.

Note: **Bias** and **Variance** are terms you will use A TON as a data scientist! Exciting times!



We assume the true predictor/target relationship is given by an unknown function plus some sampling error:

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

We estimate the true (unknown) function by fitting a model over the training set.

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

Let's evaluate this model using a test observation **(x_0, y_0)** drawn from the population. What is the model's expected squared prediction error on this test observation?

$$E[(y_o - \hat{f}(x_0))^2] = \ldots$$

Our model's expected squared prediction error will depend on (1) the variability of $\mathbf{y_0}$ and (2) the variability of the training set used to train our model. We can break this into three pieces:

$$E[(y_o - \hat{f}(x_0))^2] = \ldots = \mathrm{Var}(\hat{f}(x_0)) + \mathrm{Bias}^2(\hat{f}(x_0)) + \mathrm{Var}(\epsilon)$$

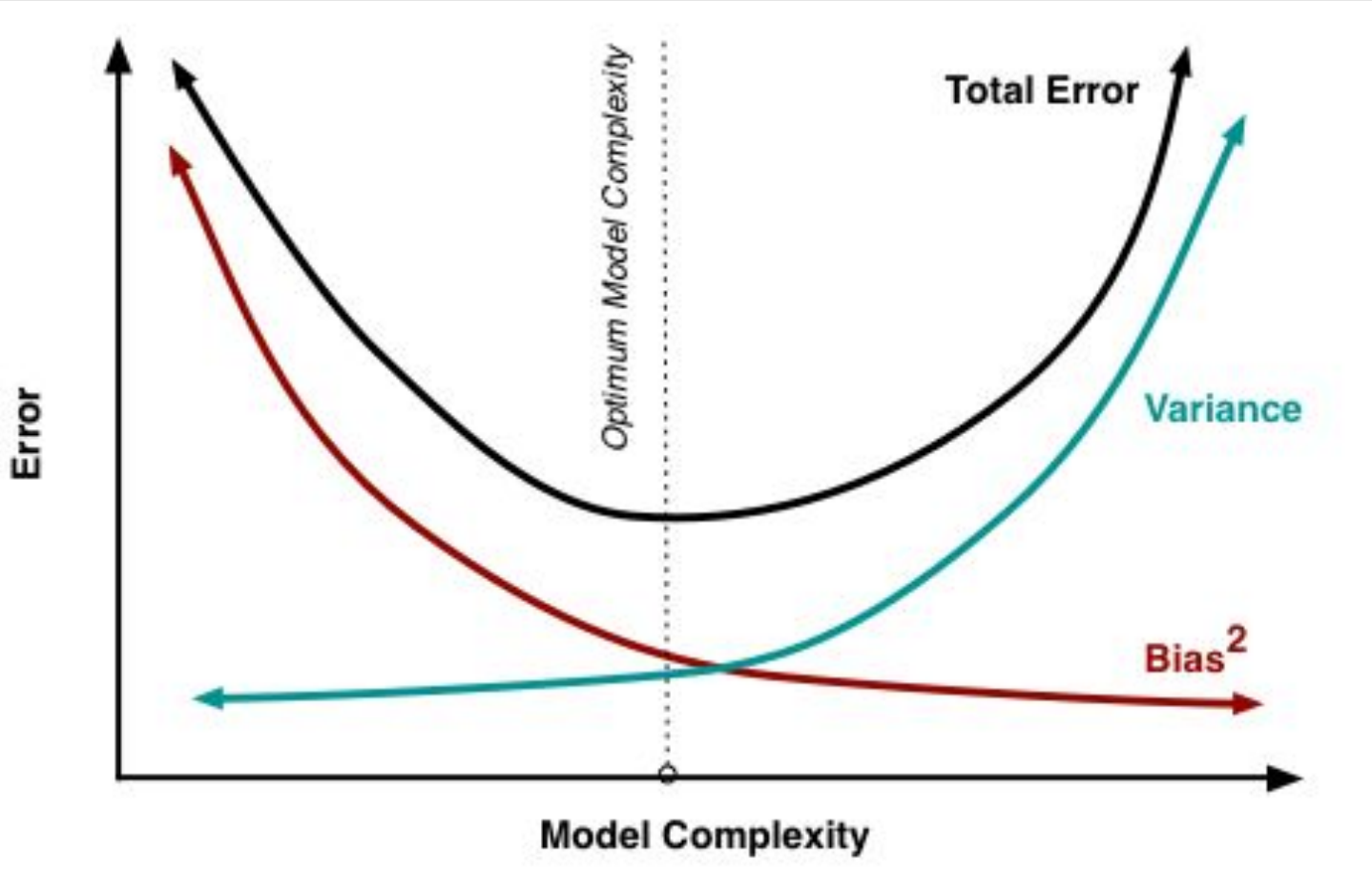
The variance of our model's prediction of $\mathbf{x_0}$ over all possible training sets

The difference between the true target and our model's average prediction over all possible training sets

$$\mathrm{Bias}(\hat{f}(x_0)) = E[\hat{f}(x_0)] - f(x_0)$$

The variance of the irreducible error.

The Bias/Variance Tradeoff



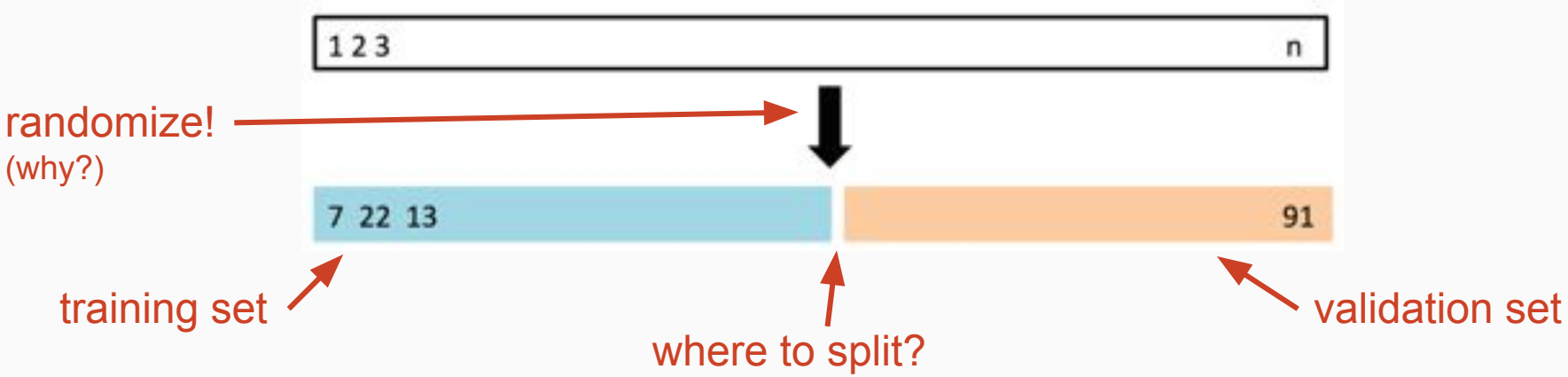
How is the **bias/variance tradeoff** related to **underfitting** and **overfitting**?

How can we find the best tradeoff point? I.e. The optimum model complexity

Cross-Validation

Main idea: **Don't use all your data for training.**

Instead: **Split your data into a "training set" and a "validation set".**



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Cross-Validation

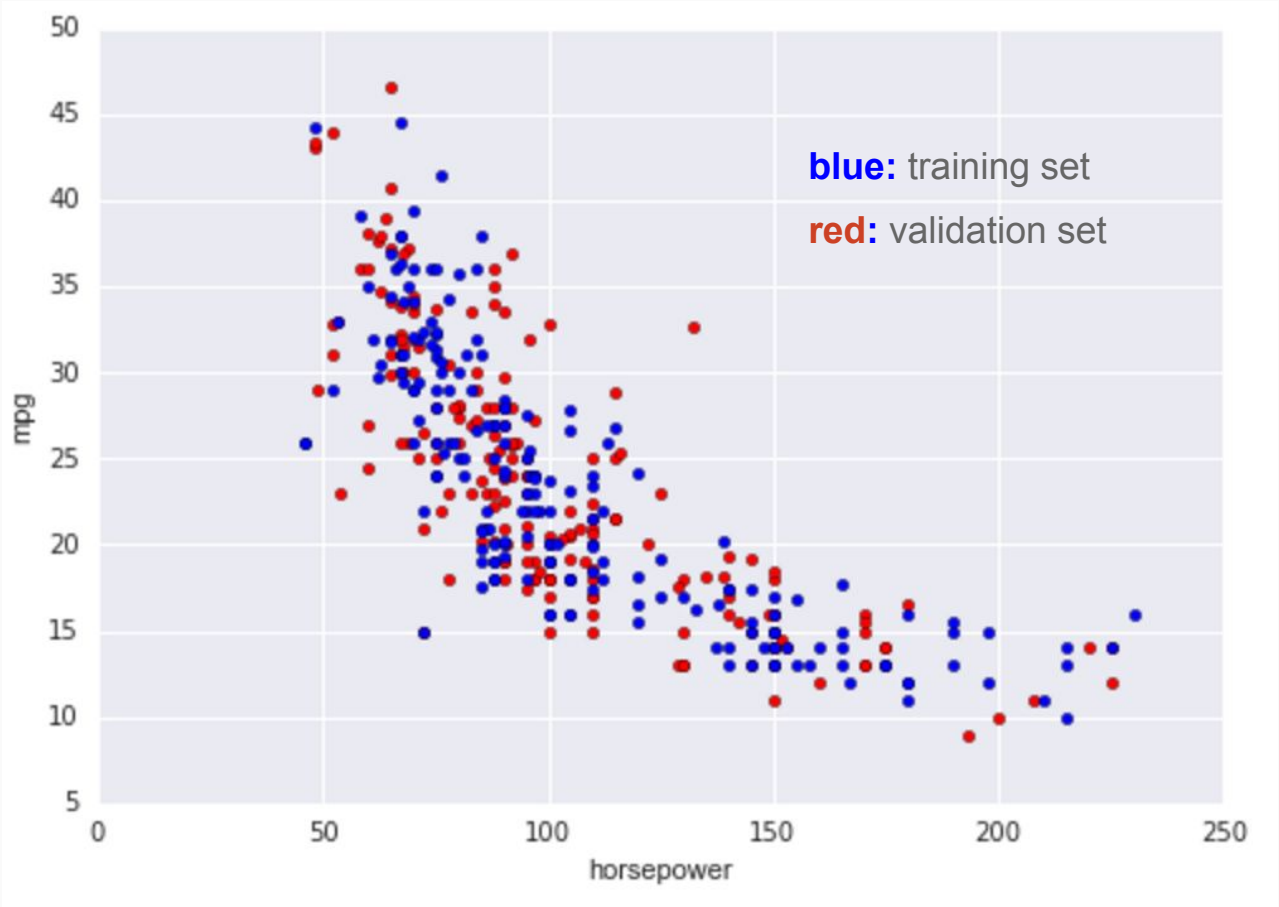
1. Split your data into training/validation sets.
   70/30 or 90/10 splits are commonly used

2. Use the training set to train several models of varying complexity.
   e.g. linear regression (w/ and w/out interaction features), neural nets, decision trees, etc.
   (we'll talk about hyperparameter tuning, grid search, and feature engineering later)

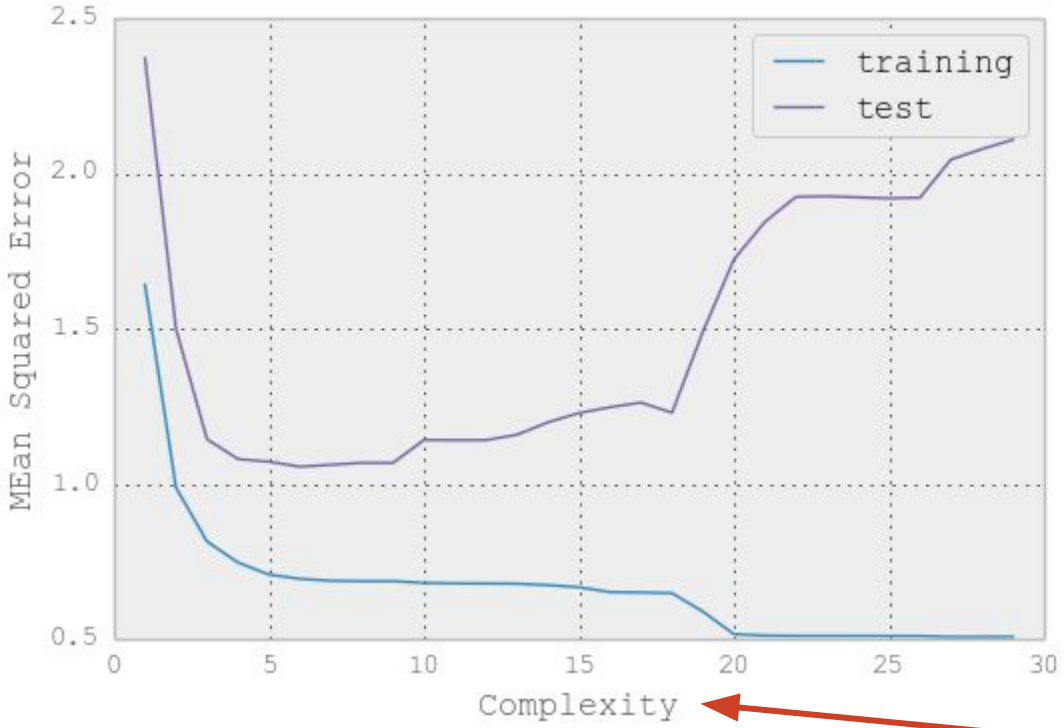
3. Evaluate each model using the validation set.
   calculate R^2, MSE, accuracy, or whatever you think is best

4. Keep the model that performs best over the **validation** set.

Let’s predict MPG from horsepower



Cross-Validation Example



You will see this shape all the time!

You will wrestle with the bias/variance tradeoff constantly...

E.g. linear regression w/ varying degree of polynomial

Recall our goal: Making accurate future predictions

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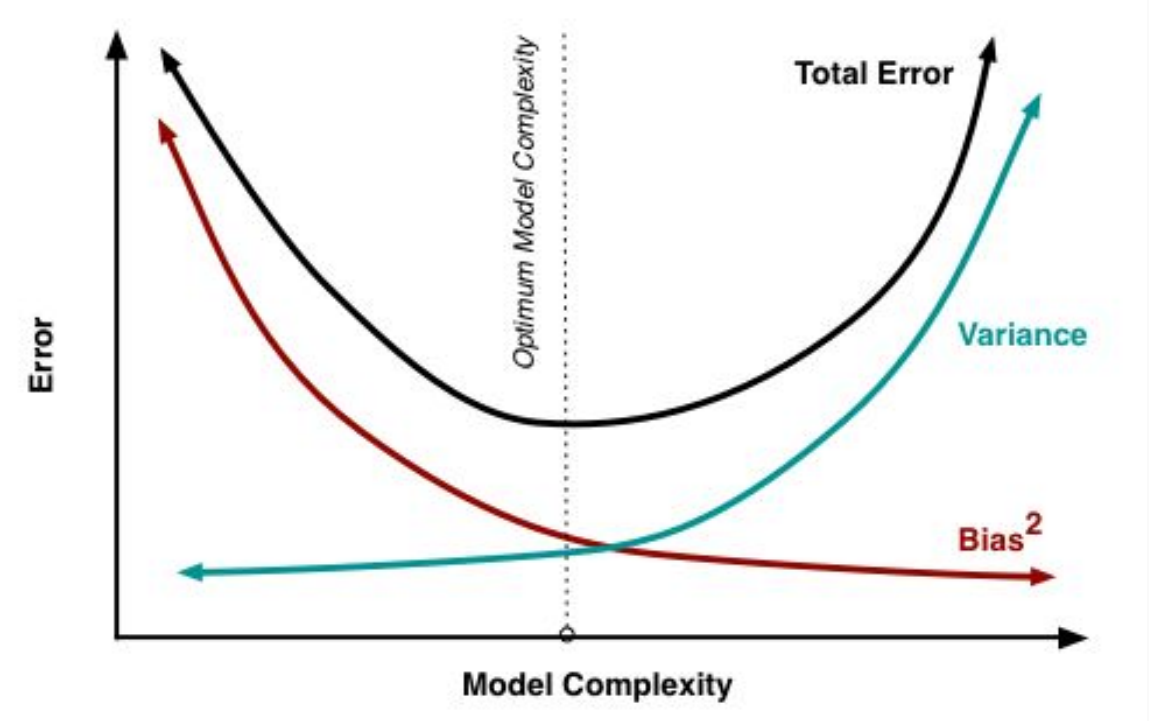
Fitting the training set perfectly is *easy*.
How?

Fitting future (unseen) data is *not easy*.

Cross validation helps us choose a model that performs well on unseen data.



k-Fold Cross-Validation

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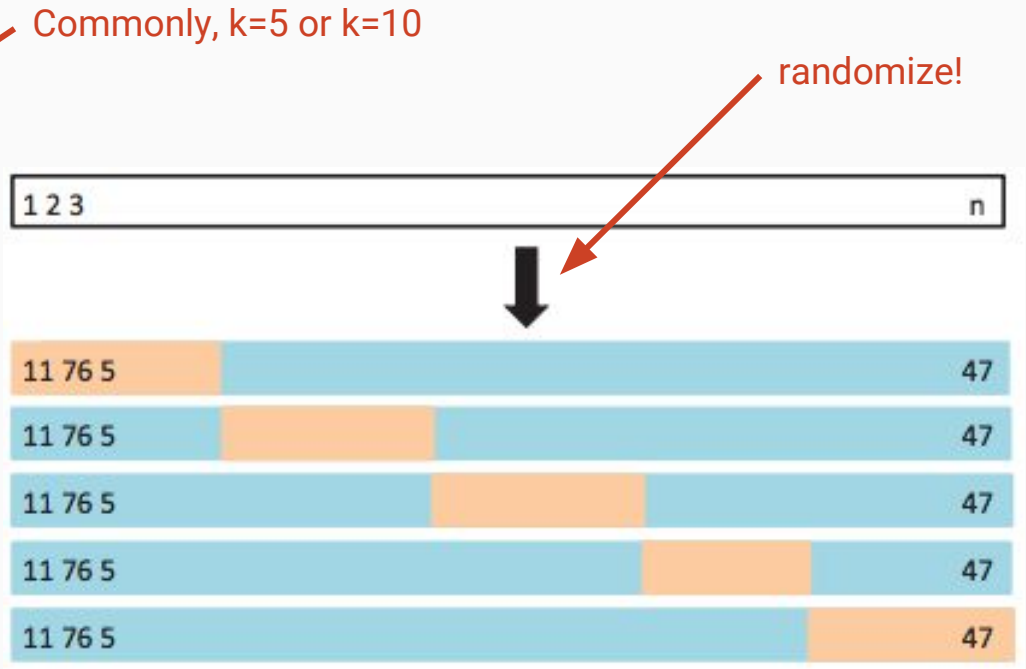
1. Split the dataset into k "folds".
2. Train using (k-1) folds. Validate using the one "leave out" fold. Record a validation metric such as RSS or accuracy.
3. Train *k* models, leaving out a different fold for each one.
4. Average the validation results.



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Example:

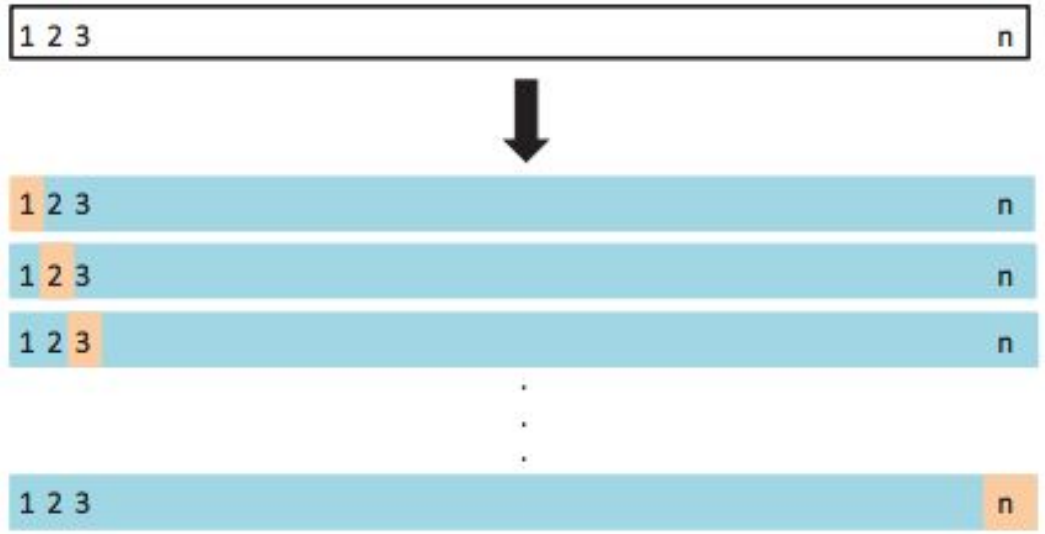
```
from sklearn.model_selection import KFold
import numpy as np

# Generate indices for k-fold selection
kf = KFold(m, n_folds = num_folds)
kf=KFold(n_splits=4, shuffle=True)

# Toy Data
X=np.array([[1,1,1,1],[2,2,2,2],[3,3,3,3],
    [4,4,4,4],[5,5,5,5]])
y=np.array([100,200,300,400,500])

for train_idx, test_idx in kf.split(X):
    X_train, X_test=X[train_idx],X[test_idx]
    y_train, y_test=y[train_idx],y[test_idx]
    print ('X train, X_test: ')
    print (X_train)
    print (X_test)
    print ('y_train, y_test: ')
    print (y_train, y_test)
```

Leave-one-out Cross-Validation

Assume we have *n* training examples.

A special case of k-fold CV is when k=n. This is called *leave-one-out cross-validation*.

Useful (only) if you have a tiny dataset where you can't afford a large validation set.



Overfitting in high dimensions is easy, even with simple models.

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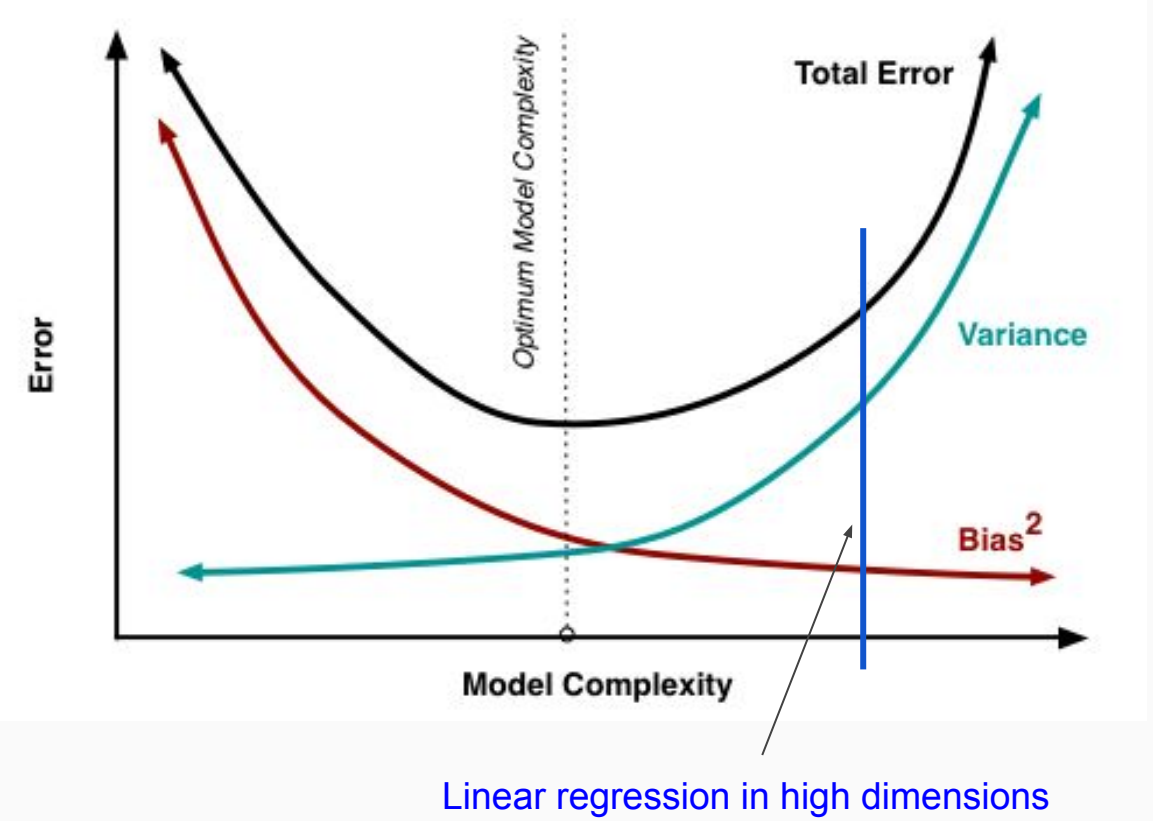
If our data has high dimensionality (many many predictors), then it becomes easy to overfit the data.

This is one result of the so-called **Curse of Dimensionality** (look it up).

Even linear regression might be too complex of a model for high dimensional data (and the smaller the dataset, the worse this problem is).



You have a few options.

1. Get more data… (not usually possible/practical)
2. **Subset Selection:** keep only a subset of your predictors (i.e, dimensions)
3. **Regularization:** restrict your model’s parameter space
4. **Dimensionality Reduction:** project the data into a lower dimensional space

Subset Selection

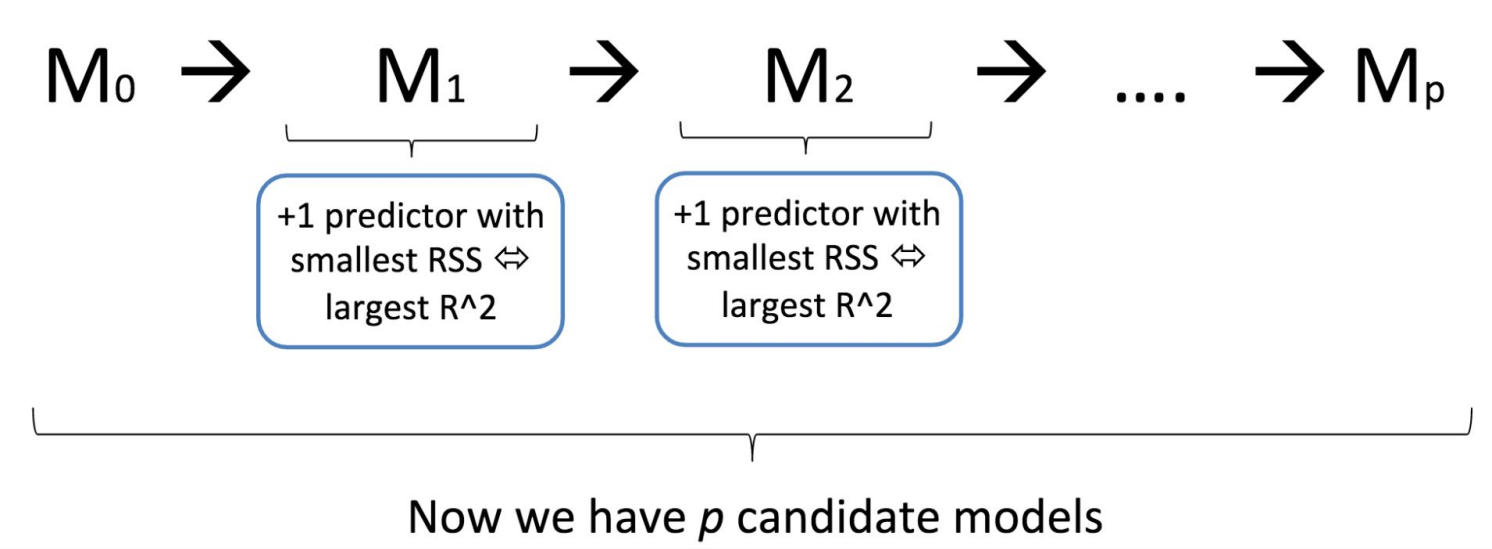
Best subset: Try every model. Every possible combination of *p* predictors

- Computationally intensive. 2^p possible subsets of *p* predictors
- High chance of finding a “good” model by random chance.

  … A sort-of monkeys-Shakespeare situation …

Stepwise: Iteratively pick predictors to be in/out of the final model.

- Forward, backward, forward-backward strategies



Are RSS and R^2 good ways to decide amongst the resulting *(p+1)* candidates?

Answer: Don't use RSS or R^2 for this part.
Use Mallow's C_p, or AIC, or BIC, or Adjusted R^2.

… or just use cross-validation with any error measurement.

Subset Selection: Comparing models of varying number of predictors...

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$$C_p = \frac{1}{n}(RSS + 2p\hat{\sigma}^2)$$

Mallow's Cp
p is the total # of parameters
$\hat{\sigma}^2$ is an estimate of the variance of the error, ε

$$AIC = -2logL + 2 \cdot p$$

L is the maximized value of the likelihood function for the model estimated

$$BIC = \frac{1}{n}(RSS + log(n)p\hat{\sigma}^2)$$

This is Cp, except 2 is replaced by log(n). log(n) > 2 for n>7, so BIC generally exacts a heavier penalty for more variables

$$Adjusted\ R^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$$

Similar to R^2, but pays price for more variables

Side Note: Can show AIC and Mallow's Cp are equivalent for linear case

Subset Selection: Comparing models of varying number of predictors...

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OLS Regression Results

Dep. Variable:	y	R-squared:	0.933
Model:	OLS	Adj. R-squared:	0.928
Method:	Least Squares	F-statistic:	211.8
Date:	Mon, 03 Nov 2014	Prob (F-statistic):	6.30e-27
Time:	14:45:06	Log-Likelihood:	-34.438
No. Observations:	50	AIC:	76.88
Df Residuals:	46	BIC:	84.52
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[95.0% Conf.	Int.]
x1	0.4687	0.026	17.751	0.000	0.416	0.522
x2	0.4836	0.104	4.659	0.000	0.275	0.693
x3	-0.0174	0.002	-7.507	0.000	-0.022	-0.013
const	5.2058	0.171	30.405	0.000	4.861	5.550

Omnibus:	0.655	Durbin-Watson:	2.896
Prob(Omnibus):	0.721	Jarque-Bera (JB):	0.360
Skew:	0.207	Prob(JB):	0.835
Kurtosis:	3.026	Cond. No.	221.

In groups of 2 or 3, try to give *your answer* to your partners:
What you think the bias and variance tradeoff means?

Why do we perform cross validation? (2-min)

Why is k-folds cross validation better than a single train-validation split? (2-min)

Why do we keep a completely separate test set? (2-min)

Regularized Linear Regression

Mark Llorente, Based on Previous Work of RH

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- Shortcomings of Ordinary Linear Regression
- Ridge Regression
- Lasso Regression
- When to use each!

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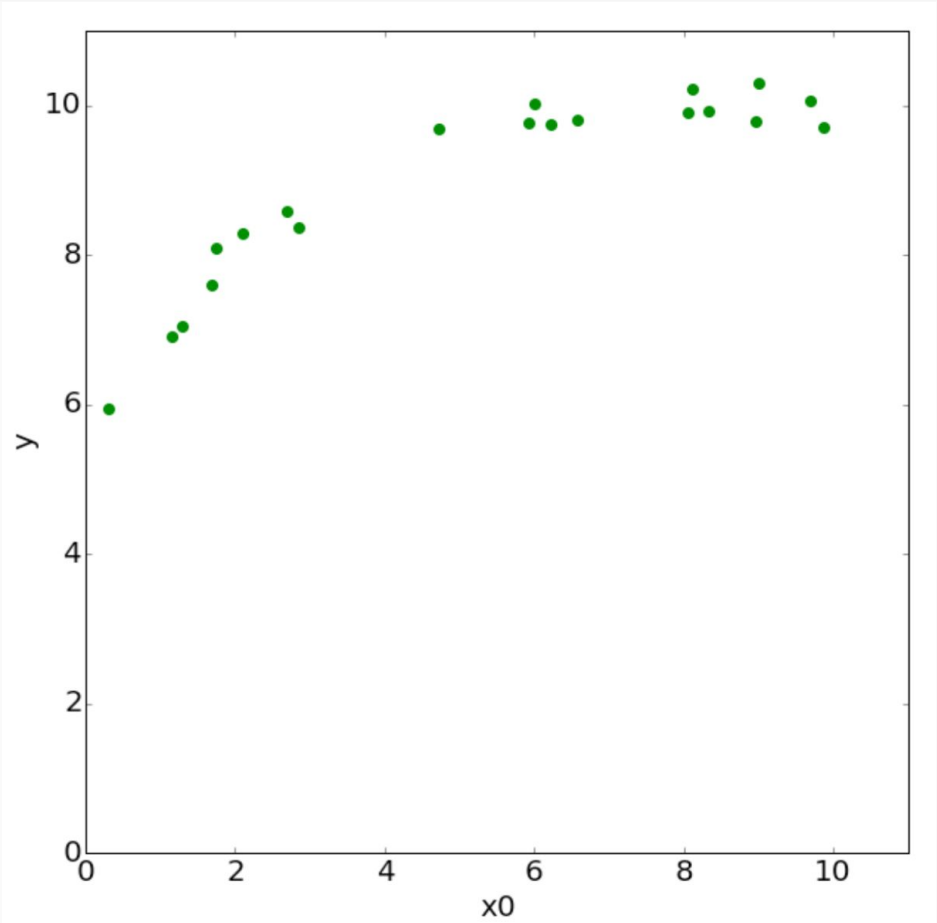
Linear Regression Example

Data: 20 examples x 10 features

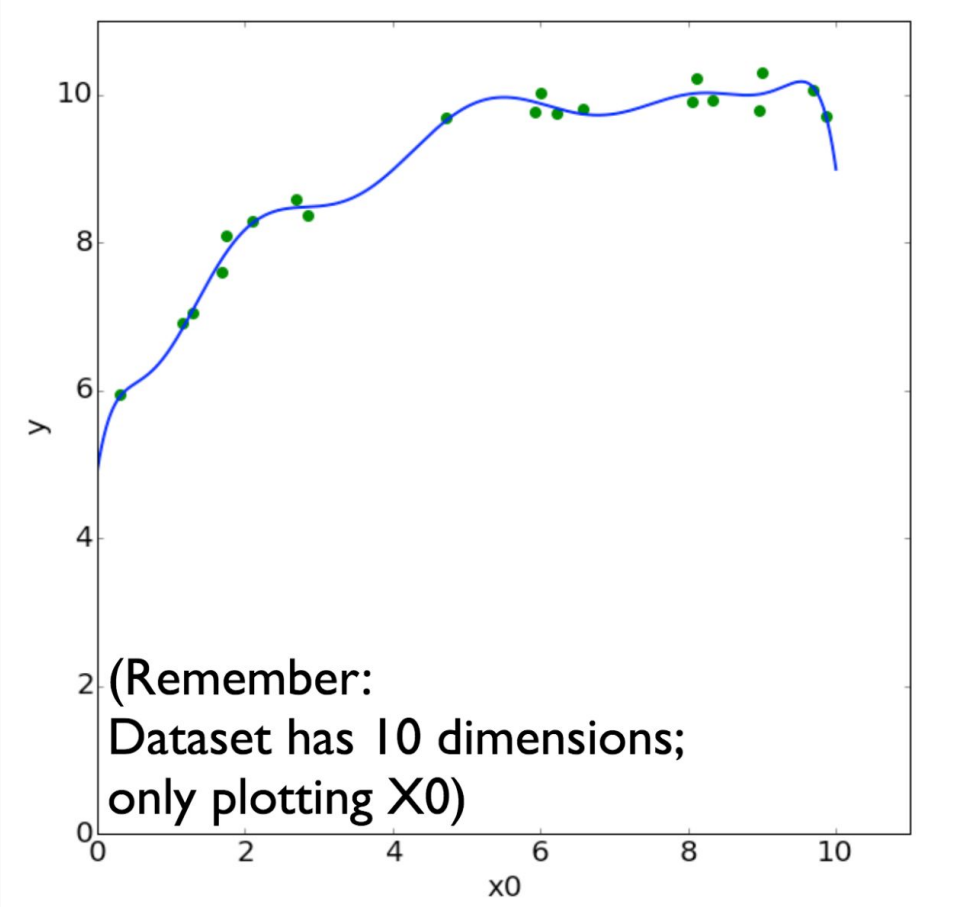
Predict: *y*

y	x0	x1	x2	x3	...
9.92	8.33	69.39	578.0	4815.	...
8.58	2.69	7.26	19.54	52.64	...
8.07	1.75	3.06	5.35	9.36	...
8.29	2.11	4.46	9.41	19.86	...
...	...	...	...	...	...

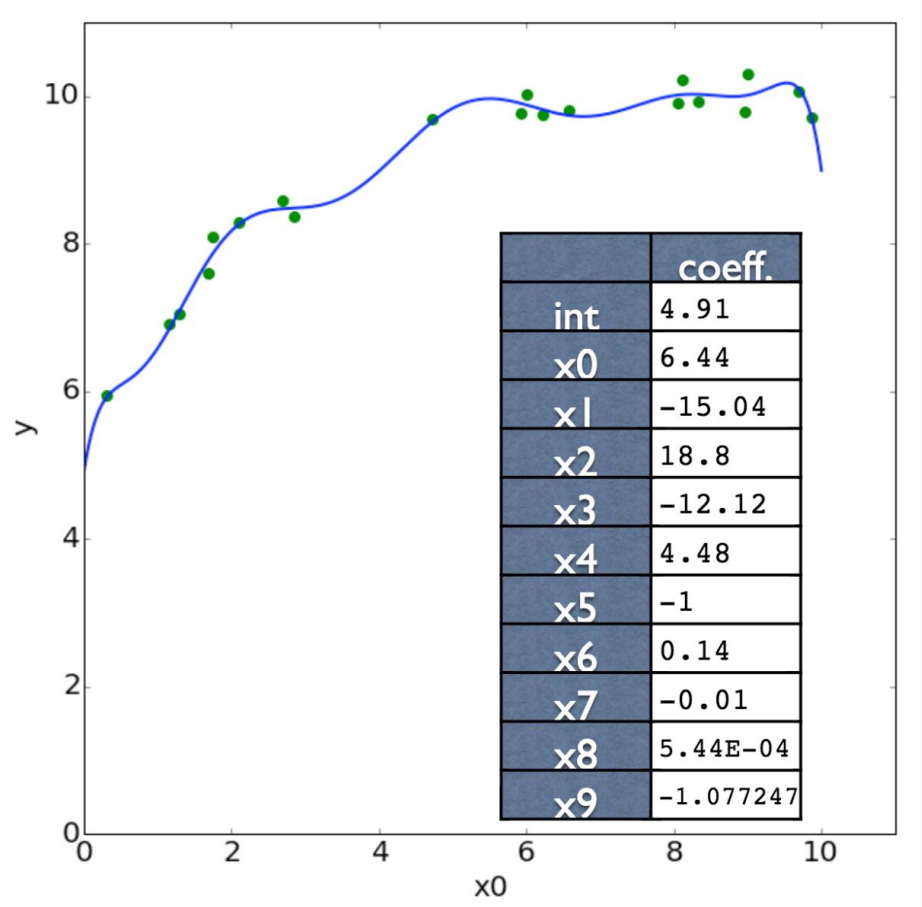
Linear Regression Example (x0 vs y)



Linear Regression Example (x0 vs y, model over all features)

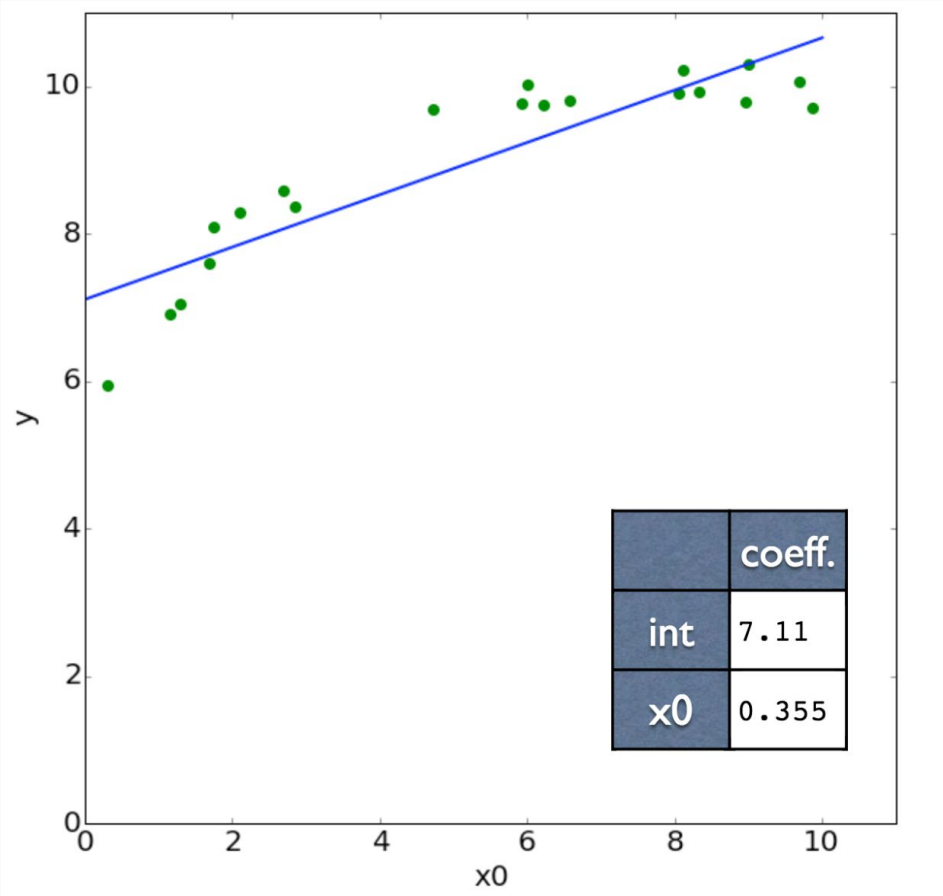


Linear Regression Example (x0 vs y, model over all features)



	coeff.
int	4.91
x0	6.44
x1	-15.04
x2	18.8
x3	-12.12
x4	4.48
x5	-1
x6	0.14
x7	-0.01
x8	5.44E-04
x9	-1.077247

Linear Regression Example (x0 vs y, model over only x0 features)



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In high dimensions, data is (usually) sparse

Again… the **Curse of Dimensionality** bites us.
(we'll talk more about this is a later lecture)

Linear regression can have high variance (i.e. tends to overfit) on high dimensional data…
We'd like to restrict ("normalize", or "regularize") the model so that it has less variance.

Take the 20 example x 10 feature dataset as an example… when we fit over all features, the complexity of the model grew dramatically.
(and keep in mind, some datasets have thousands of features)

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Linear Regression (another review)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

We estimate the model parameters by minimizing:

$$\sum_{i=1}^{N} (y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij} \hat{\beta}_j)^2$$

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Ridge Regression
(Linear Regression w/ Tikhonov (L2) Regularization)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

(same as before)

We estimate the model parameters by minimizing:

$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$$

(the “regularization” parameter)

(new term!)

Ridge Regression

$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$$

What if we set the lambda equal to zero?

What does the new term accomplish?

What happens to a features whose corresponding coefficient value (beta) is zero?

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Ridge Regression

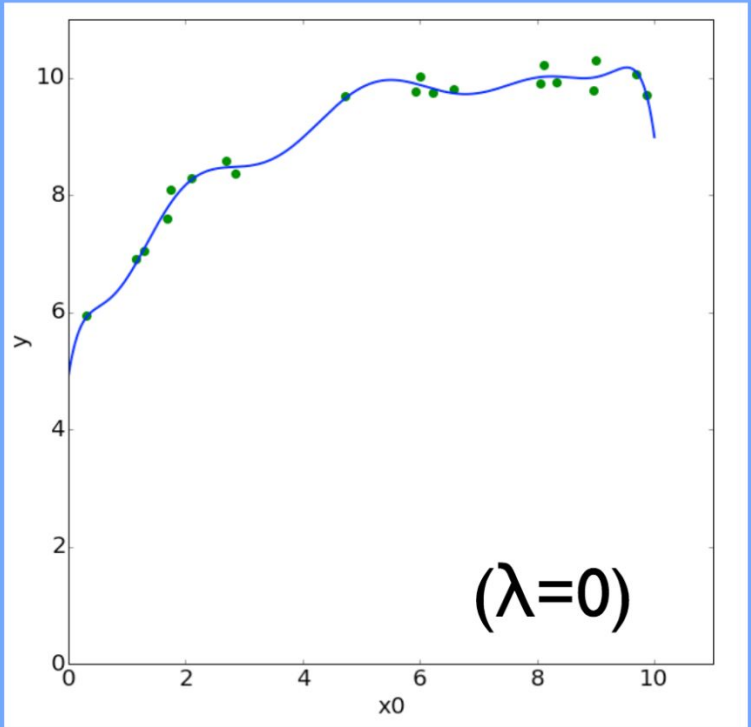
$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$$

Notice, we do not penalize B_0.

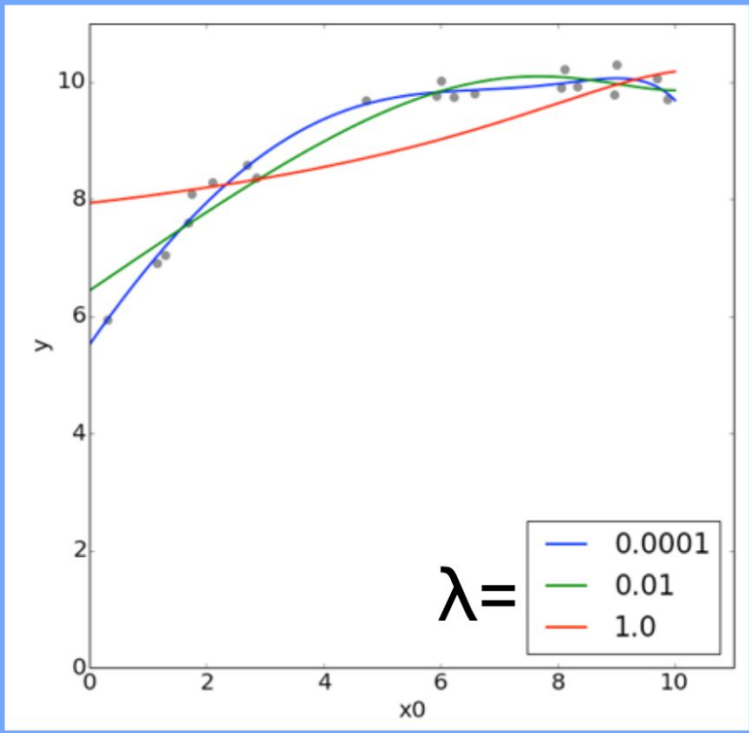
Changing lambda changes the amount that large coefficients are penalized.

Increasing lambda increases the model's bias and decreases its variance. ← this is cool!

Linear Regression



Ridge Regression



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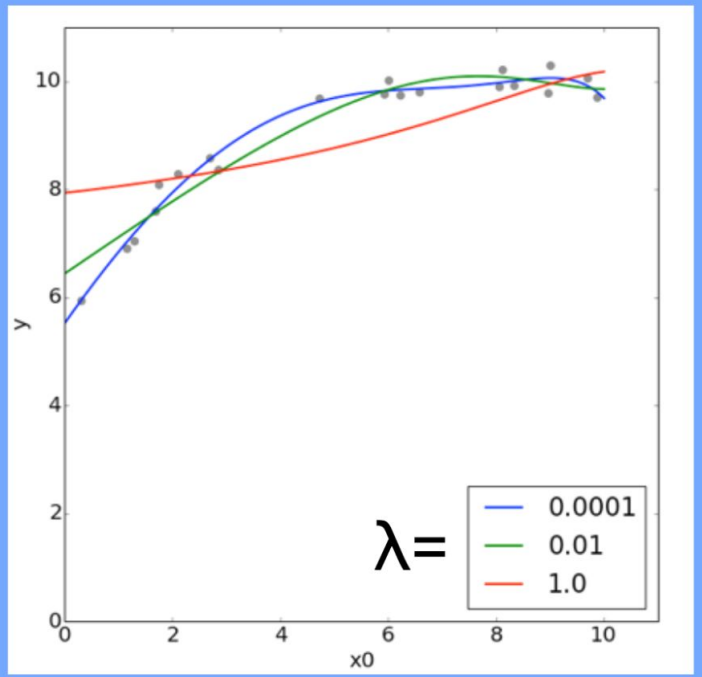
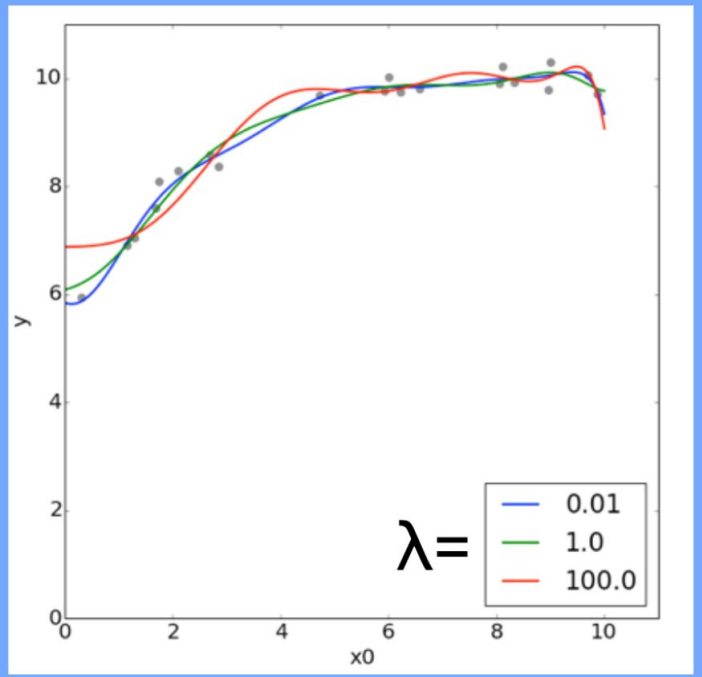
Normalized Data



Non-Normalized Data



Single value for λ assumes features are on the same scale!!

LASSO Regression
(Linear Regression w/ LASSO (L1) Regularization)

We model the world as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_p X_p + \epsilon$$

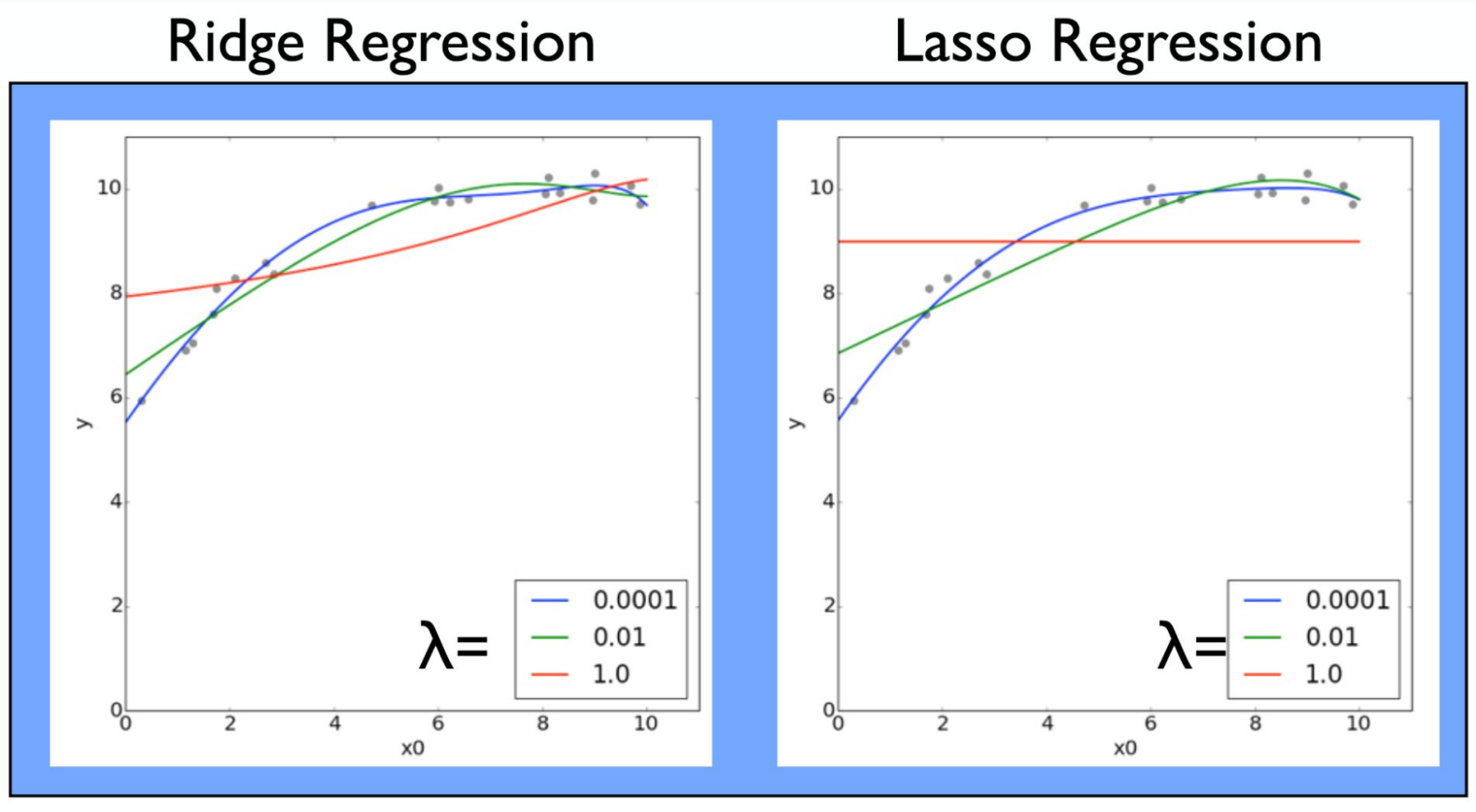
(same as before)

We estimate the model parameters to minimizing:

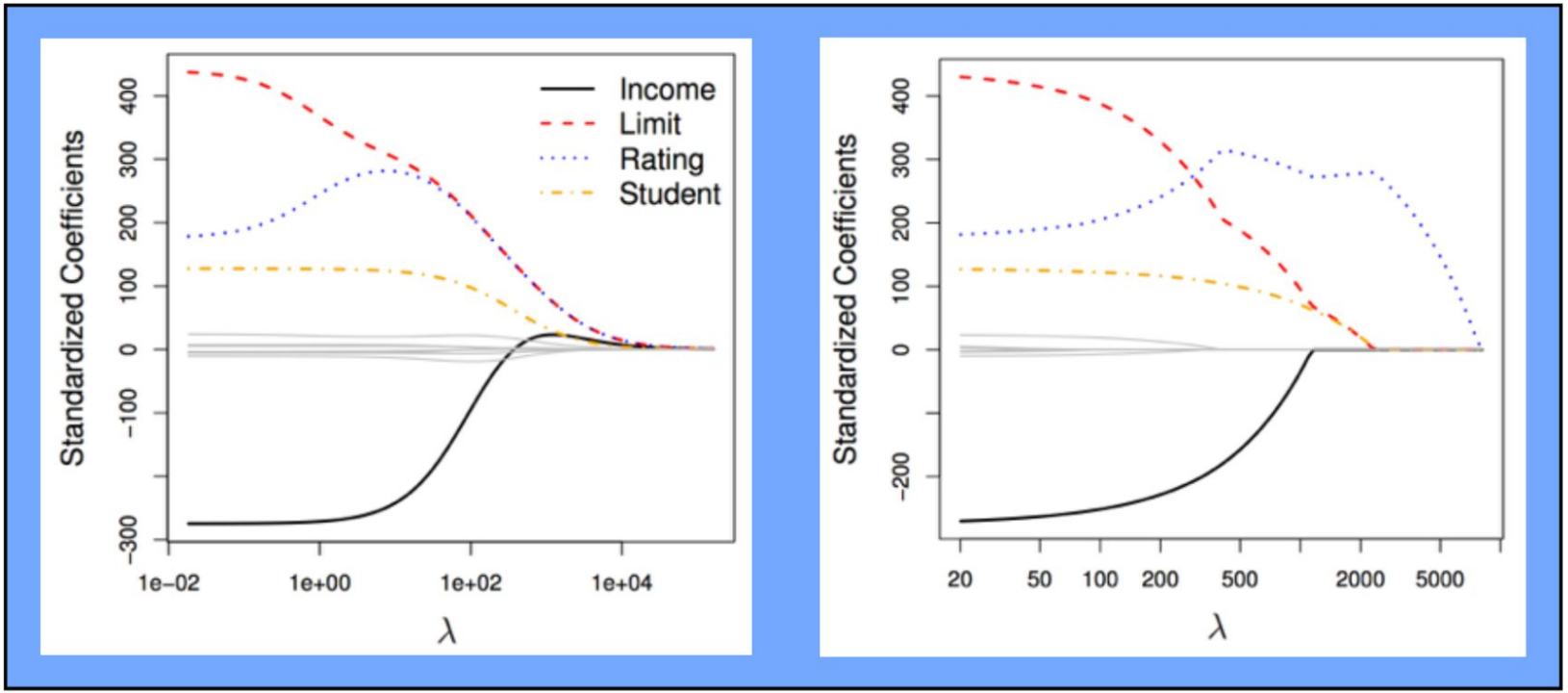
$$\sum_{i=1}^{N}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ij}\hat{\beta}_j)^2 + \lambda \sum_{i=1}^{p} |\hat{\beta}_i|$$

(the “regularization” parameter)

(absolute value instead of squared)


Ridge Regression
Lasso Regression
y
x0
λ=
0.0001
0.01
1.0

Ridge vs. Lasso

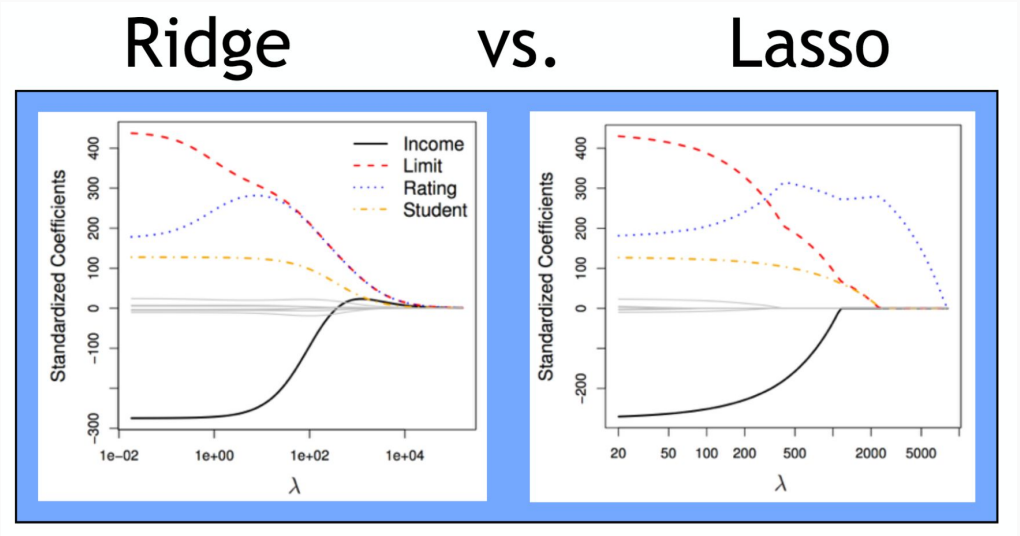


Ridge vs LASSO

- Ridge forces parameters to be small + Ridge is computationally easier because it is differentiable
- Lasso tends to set coefficients exactly equal to zero
  - This is useful as a sort-of “automatic feature selection” mechanism,
  - leads to “sparse” models, and
  - serves a similar purpose to stepwise features selection

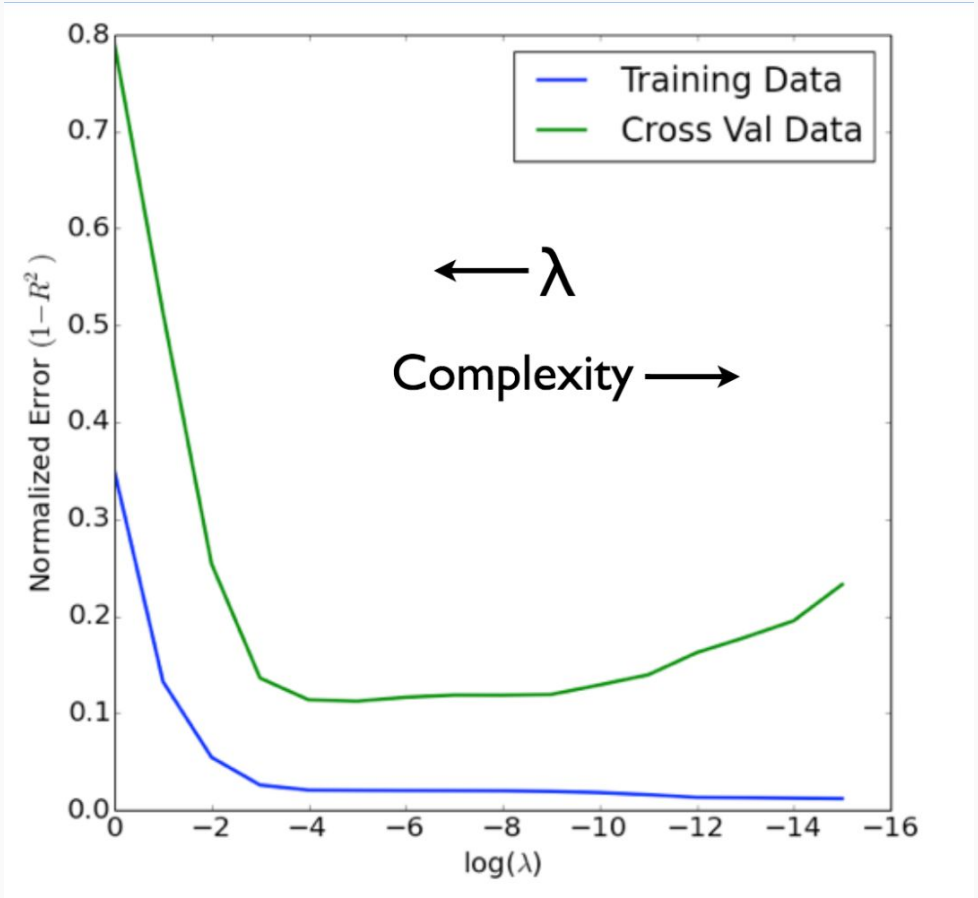
Which is better depends on your dataset!

True sparse models will benefit from lasso; true dense models will benefit from ridge.



- Jupyter Notebook Time!

Chose lambda via Cross-Validation



scikit-learn

Classes:

- sklearn.linear_model.**LinearRegression**(...)
- sklearn.linear_model.**Ridge**(alpha=my_alpha, ...)
- sklearn.linear_model.**Lasso**(alpha=my_alpha, ...)

All have these methods:

- fit(X, y)
- predict(X)
- score(X, y)