CSE/STAT 416

Cross Validation; Ridge Regression

Pre-Class Videos (lecture slides below)

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University of Washington
June 26, 2024

Bias-Variance Tradeoff

Tradeoff between bias and variance:

Simple models: High bias + Low variance

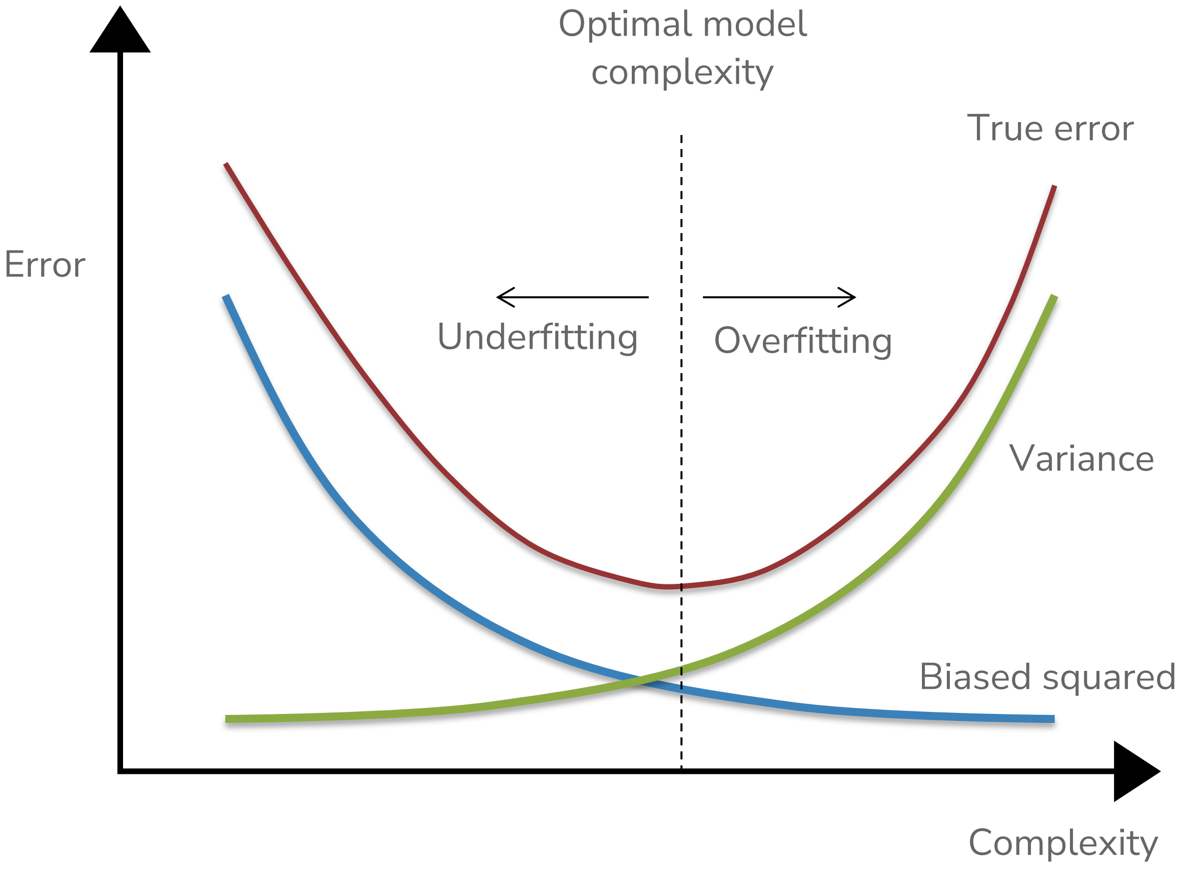
Complex models: Low bias + High variance

Source of errors for a particular model $\hat{f}$ using MSE loss function:

$$\mathbb{E}[(y - \hat{f}(x))^2] = \mathrm{bias}[\hat{f}(x)]^2 + \mathrm{var}(\hat{f}(x)) + \sigma_\epsilon^2$$

Error = Biased squared + Variance + Irreducible Error

Bias – Variance Tradeoff



Dataset Size

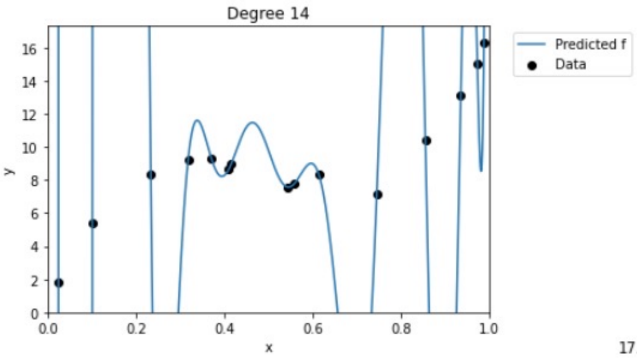
So far our entire discussion of error assumes a fixed amount of data. What happens to our error (true error and training error) as we get more data?

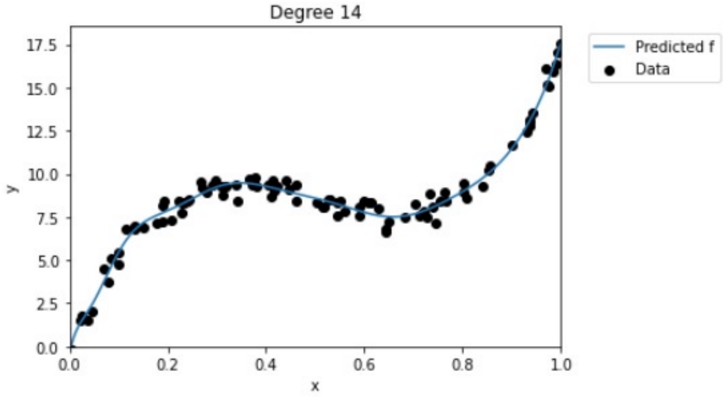
Error
Size of train set

Dataset Size

Model complexity doesn't depend on the size of the training set

The larger the training set, the lower the variance of the model, thus less overfitting





Demo

Bias-Variance Tradeoff

Training a linear regression model in Python

Observing the effect of the bias-variance tradeoff as compared to model complexity

Brain Break

Choosing Complexity

Choosing Complexity

So far we have talked about the affect of using different complexities on our error. Now, how do we choose the right one?

Poll Everywhere

Think

1 min

pollev.com/cs416

Suppose I wanted to figure out the right degree polynomial for my dataset (we'll try p from 1 to 20). What procedure should I use to do this? Pick the best option

For each possible degree polynomial p:

- Train a model with degree p on the training set, pick p that has the lowest test error
- Train a model with degree p on the training set, pick p that has the highest test error
- Train a model with degree p on the test set, pick p that has the lowest test error
- Train a model with degree p on the test set, pick p that has the highest test error
- None of the above

Poll Everywhere

Think

2 min

pollev.com/cs416

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Train a model with degree p on the test set, pick p that has the highest test error

None of the above

Choosing Complexity

We can't just choose the model that has the lowest **train** error because that will favor models that overfit!

It then seems like our only other choice is to choose the model that has the lowest **test** error (since that is our approximation of the true error)

> This is almost right. However, the test set has been **tampered**, thus is no longer is an unbiased estimate of the true error.
>
> We didn't technically train the model on the test set (that's good), but we chose **which model** to use based on the performance of the test set.
>
> - It's no longer a stand in for "the unknown" since we probed it many times to figure out which model would be best.

NEVER EVER EVER touch the test set until the end. You only use it ONCE to evaluate the performance of the best model you have selected during training.

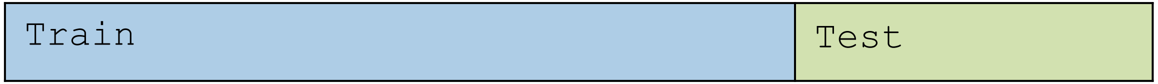
Choosing Complexity

We will talk about two ways to pick the model complexity without ruining our test set.

- Using a validation set
- Doing (k-fold) cross validation

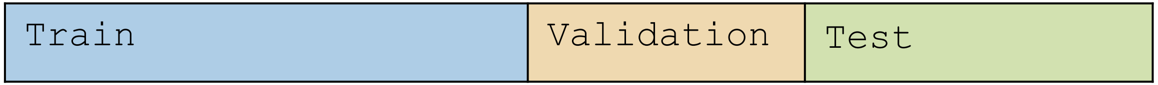
Validation Set

So far we have divided our dataset into train and test



Train Test

We can’t use Test to choose our model complexity, so instead, break up Train into ANOTHER dataset



Train Validation Test

We will pick the model that does best on validation. Note that this now makes the validation error of the “best” model a biased estimate of true error. The test error will be an unbiased estimate though since we never looked at it!

Validation Set

The process generally goes

```
train, validation, test = random_split(dataset)
for each model complexity p:
    model = train_model(model_p, train)
    val_err = error(model, validation)
    keep track of p and model with smallest val_err
return best p & error(model, test)
```

Validation Set

Pros

Easy to describe and implement

Pretty fast

- Only requires training a model and predicting on the validation set for each complexity of interest

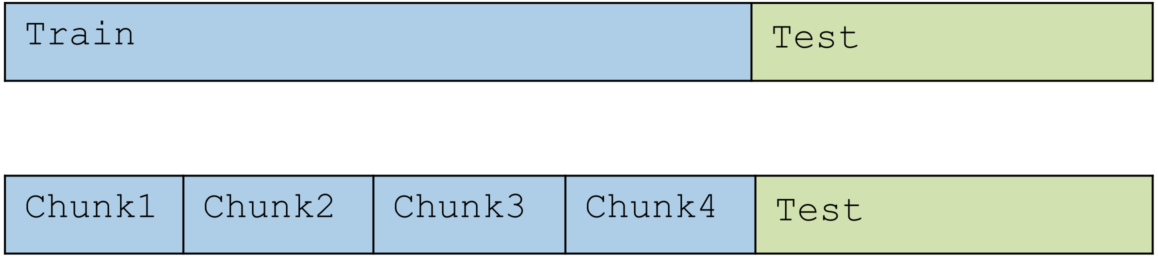
Cons

- Have to sacrifice even more training data
- Prone to overfitting*

Cross-Validation

Clever idea: Use many small validation sets without losing too much training data.

Still need to break off our test set like before. After doing so, break the training set into k chunks.



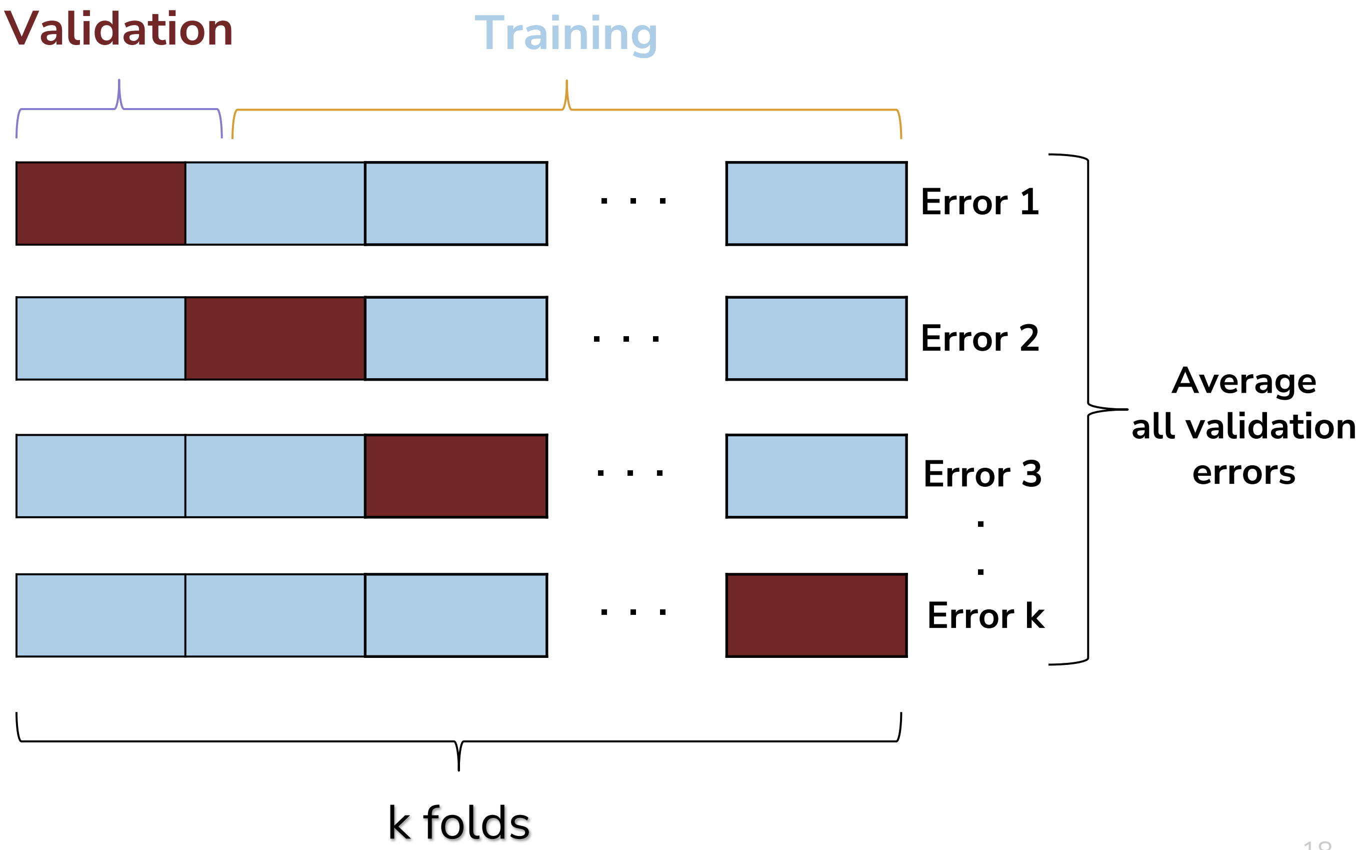
Train | Test

Chunk1 | Chunk2 | Chunk3 | Chunk4 | Test

For a given model complexity, train it k times. Each time use all but one chunk and use that left out chunk to determine the validation error.

Cross Validation

For a set of hyperparameters, perform Cross Validation on k folds



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Cross-Validation

Pros

- Prevent overfitting: By training the model on multiple folds instead of only 1 training set, this learns the model with the best generalization capabilities.
- Don’t have to actually get rid of any training data!

Cons

- Slow. For each model selection, we have to train k times
- Very computationally expensive

Cross-Validation

Generally, the more folds you use the better as you aren’t relying on the specifics of a single validation fold.

Theoretical best estimator* is to use $k = n$

- Called "**Leave One Out Cross Validation**” (LOOCV)

In practice, people use $k = 5$ to 10 for computational simplicity

Recap

Theme: Assess the performance of our models

Ideas:

Model complexity

Train vs. Test vs. True error

Overfitting and Underfitting

Bias-Variance Tradeoff

Error as a function of train set size

Choosing best model complexity

- Validation set
- Cross Validation

Pre-Class Video 1:

Cross Validation

Validation Set

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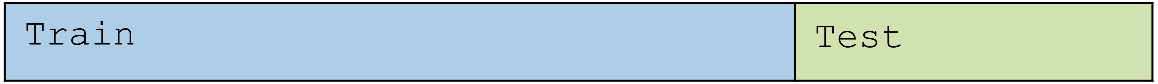

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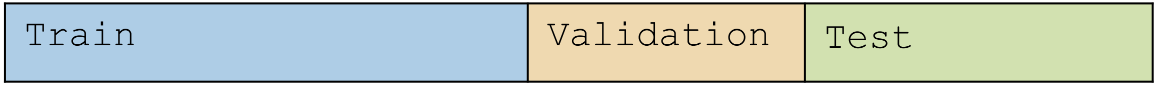

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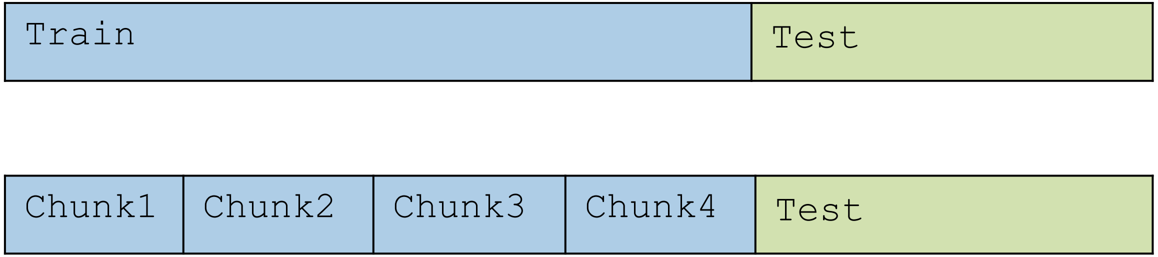

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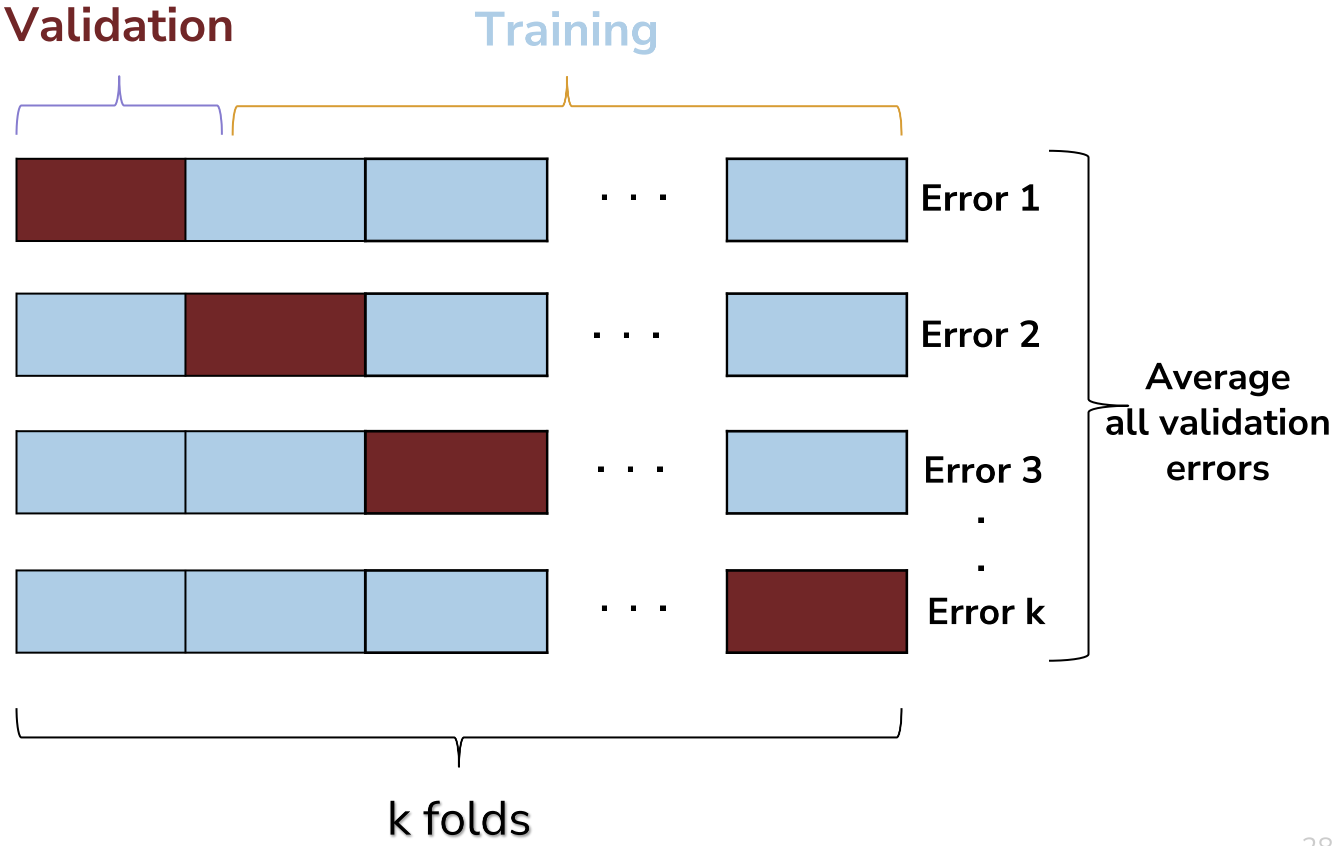

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Cross-Validation

What size of k?

Theoretical best estimator is to use $k = n$

- Called "Leave One Out Cross Validation”

In practice, people use $k = 5$ to 10.

Pre-Class Video 1:

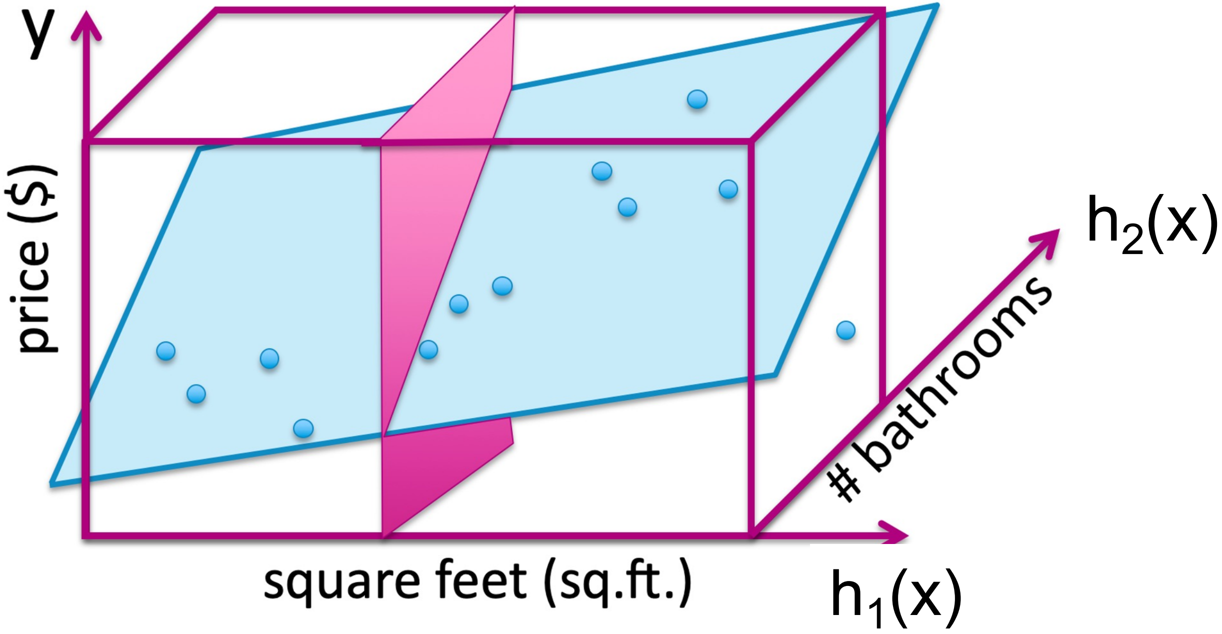
Cross Validation

Interpreting Coefficients

Interpreting Coefficients – Multiple Linear Regression

$$\hat{y} = \hat{w}_0 + \hat{w}_1 h_1(x) + \hat{w}_2 h_2(x)$$

Fix



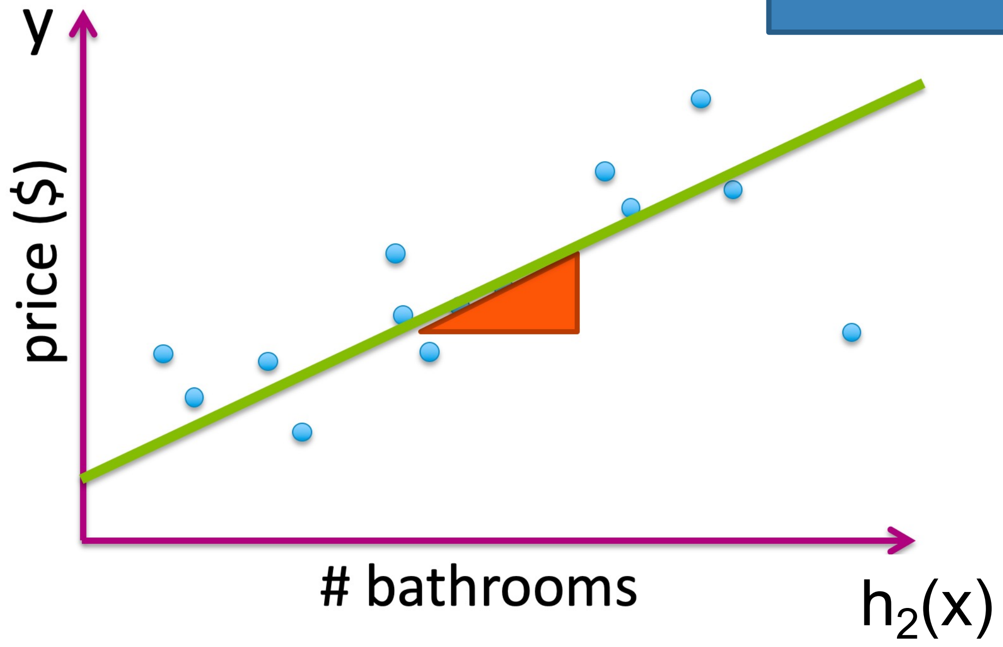
Interpreting Coefficients

Interpreting Coefficients – Multiple Linear Regression

$$\hat{y} = \hat{w}_0 + \hat{w}_1 h_1(x) + \hat{w}_2 h_2(x)$$

Fix

Holding $h_1(x)$ fixed!



Interpreting Coefficients

This also extends for multiple regression with many features!

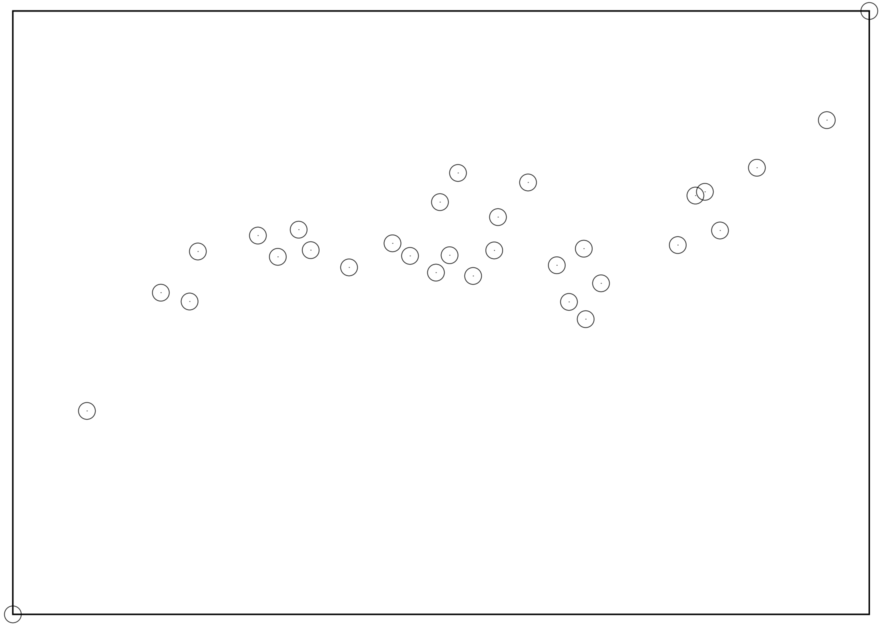
$$\hat{y} = \hat{w}_0 + \sum_{j=1}^{D} \hat{w}_j h_j(x)$$

Interpret $\hat{w}_j$ as the change in y per unit change in $h_j(x)$ if all other features are held constant.

This is generally not possible for polynomial regression or if other features use same data input!

Can't "fix" other features if they are derived from same input.

Overfitting

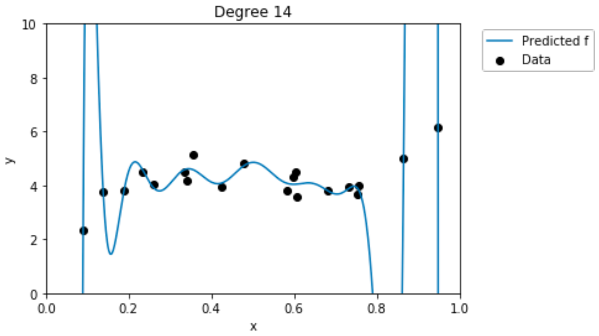


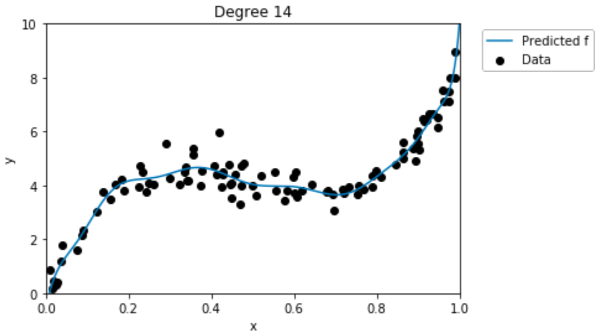
Often, overfitting is associated with very large estimated parameters $\hat{w}$!

Number of Features

Overfitting is not limited to polynomial regression of large degree. It can also happen if you use a large number of features!

Why? Overfitting depends on whether the amount of data you have is large enough to represent the true function's complexity.





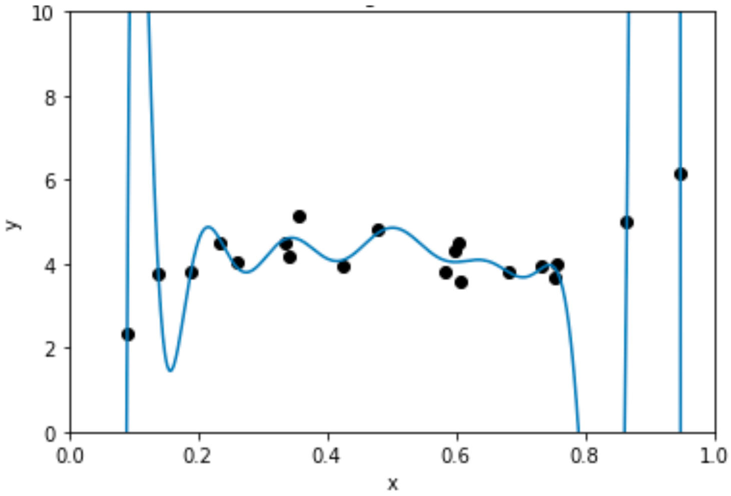
Number of Features

How do the number of features affect overfitting?

1 feature

Data must include representative example of all $(h_1(x), y)$ pairs to avoid overfitting

HARD



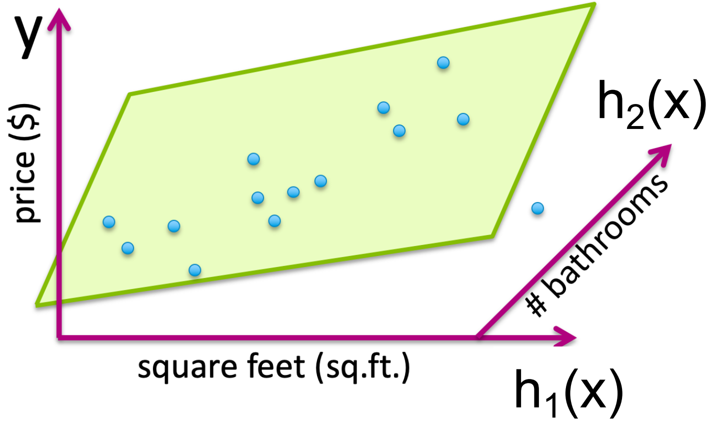
Number of Features

How do the number of features affect overfitting?

D features

Data must include representative example of all $\big((h_1(x), h_2(x), \ldots, h_D(x)\ ), y\big)$ combos to avoid overfitting!

MUCH HARDER!!



Introduction to the **Curse of Dimensionality**.
We will come back to this later in the quarter!

Prevent Overfitting

Last time, we **trained multiple models**, using cross validation / validation set, to find one that was less likely to overfit

For selecting polynomial degree, we train p models.

For selecting which features to include, we'd have to train ____ models!

Can we **train one model** that isn't prone to overfitting in the first place?

Big Idea: Have the model self-regulate to prevent overfitting by making sure its coefficients don't get ”too large”

This idea is called **regularization**.

CSE/STAT 416

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❓ **Questions?** Raise hand or **sli.do #cs416**
💬 **Before Class:** What is your favorite coffee/tea/boba/beverage shop near campus?
🎵 **Listening to:** [Sammy Rae & The Friends]()

Administrivia

HW0 due today, late due Friday night at 11:59 pm on Ed and Gradescope

- See late day policy if you need more time

Office Hours (see schedule on website) started this week

- make use of those
- Longer wait times closer to assignment due dates

Ed Discussion Board

- Respond to other student’s questions and in Megathread
- Post privately if you’re question is very detailed to your answer
- Do not post solutions to assignments publicly

Learning Reflection specifications are constant week-to-week, so you can start building LR1 now even if the turn in isn’t open yet!

HW1 Walkthrough

Recap

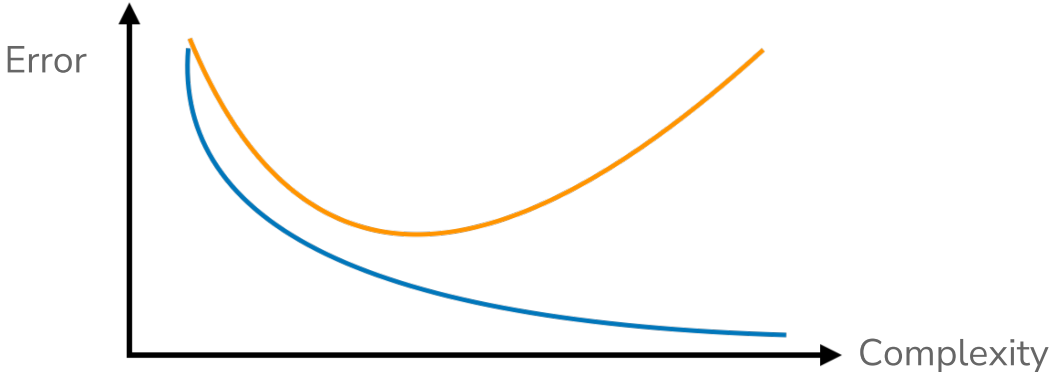
Overfitting

Overfitting happens when we too closely match the training data and fail to generalize.

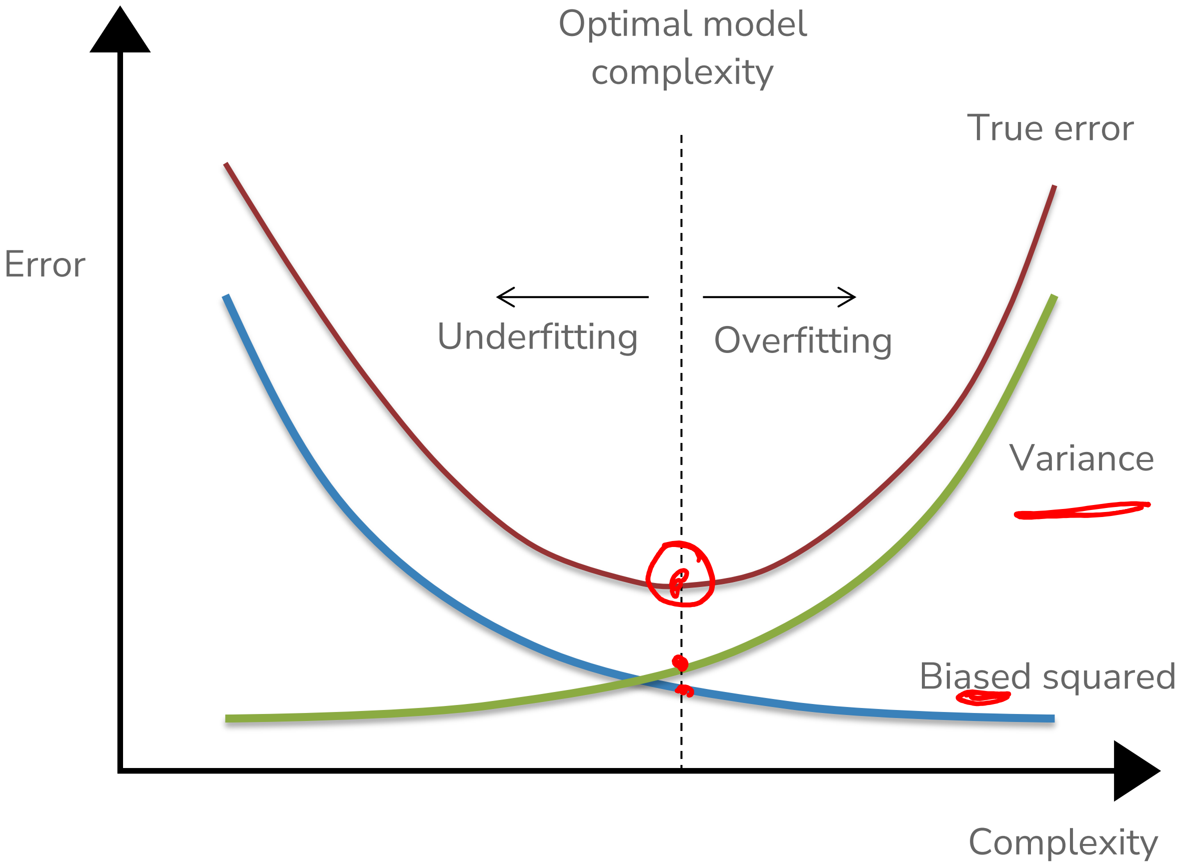
Overfitting occurs when you train a predictor $\hat{w}$ but there exists another predictor w' from the same model class such that:

$$error_{true}(w') < error_{true}(\hat{w})$$

$$error_{train}(w') > error_{train}(\hat{w})$$



Bias – Variance Tradeoff



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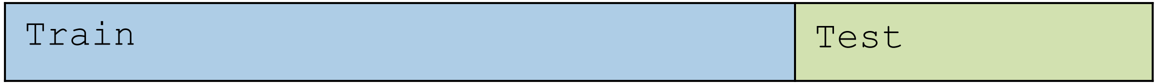

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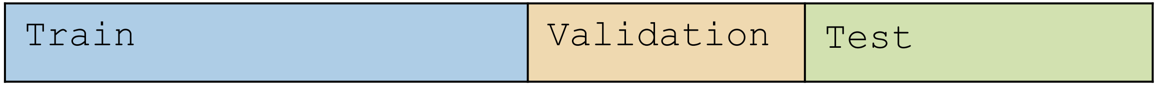

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Cross Validation

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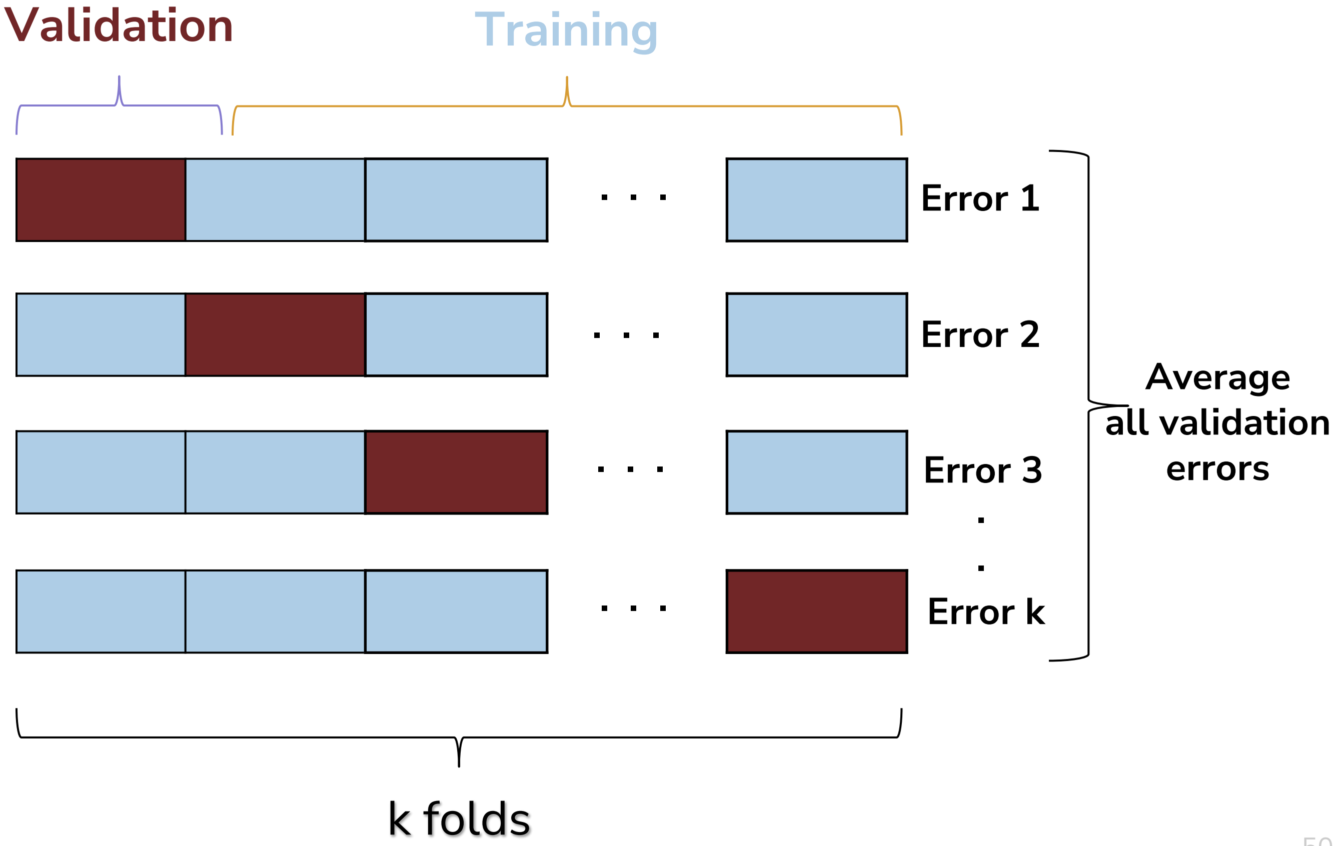

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slido

Think

1 min

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Say we are testing p different polynomial degrees, using the pseudocode for k-fold cross-validation.

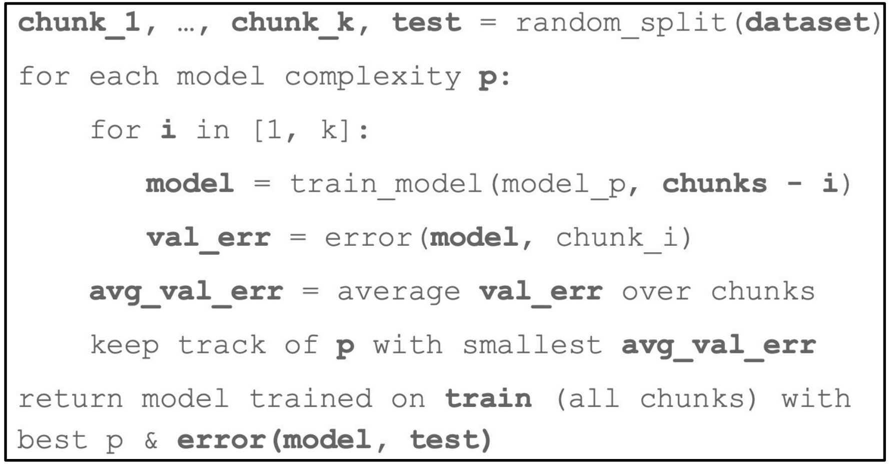
How many models would we train?

a) pk

b) $p(k-1)$

c) p^k

[✓ d) $\underline{pk} + \boxed{1}$]



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Group

1 min

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How many models would we train?

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d) $pk+1$

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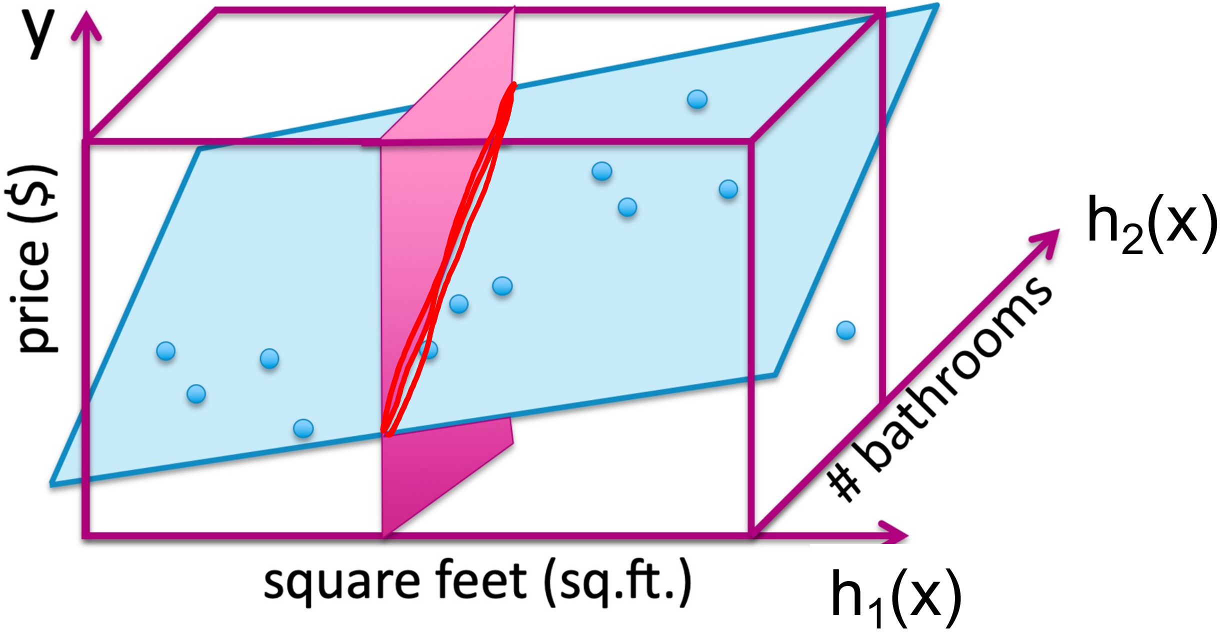
Coefficients and Overfitting

Interpreting Coefficients

Interpreting Coefficients – Multiple Linear Regression

$$\hat{y} = \hat{w}_0 + \hat{w}_1 h_1(x) + \hat{w}_2 h_2(x)$$

Fix



Overfitting

$w_1 h_1(x)$

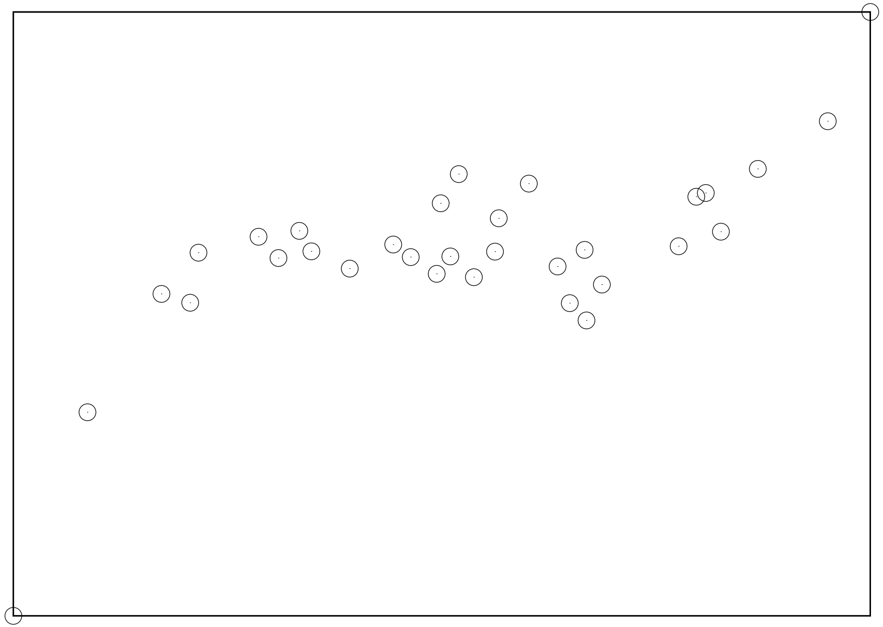
$x : 1$

$=$

1m

0.1

100k



Often, overfitting is associated with very large estimated parameters $\hat{w}$!

slido

Group

2 Minutes

sli.do #cs416

What characterizes overfitting?

([✓ Low] / High) Train Error, **(Low / [✓ High])** Test Error

([✓ Low] / High) Bias, **(Low / [✓ High])** Variance

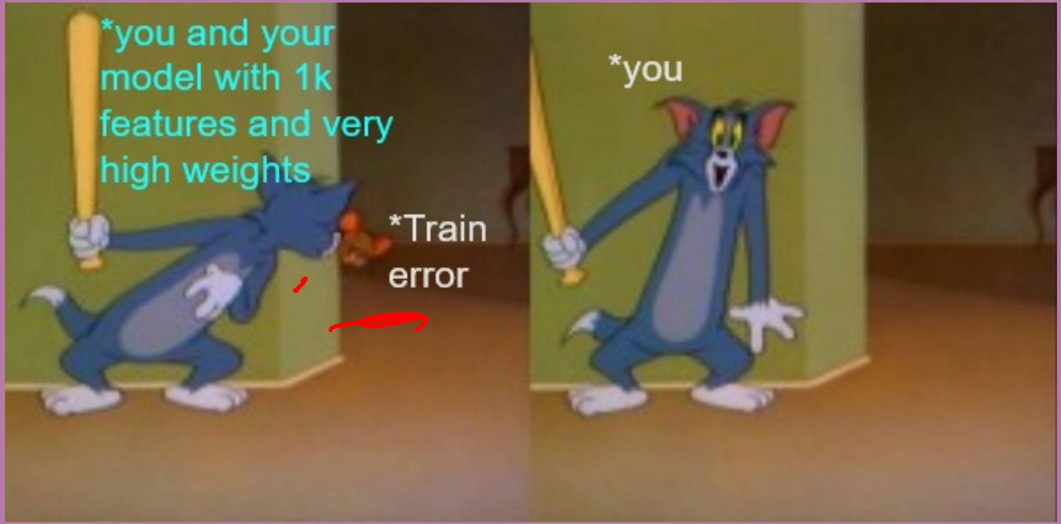
In which scenario is it more likely for a model to overfit?

(Few / [✓ Many]) Features

(Few / [✓ Many]) Parameters

(Small / [✓ Large]) Polynomial Degree

([✓ Small] / Large) Dataset



Overfitting in a nutshell

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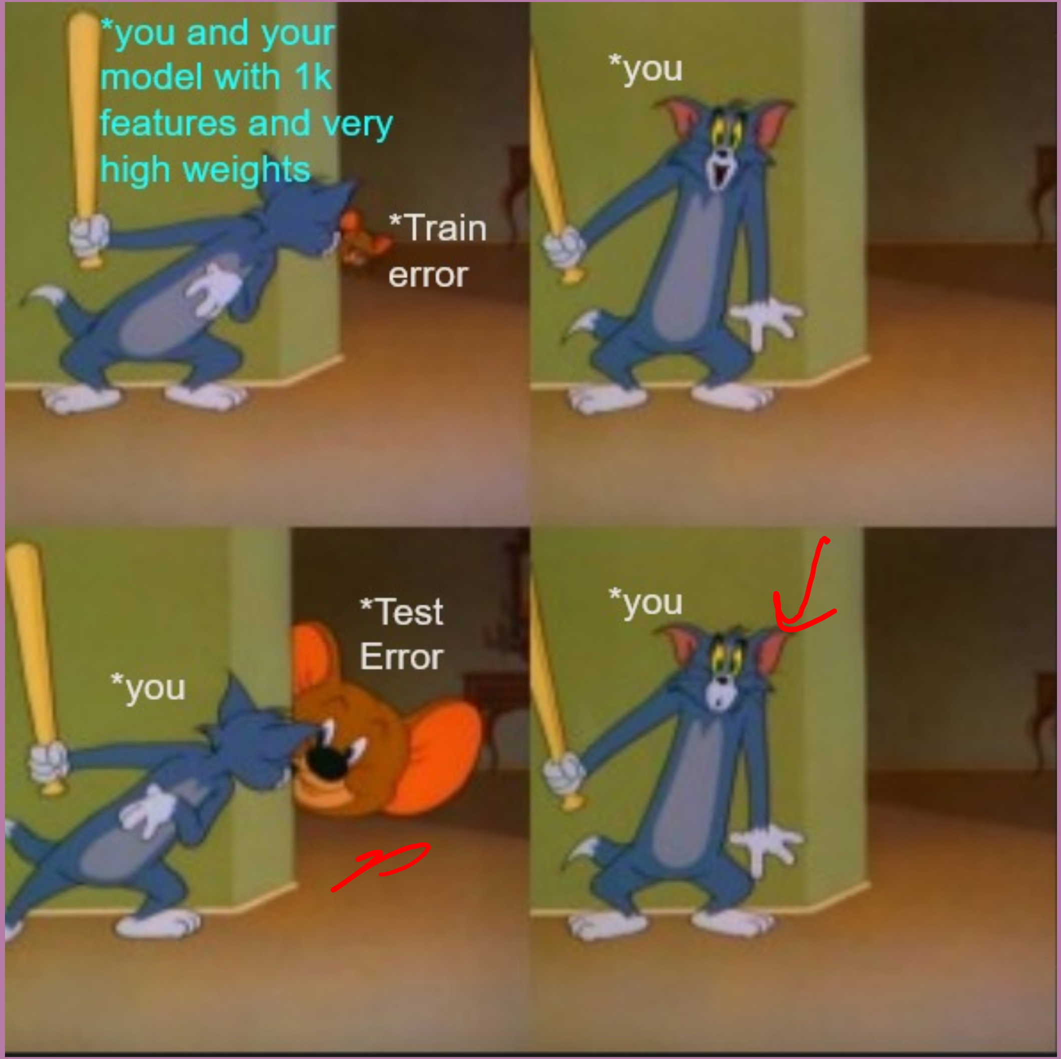


Prevent Overfitting

↓

d

2

Last time, we **trained multiple models**, using cross validation / validation set, to find one that was less likely to overfit

✓ For selecting polynomial degree, we train p models.

For selecting which features to include, we'd have to train ____ models!

Can we **train one model** that isn't prone to overfitting in the first place?

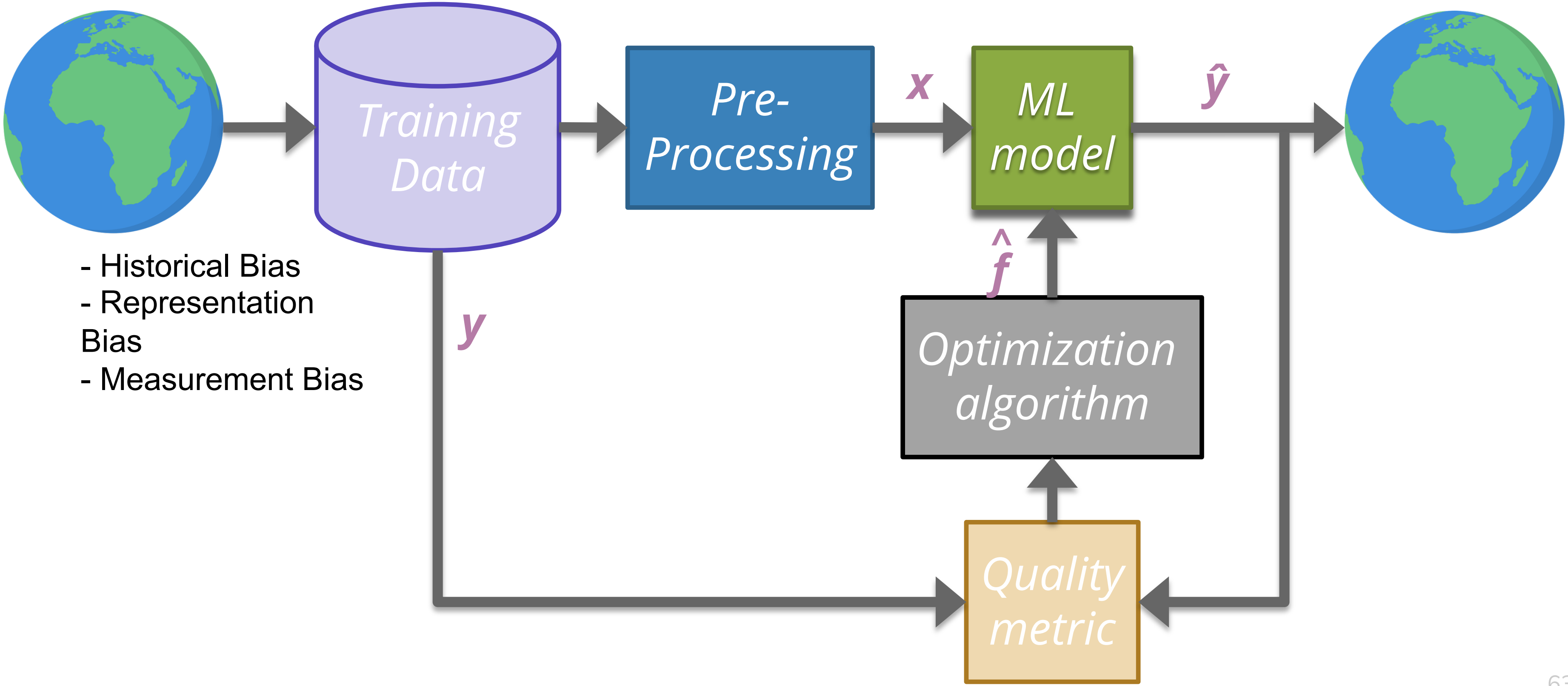
Big Idea: Have the model self-regulate to prevent overfitting by making sure its coefficients don't get "too large"

This idea is called **regularization**.

$$\underbrace{2 \cdot 2 \cdot 2 \cdot \ldots \cdot 2}_{\leftarrow d \text{ times} \rightarrow} = \boxed{2^d}$$

Regularization

ML Pipeline



- Historical Bias
- Representation Bias
- Measurement Bias

- Deployment Bias

Regularization

Before, we used the quality metric that minimized loss

$$\boxed{\hat{w} = \underset{w}{\operatorname{argmin}}\, L(w)}$$

Change quality metric to balance loss with measure of overfitting

- $L(w)$ is the measure of fit
- $R(w)$ measures the magnitude of coefficients

$$\hat{w} = \underset{w}{\operatorname{argmin}}\, \boxed{L(w) + \lambda\, R(w)}$$

λ: regularization parameter

How do we actually measure the magnitude of coefficients?

Magnitude

$w_1 = +1m$

$w_2 = -1m$

Come up with some number that summarizes the magnitude of the coefficients in w.

Sum? $w_1 + w_2 + \dots + w_d$

Sum of absolute values? Lasso $\sum_{i=1}^{d} |w_i| = R(w)$

Sum of squares? $\sum_{i=1}^{d} |w_i^2|$ → Ridge regression

Ridge Regression

Change quality metric to minimize

$$\boxed{\hat{w} = \underset{w}{\operatorname{argmin}}\, MSE(w) + \lambda\|w\|_2^2}$$

λ is a tuning **hyperparameter** that changes how much the model cares about the regularization term.

What if $\lambda = 0$?

OLS

What if $\lambda = \infty$?

$w = \emptyset$

λ in between?

$0 < w_i < \infty$

Poll Everywhere

Think

1 Minutes

How does λ affect the bias and variance of the model? For each underlined section, select “Low” or “High” appropriately.

When $\lambda = 0$

The model has **([✓ Low] / High)** Bias and **(Low / [✓ High])** Variance.

When $\lambda = \infty$

The model has **(Low / [✓ High])** Bias and **([✓ Low] / High)** Variance.

Poll Everywhere

Group

2 Minutes

How does λ affect the bias and variance of the model? For each underlined section, select “Low” or “High” appropriately.

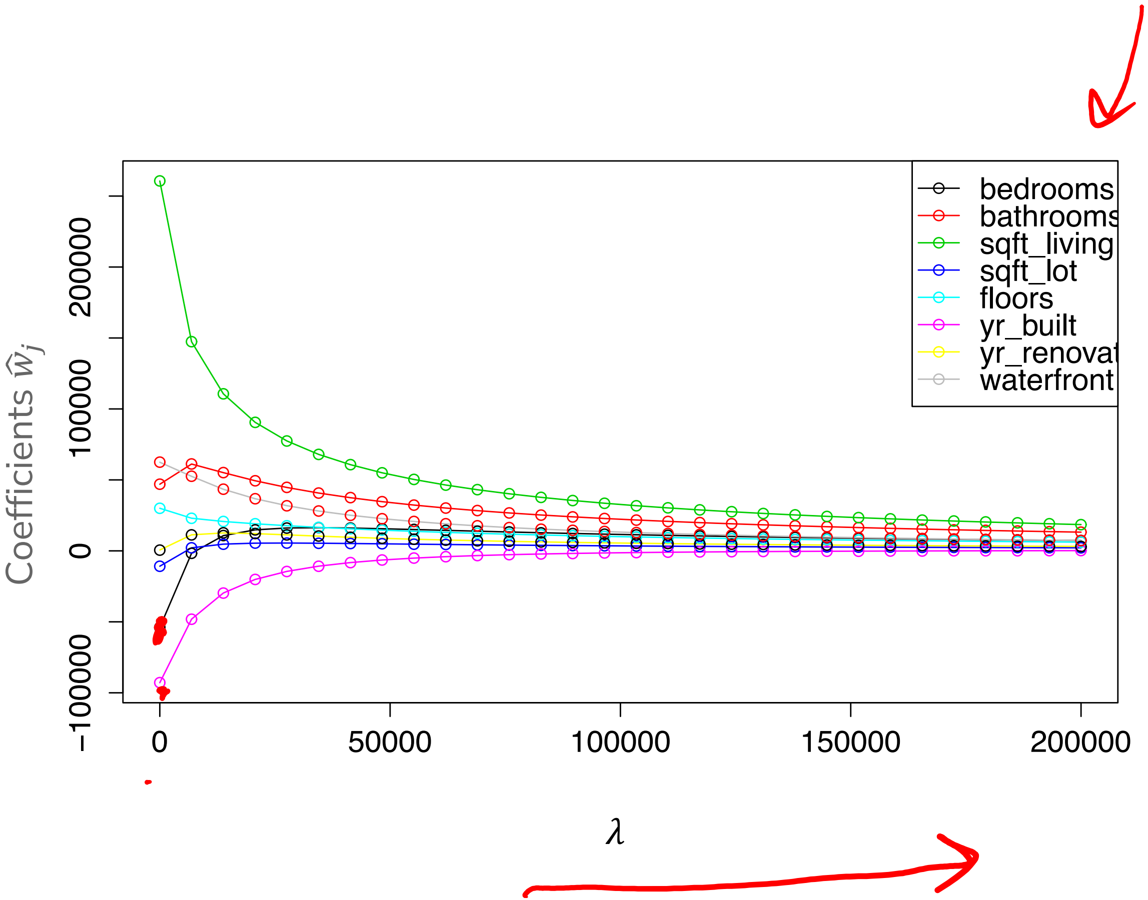
When $\lambda = 0$

The model has **(Low / High)** Bias and **(Low / High)** Variance.

When $\lambda = \infty$

The model has **(Low / High)** Bias and **(Low / High)** Variance.

Coefficient Paths



Brain Break

Demo: Ridge Regression

See Jupyter Notebook for interactive visualization.

Shows relationship between

- Regression line
- Mean Square Error
  - Also called Ordinary Least Squares
- Ridge Regression Quality Metric
- Coefficient Paths

Choosing λ

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Think

1 min

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How should we choose the best value of λ?

After we train each model with a certain λ_i and find

$\hat{w}_i = \mathrm{argmin}_w\ MSE(w) + \lambda_i ||w||_2^2$:

a) Pick the λ_i that has the smallest $MSE(\hat{w}_i)$ on the **train set**

b) Pick the λ_{i} that has the smallest $MSE(\hat{w}_i)$ on the **validation set**

c) Pick the λ_{i} that has the smallest $MSE(\hat{w}_i) + \lambda_i ||\hat{w}_i||_2^2$ on the **train set**

d) Pick the λ_{i} that has the smallest $MSE(\hat{w}_i) + \lambda_i ||\hat{w}_i||_2^2$ on the **validation set**

e) None of the above

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Group

2 min

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[✓ b)] Pick the λ_i that has the smallest $MSE(\hat{w}_i)$ on the **validation set**

c) Pick the λ_i that has the smallest $MSE(\hat{w}_i) + \lambda_i ||\hat{w}_i||_2^2$ on the **train set**

d) Pick the λ_i that has the smallest $\boxed{MSE(\hat{w}_i) + \lambda_i ||\hat{w}_i||_2^2}$ on the **validation set**

e) None of the above

Used only during Training process

Choosing λ

For any particular setting of λ, use Ridge Regression objective to train.

$$\boxed{\hat{w}_{ridge} = \underset{w}{\text{argmin}}\ \boxed{MSE(w) + \lambda||w||_2^2}}$$

If λ is too small, will overfit to **training set**. Too large, $\hat{w}_{ridge} = 0$.

How do we choose the right value of λ? We want the one that will do best on **future data.** Hence, we use the validation set.

For future data, what matters is that the model gets accurate predictions.

$MSE(w)$ measures error of predictions

$MSE(w) + \lambda||w||_2^2$ measures error of predictions & coefficient size

Regularization is a tool **used during training** to get a model that is likely to generalize. Regularization is **not used during prediction**.

Choosing λ

The process for selecting λ is exactly the same as we saw with using a validation set or using cross validation.

```
for $\lambda$ in $\lambda s$:
  Train a model using using Gradient Descent
        $\hat{w}_{ridge(\lambda)} = \underset{w}{\operatorname{argmin}}\, MSE_{train}(w) + \lambda||w||_2^2$
  Compute validation error
        $validation\_error = MSE_{val}(\hat{w}_{ridge(\lambda)})$
  Track $\lambda$ with smallest $validation\_error$
Return $\lambda^*$ & estimated future error $MSE_{test}(\hat{w}_{ridge(\lambda^*)})$
```

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Group

2 minutes

K

A model **parameter** is learnt during training (e.g., $\hat{w}$)

A **hyperparameter** is a parameter that is external to the model, whose value is used to influence the learning process.

What hyperparameters have we learned so far?

α : learning rate

λ : regu. hyperparameter

epochs

Scaling

Regularization

At this point, I've hopefully convinced you that regularizing coefficient magnitudes is a good thing to avoid overfitting!

You:

We might have gotten a bit carried away, it doesn't ALWAYS make sense…

The Intercept

For most of the features, looking for large coefficients makes sense to spot overfitting. The one it does not make sense for is the **intercept**.

We shouldn't penalize the model for having a higher intercept since that just means the y value units might be really high! Also, the intercept doesn't affect the curvature of a loss function (it's just a linear scale).

- My demo before does this wrong and penalizes w_0 as well!

Two ways of dealing with this

- Center the y values so they have mean 0
  - This means forcing w_0 to be small isn't a problem
- Change the measure of overfitting to not include the intercept

$$\underset{w_0, w_{rest}}{\operatorname{argmin}} MSE(w_0, w_{rest}) + \lambda \left|\left|w_{rest}\right|\right|_2^2$$

Other Coefficients

The L2 penalty penalizes all (non-intercept) coefficients equally

Is that reasonable?

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Think

1 Minute

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How would the coefficient change if we change the scale of our feature?

Consider our housing example with $(sq.ft., price)$ of houses

Say we learned a coefficient $\hat{w}_1$ for that feature

What happens if we change the unit of x to square **miles?** Would $\hat{w}_1$ need to change?

[✓ a) The $\hat{w}_1$ in the new model with sq. miles would be larger]

b) The $\hat{w}_1$ in the new model with sq. miles would be smaller

c) The $\hat{w}_1$ in the new model with sq. miles would stay the same

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Group

1 Minute

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c) The $\hat{w}_1$ in the new model with sq. miles would stay the same

Scaling Features

The other problem we overlooked is the “scale” of the coefficients.

Remember, the coefficient for a feature increase per unit change in that feature (holding all others fixed in multiple regression)

Consider our housing example with $(sq.ft., price)$ of houses

Say we learned a coefficient $\hat{w}_1$ for that feature

What happens if we change the unit of x to square **miles?** Would $\hat{w}_1$ need to change?

- It would need to get bigger since the prices are the same but its inputs are smaller

This means we accidentally penalize features for having large coefficients due to having small value inputs!

Scaling Features

Fix this by **normalizing** the features so all are on the same scale!

$$\boxed{\tilde{h}_j(x_i) = \frac{h_j(x_i) - \mu_j(x_1, \dots, x_N)}{\sigma_j(x_1, \dots, x_N)}}$$

Where

The mean of feature j:

$$\mu_j(x_1, \dots, x_N) = \frac{1}{N}\sum_{i=1}^{N} h_j(x_i)$$

The standard devation of feature j:

$$\sigma_j(x_1, \dots, x_N) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(h_j(x_i) - \mu_j(x_1, \dots, x_N)\right)^2}$$

Important: Must scale the test data and all future data using the means and standard deviations **of the training set!**

Otherwise the units of the model and the units of the data are not comparable!

LASSO Regression

Change quality metric to minimize

$$\hat{w} = \underset{w}{\operatorname{argmin}}\, MSE(w) + \lambda \underline{||w||_1}$$

λ is a tuning parameter that changes how much the model cares about the regularization term.

What if $\lambda = 0$?

OLS

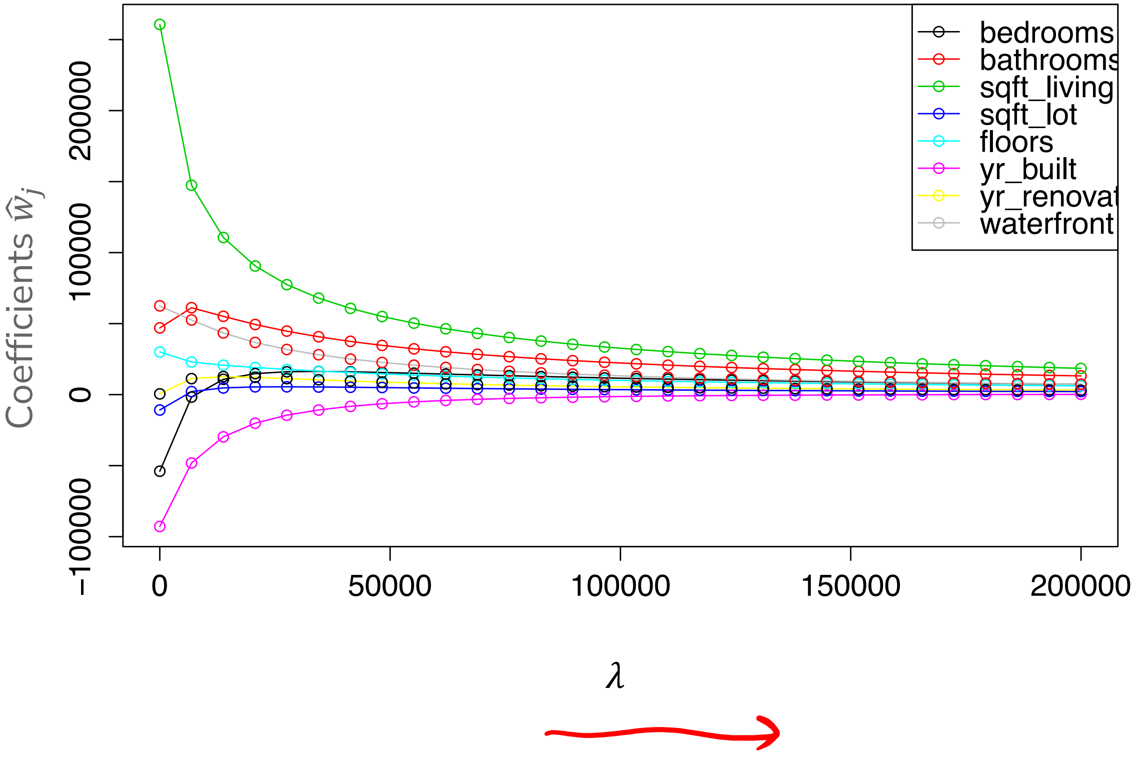
What if $\lambda = \infty$?

$w \rightarrow \emptyset$

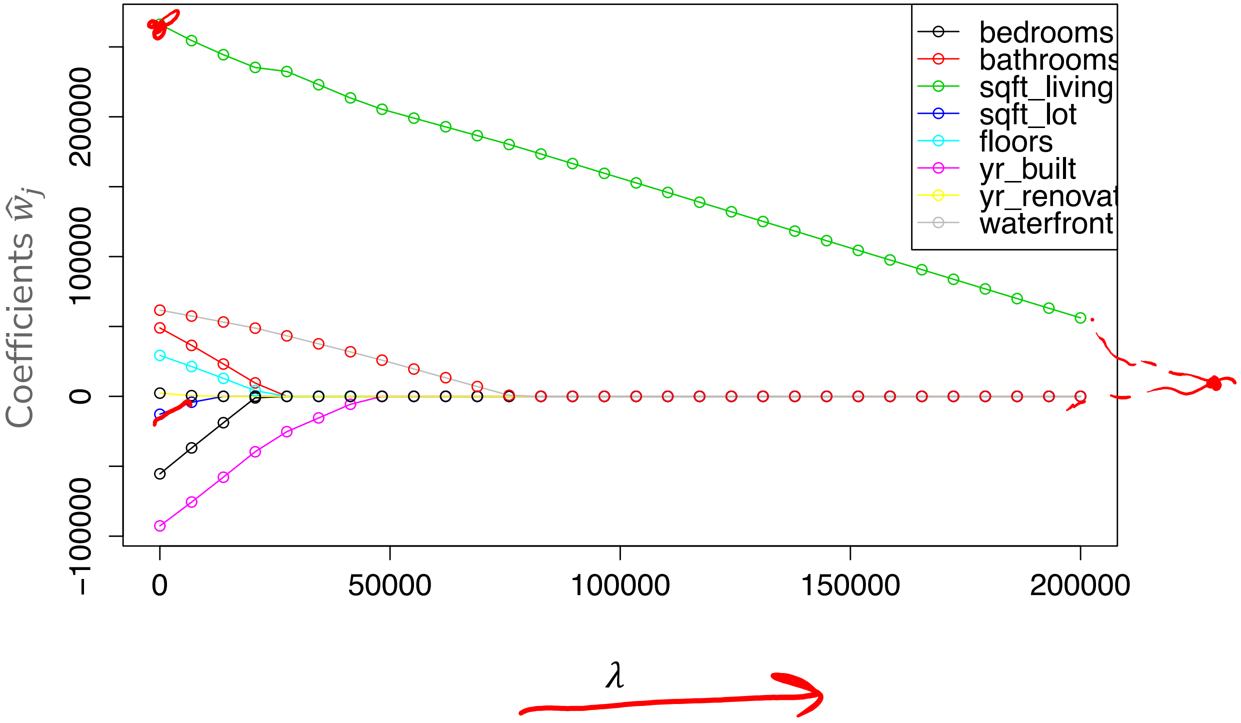
λ in between?

$0 < w < \infty$

Ridge (L2) Coefficient Paths

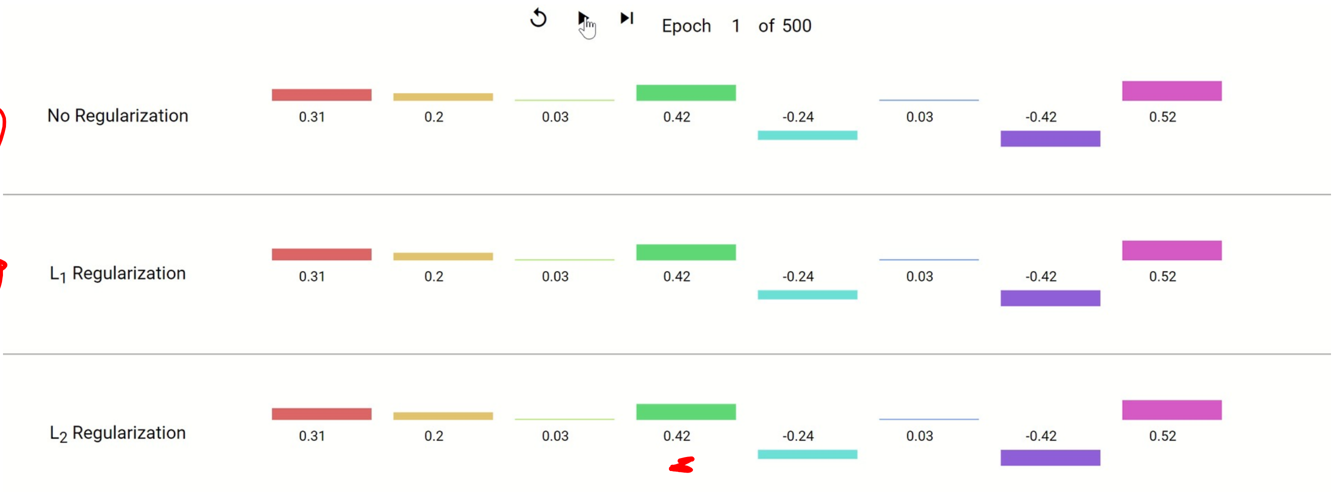


LASSO (L1) Coefficient Paths



Coefficient Paths – Another View

Example from Google's Machine Learning Crash Course



No Regularization	0.31	0.2	0.03	0.42	-0.24	0.03	-0.42	0.52
L_1 Regularization	0.31	0.2	0.03	0.42	-0.24	0.03	-0.42	0.52
L_2 Regularization	0.31	0.2	0.03	0.42	-0.24	0.03	-0.42	0.52

Demo

Similar demo to last time’s with Ridge but using the LASSO penalty

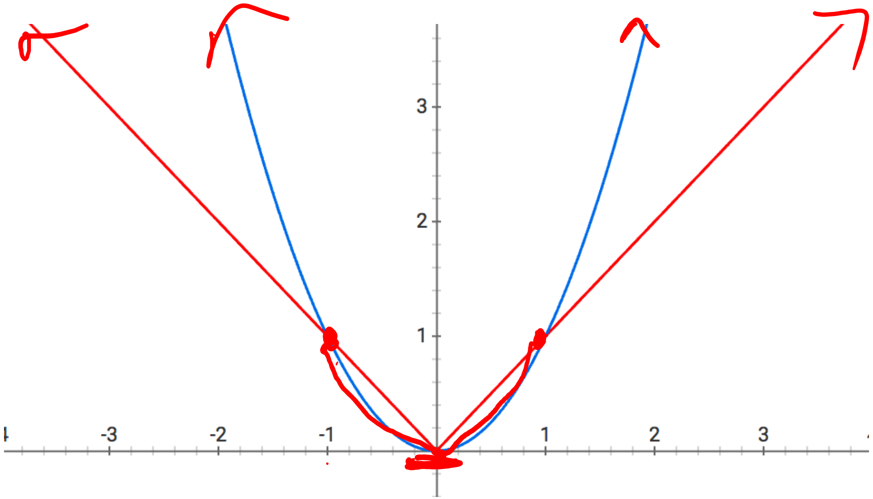
Poll Everywhere

Think

2 minutes

No poll

Why might the shape of the L1 penalty cause more sparsity than the L2 penalty?

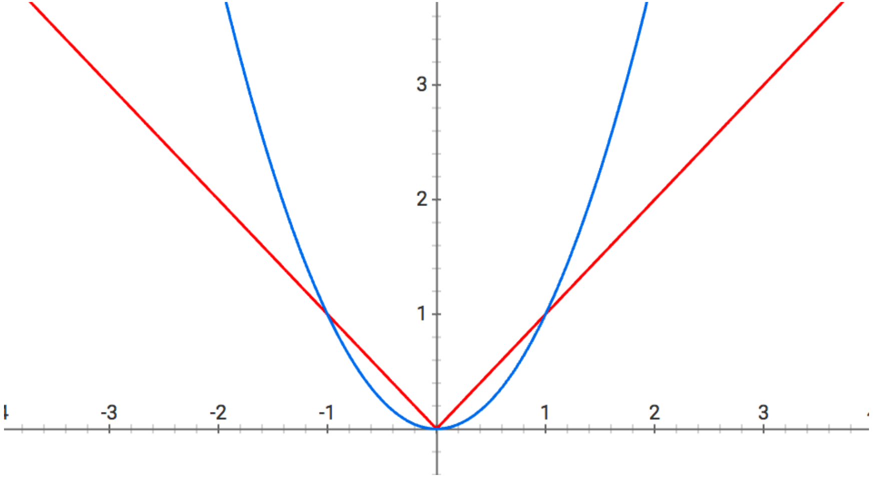


Sparsity

$[0, w_1, 0, w_2]$

When using the L1 Norm ($||w||_1$) as a regularizer, it favors solutions that are **sparse**. Sparsity for regression means many of the learned coefficients are 0.

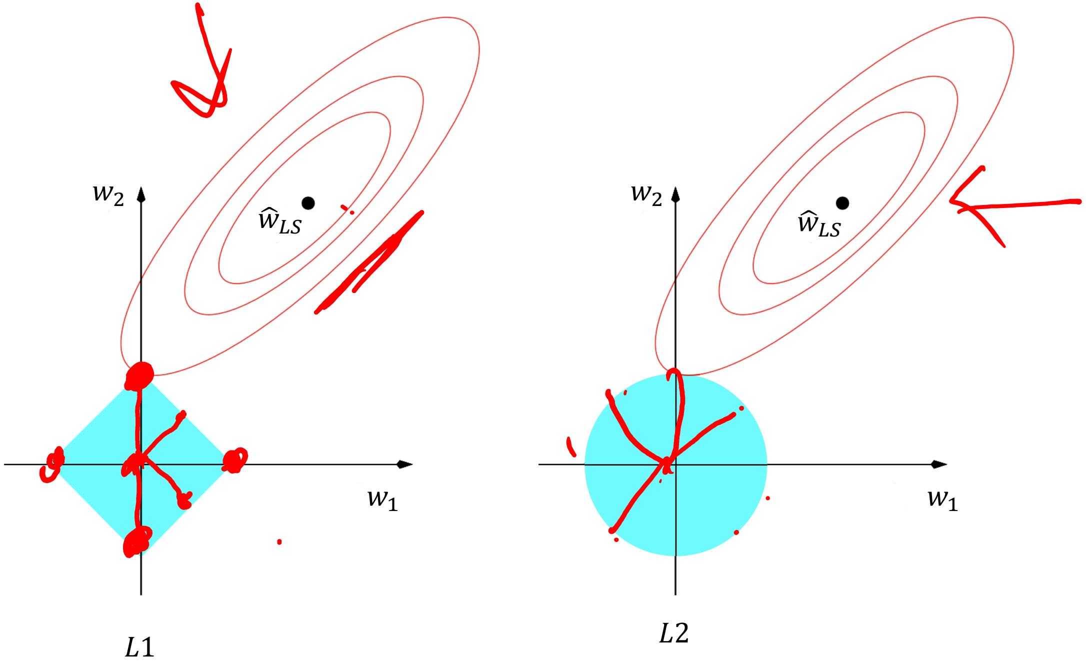
This has to do with the shape of the norm



When w_j is small, w_j^2 is VERY small! Diminishing returns on decreasing w_j with Ridge penalty

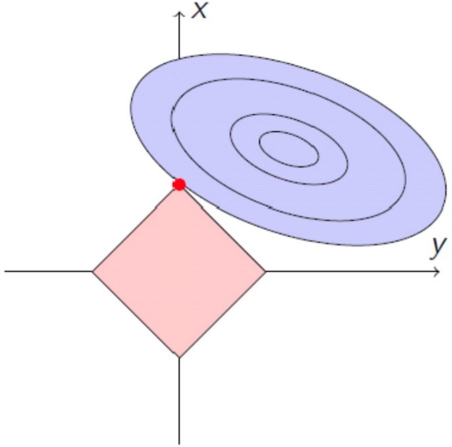
Sparsity Geometry

Another way to visualize why LASSO prefers sparse solutions

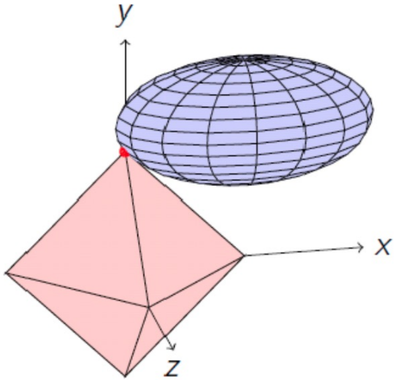


The L1 ball has spikes (places where some coefficients are 0)

Sparsity Geometry



$L1$ (2 features)



$L1$ (3 features)

Brain Break

Poll Everywhere

Think

1 min

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How should we choose the best value of λ for LASSO?

a) Pick the λ that has the smallest $MSE(\hat{w})$ on the **validation set**

b) Pick the λ that has the smallest $MSE(\hat{w}) + \lambda||\hat{w}||_2^2$ on the **validation set**

c) Pick the λ that results in the most zero coefficients

d) Pick the λ that results in the fewest zero coefficients

e) None of the above

Choosing λ

Exactly the same as Ridge Regression :)

This will be true for almost every **hyper-parameter** we talk about

A **hyper-parameter** is a parameter you specify for the model that influences which parameters (e.g. coefficients) are learned by the ML aglorithm

LASSO in Practice

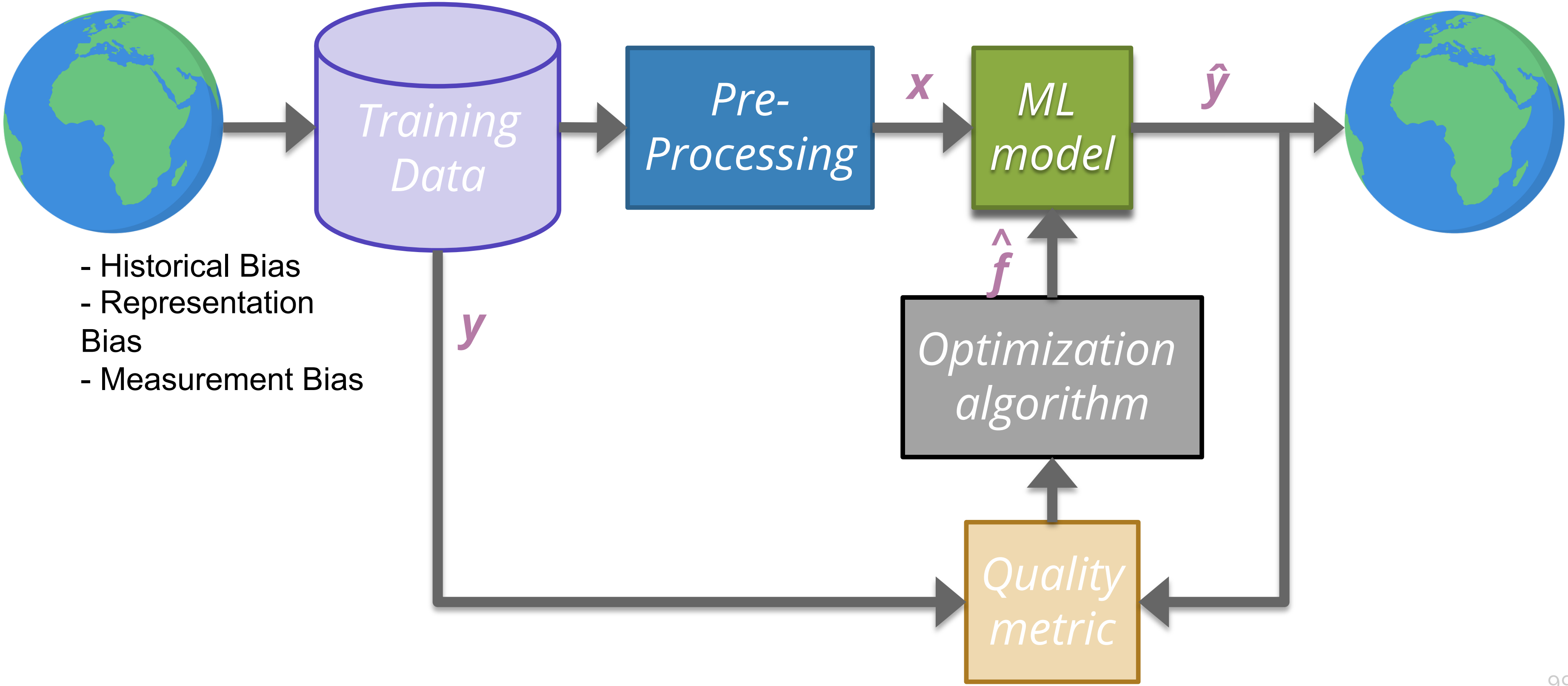
A very common usage of LASSO is in feature selection. If you have a model with potentially many features you want to explore, you can use LASSO on a model with all the features and choose the appropriate λ to get the right complexity.

Then once you find the non-zero coefficients, you can identify which features are the most important to the task at hand*

* e.g., using domain-specific expertise

ML Pipeline

- Deployment Bias



- Historical Bias
- Representation Bias
- Measurement Bias

De-biasing LASSO

LASSO (and Ridge) adds bias to the Least Squares solution (this was intended to avoid the variance that leads to overfitting)

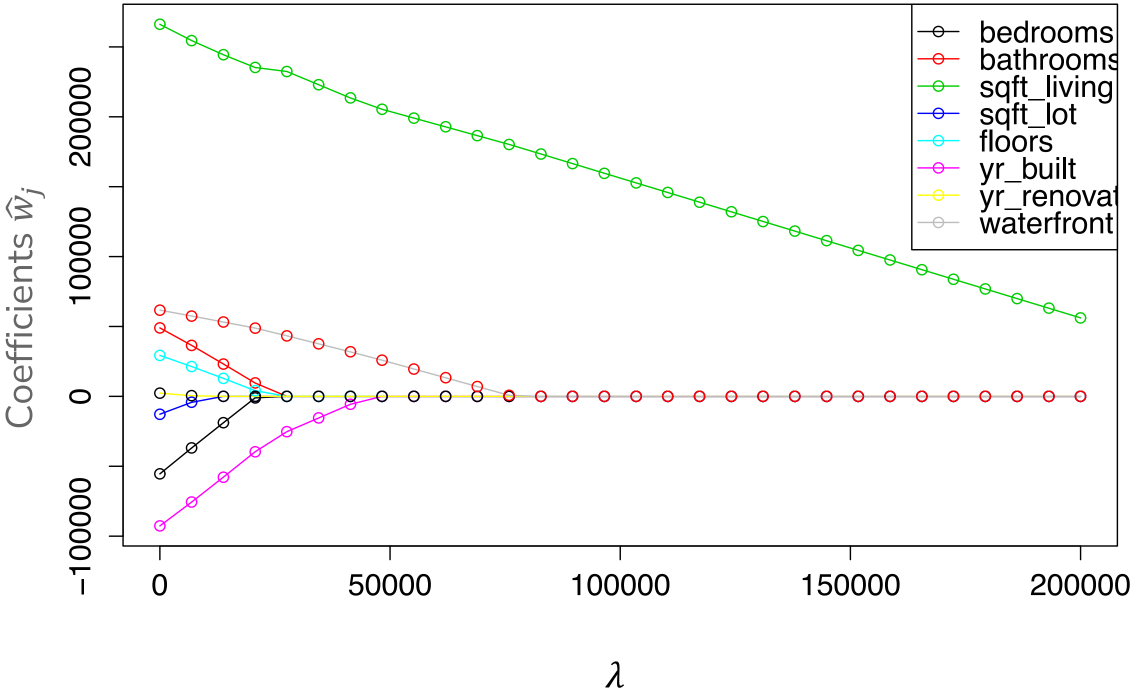
Recall Bias-Variance Tradeoff

It's possible to try to remove the bias from the LASSO solution using the following steps

1. Run LASSO to select which features should be used (those with non-zero coefficients)
2. Run regular Ordinary Least Squares on the dataset with only those features

Coefficients are no longer shrunk from their true values

LASSO (L1) Coefficient Paths



(De-biased) LASSO In Practice

1. Split the dataset into train, val, and test sets
2. Normalize features. Fit the normalization on the train set, apply that normalization on the train, val, and test sets.
3. Use validation or cross-validation to find the value of λ that that results in a LASSO model with the lowest validation error.
4. Select the features of that model that have non-zero weights.
5. Train a Linear Regression model with only those features.
6. Evaluate on the test set.

Issues with LASSO

1. Within a group of highly correlated features (e.g. # bathroom and # showers), LASSO tends to select amongst them arbitrarily.
   - Maybe it would be better to select them all together?
2. Often, empirically Ridge tends to have better predictive performance

Elastic Net aims to address these issues

$$\hat{w}_{ElasticNet} = \underset{w}{\operatorname{argmin}}\, MSE(w) + \lambda_1 ||w||_1 + \lambda_2 ||w||_2^2$$

Combines both to achieve best of both worlds!

A Big Grain of Salt

Be careful when interpreting the results of feature selection or feature importance in Machine Learning!

- Selection only considers features included
- Sensitive to correlations between features
- Results depend on the algorithm used!

At the end of the day, the best models combine statistical insights with domain-specific expertise!

Differences between L1 and L2 regularizations

L1 (LASSO):

- Introduces more sparsity to the model
- Less sensitive to outliers
- Helpful for feature selection, making the model more interpretable
- More computational efficient as a model (due to the sparse solutions, so you have to compute less dot products)

L2 (Ridge):

- Makes the weights small (but not 0)
- More sensitive to outliers (due to the squared terms)
- Usually works better in practice

Recap

Theme: Use regularization to prevent overfitting

Ideas:

How to interpret coefficients

How overfitting is affected by number of data points

Overfitting affecting coefficients

Use regularization to prevent overfitting

How L2 penalty affects learned coefficients

Visualizing what regression is doing

Practicalities: Dealing with intercepts and feature scaling

Formulate LASSO objective

Describe how LASSO coefficients change as hyper-parameter λ is varied

Interpret LASSO coefficient path plot

Compare and contrast LASSO (L1) and Ridge (L2)