

Administrivia

Last lecture in the “Regression” case study!

- Next 2 weeks: Classification
- Following 1 week: Deep Learning

Section Tomorrow:

- Coding up RIDGE and Lasso (helpful for HW2!)

Upcoming Deadlines:

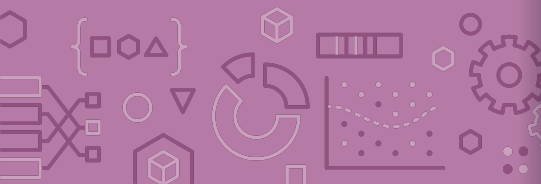
- HW1 Late deadline Thurs 7/7 11:59PM (if using 2 late days)
- HW2 out now, due Tues 7/12 11:59PM
- Learning Reflection 3 due Fri 11:59PM

Please monitor your grades on Canvas and reach out ASAP if there are any discrepancies. Canvas is the “final” gradebook.

OH is a great place to ask your learning reflection questions!

Reminder that we have lecture notes! Particularly recommended pre-lecture.

Poll on Brain Breaks.



Think 

30 sec

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Would you prefer one ~10 min brain break, or two ~5 min brain breaks?



HW2

Walkthrough

Recap Ridge Regression & Address LR Uncertainties

What is min /
argmin?

$$\min_x f(x)$$

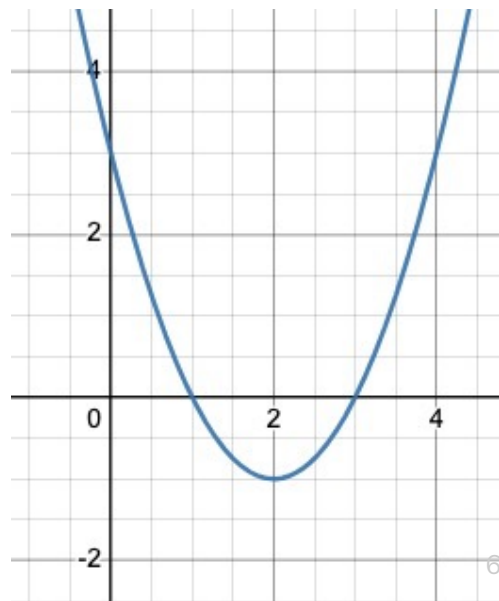
returns the minimum value of $f(x)$

$$\operatorname{argmin}_x f(x)$$

returns the value of x
for which $f(x)$ attains its minimum

Several Lec3 slides had min
instead of argmin. I've fixed it on
the website

$$f(x) = x^2 - 4x + 3$$



This should be randomized!

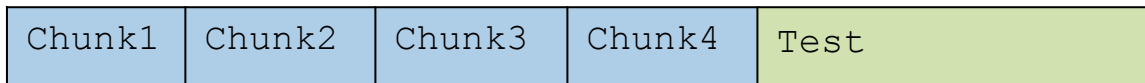
Cross-Validation

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.

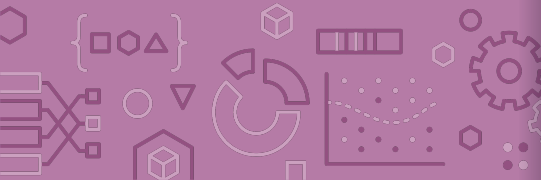
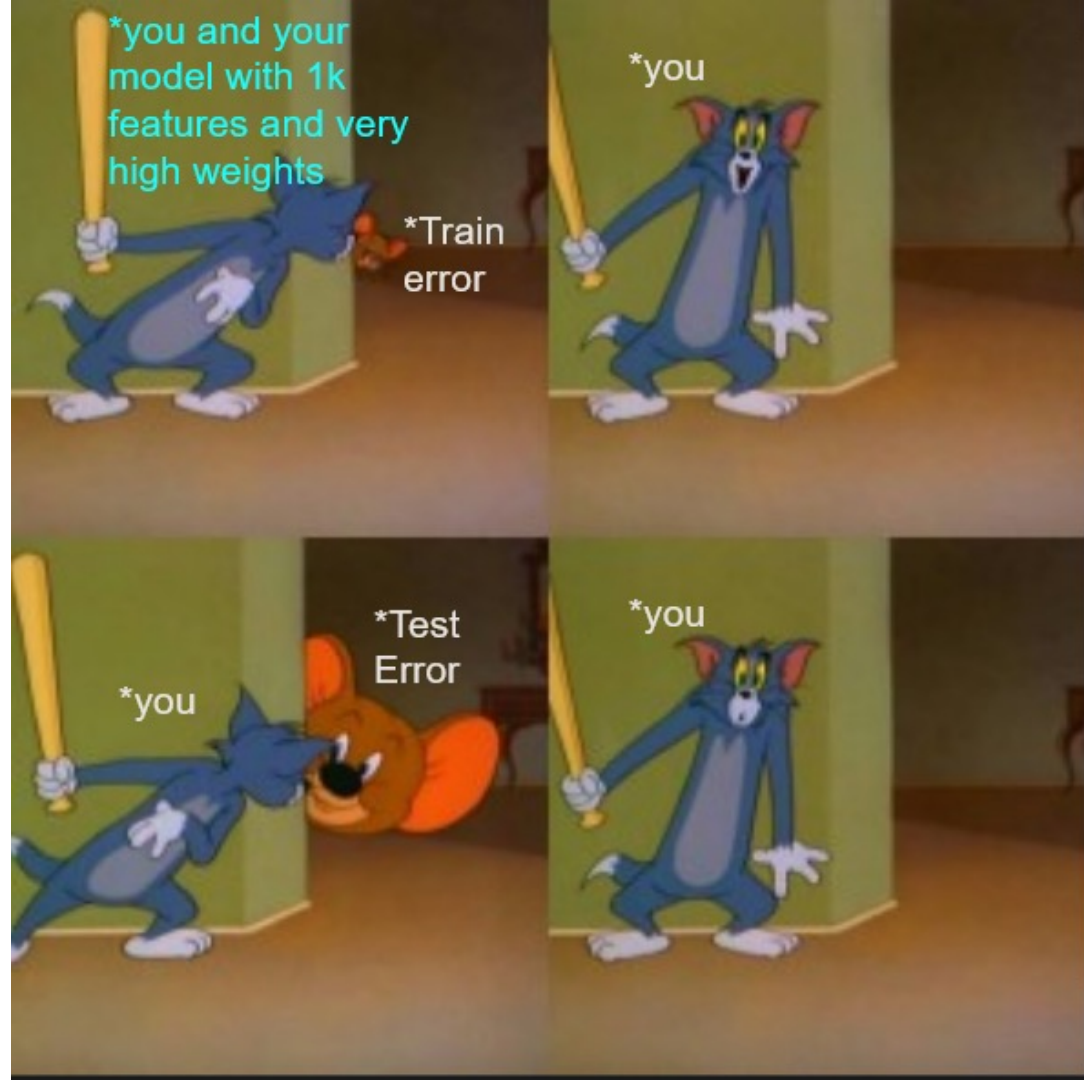


k chunks



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.

Overfitting In a Nutshell

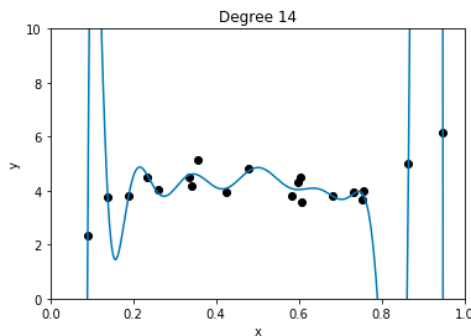


Number of Features

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

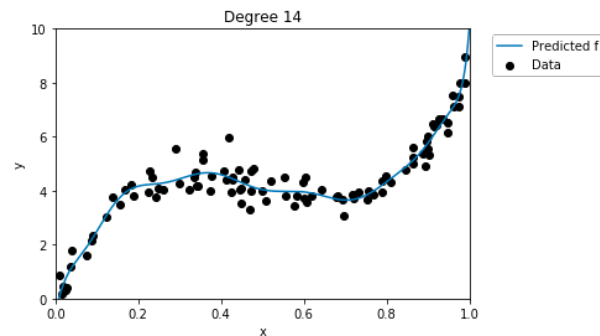
Why? Overfitting depends on whether the amount of data you have is large enough to represent the true function's complexity.

large $|\hat{\omega}_j|$



≈ 20 pts

moderate $|\hat{\omega}_j|$



≈ 100 pts

Ridge Regression

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

Change quality metric to minimize

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

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

What if $\lambda = 0$?

$$\begin{aligned}\hat{\omega} &= \underset{\omega}{\operatorname{argmin}} \operatorname{MSE}(\omega) \\ &= \hat{\omega}_{\text{OLS}}\end{aligned}$$

Ordinary
Least
Square (OLS)

What if $\lambda = \infty$?

$$\text{essentially : } \hat{\omega} = \underset{\omega}{\operatorname{argmin}} \lambda \|\omega\|_2^2 = \vec{0}$$

λ in between?

$$0 \leq \|\hat{\omega}_{\text{ridge}}\|_2 \leq \|\hat{\omega}_{\text{OLS}}\|_2$$

Poll Everywhere

Think 

~~5~~ Minutes
2

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

When $\lambda = 0 \Rightarrow$ *Complex*

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

When $\lambda = \infty \Rightarrow$ *Simple*

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



3:00

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 Gradient Descent
```

$$\hat{w}_{ridge(\lambda)} = \underset{w}{\operatorname{argmin}} MSE_{train}(w) + \lambda \|w_{1:D}\|_2^2$$

```
    Compute validation error
```

```
* validation_error = MSE_val( $\hat{w}_{ridge(\lambda)}$ ) *
```

```
    Track  $\lambda$  with smallest validation_error
```

```
Return  $\lambda^*$  & estimated future error  $MSE_{test}(\hat{w}_{ridge(\lambda^*)})$ 
```

Scaling Features

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

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

For feature j :
 μ_j mean
 σ_j std. dev.

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 deviation of feature j :

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

$$\tilde{h}_j(x) = \frac{h_j(x) - \mu_j}{\sigma_j}$$

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!

Think

1 min

What are some real-world / human analogies for each of these concepts?

Overfitting / Underfitting

Train Set / Test Set

Bias

Variance

Regularization

Poll Everywhere

Group 

2 mins

What are some real-world / human analogies for each of these concepts?

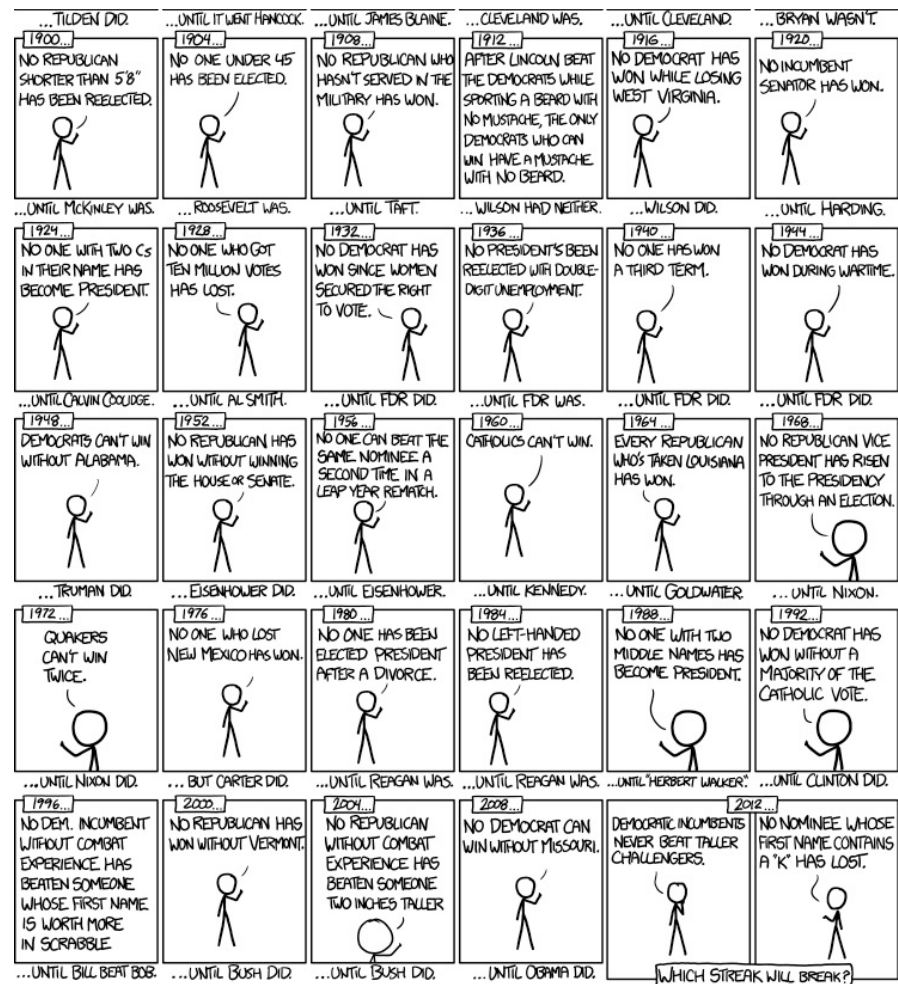
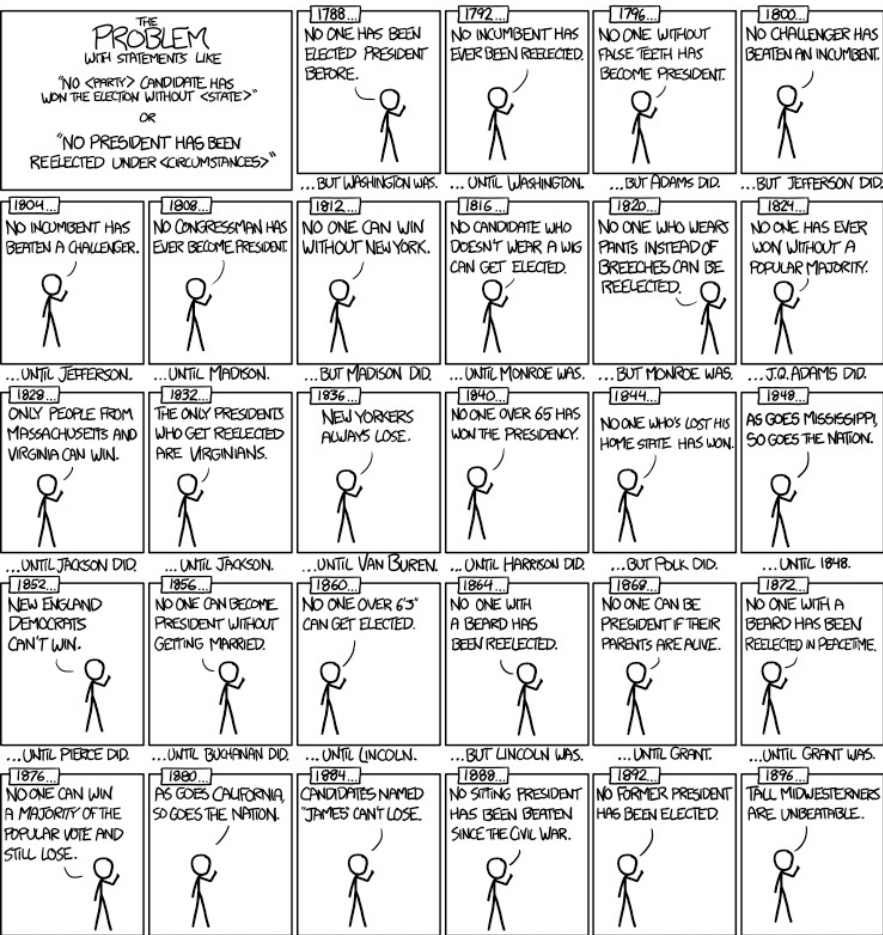
Overfitting / Underfitting

Train Set / Test Set

Bias

Variance

Regularization



Feature Selection & All Subsets

Benefits

Why do we care about selecting features? Why not use them all?

Complexity

Models with too many features are more complex. Might overfit!

Interpretability

Can help us identify which features carry more information.

Efficiency

Imagine if we had MANY features (e.g. DNA). $\hat{\mathbf{w}}$ could have 10^{11} coefficients. Evaluating $\hat{y} = \hat{\mathbf{w}}^T \mathbf{h}(x)$ would be very slow!

If $\hat{\mathbf{w}}$ is **sparse**, only need to look at the non-zero coefficients

$$\hat{y} = \sum_{\hat{w}_j \neq 0} \hat{w}_j h_j(x)$$

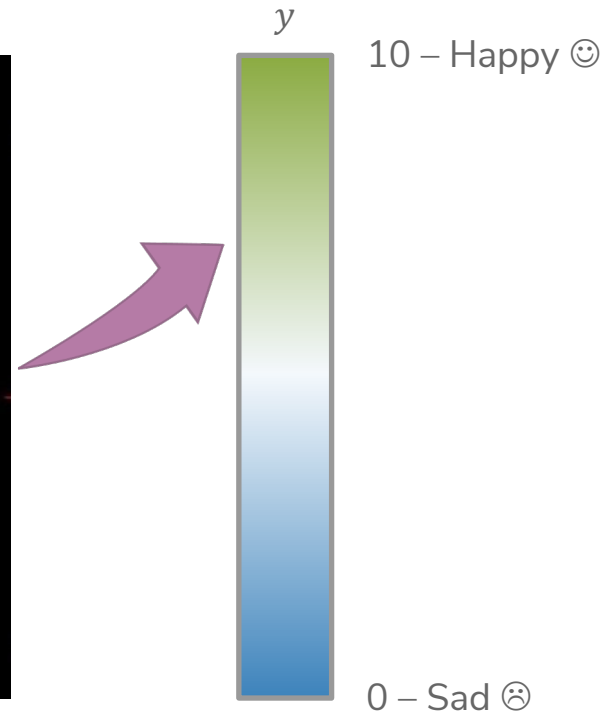
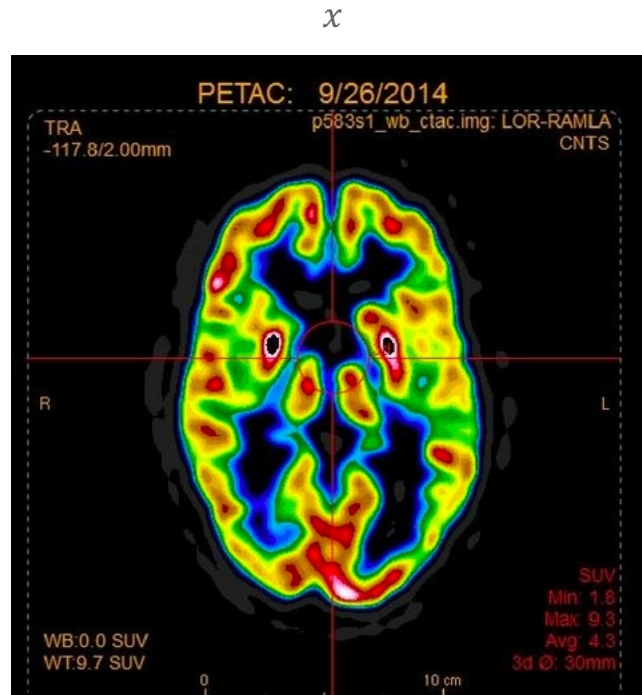
Sparsity: Housing

Might have many features to potentially use. Which are useful?

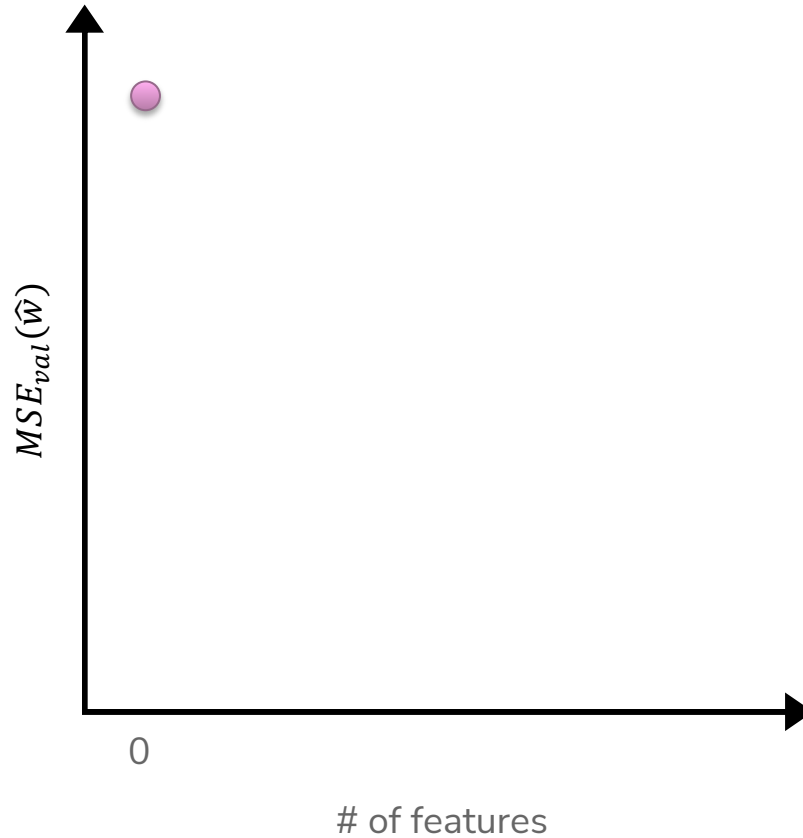
Lot size	Dishwasher
Single Family	Garbage disposal
Year built	Microwave
Last sold price	Range / Oven
Last sale price/sqft	Refrigerator
Finished sqft	Washer
Unfinished sqft	Dryer
Finished basement sqft	Laundry location
# floors	Heating type
Flooring types	Jetted Tub
Parking type	Deck
Parking amount	Fenced Yard
Cooling	Lawn
Heating	Garden
Exterior materials	Sprinkler System
Roof type	...
Structure style	

Sparsity: Reading Minds

How happy are you? What part of the brain controls happiness?



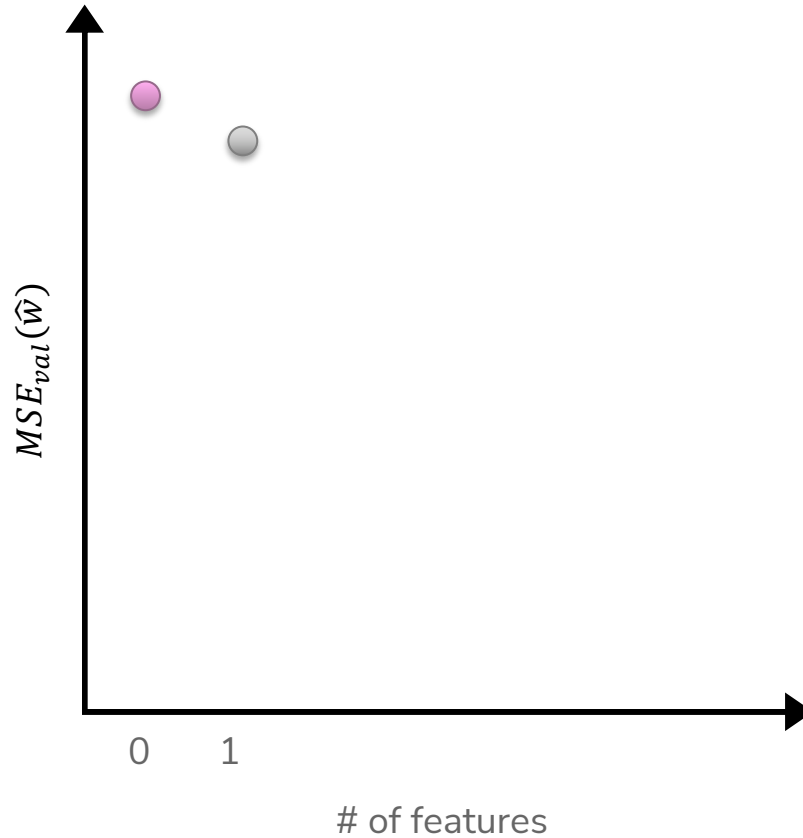
Best Model Size 0



Features

bathrooms
bedrooms
sq.ft. living
sq.ft lot
floors
year built
year renovated
waterfront

Best Model Size 1



Features

bathrooms

bedrooms

sq.ft. living

sq.ft lot

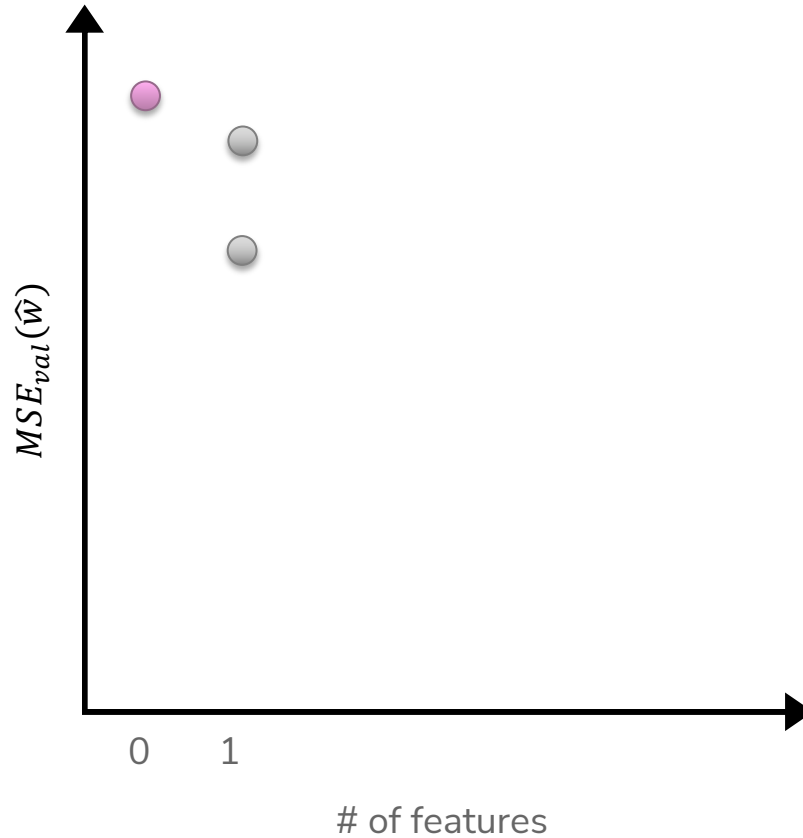
floors

year built

year renovated

waterfront

Best Model Size 1



Features

bathrooms

bedrooms

sq.ft. living

sq.ft lot

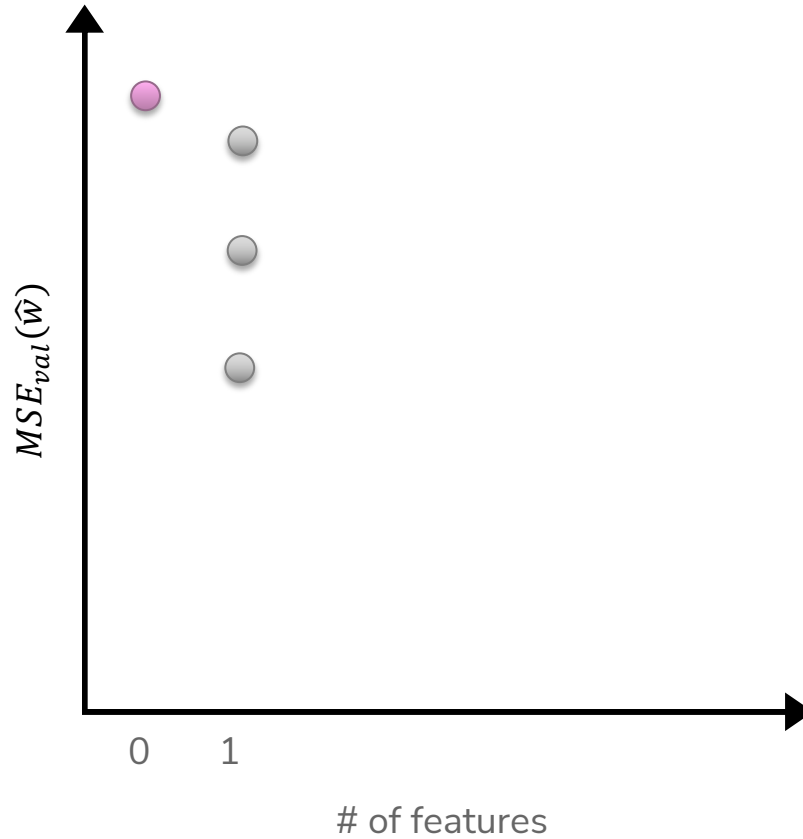
floors

year built

year renovated

waterfront

Best Model Size 1



Features

bathrooms

bedrooms

sq.ft. living

sq.ft lot

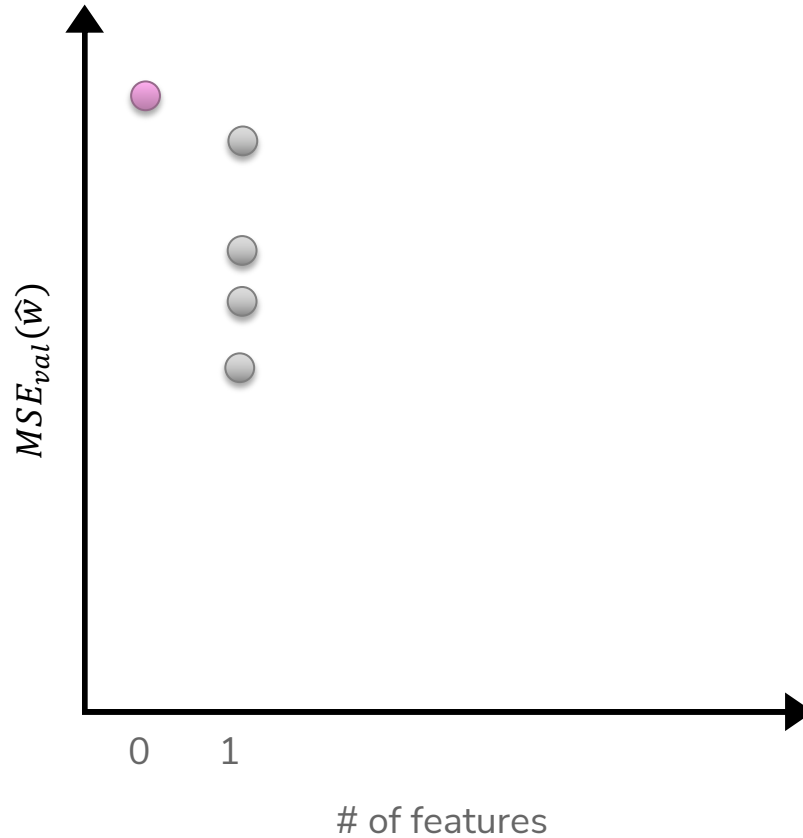
floors

year built

year renovated

waterfront

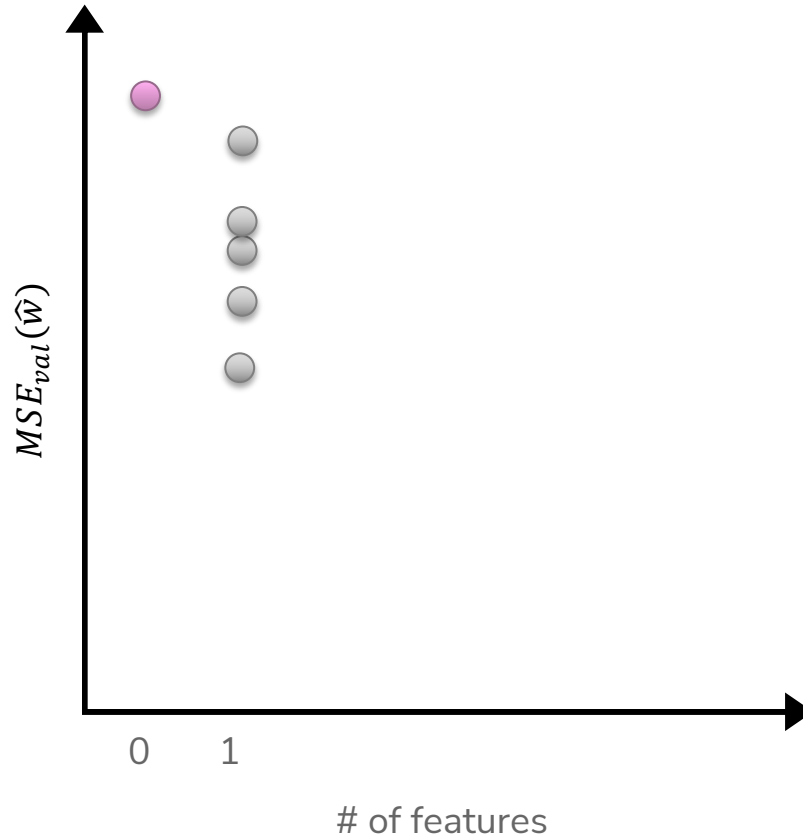
Best Model Size 1



Features

bathrooms
bedrooms
sq.ft. living
sq.ft. lot
floors
year built
year renovated
waterfront

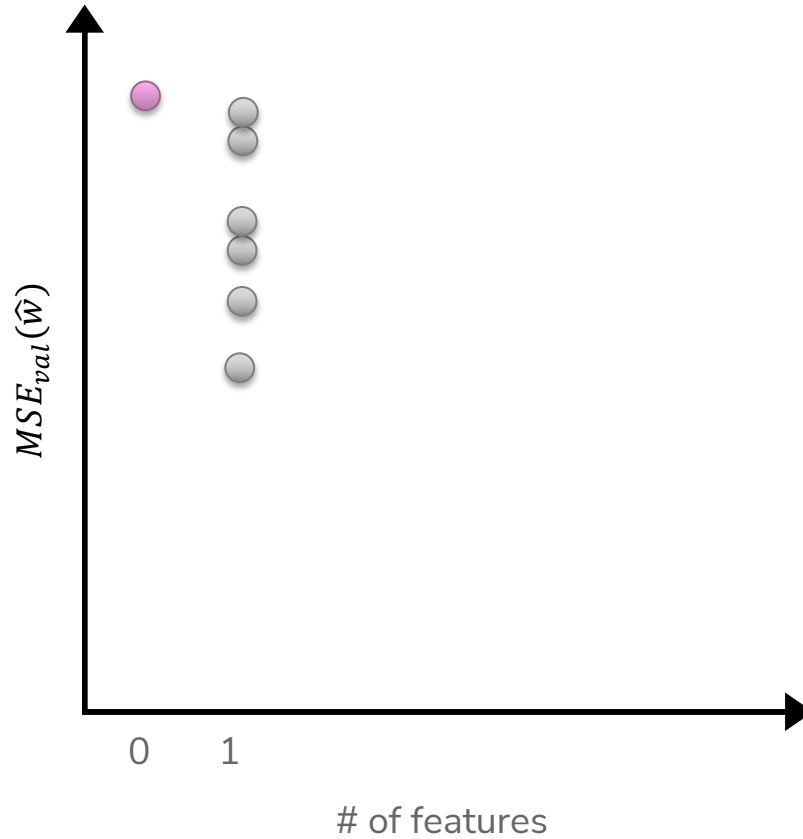
Best Model Size 1



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

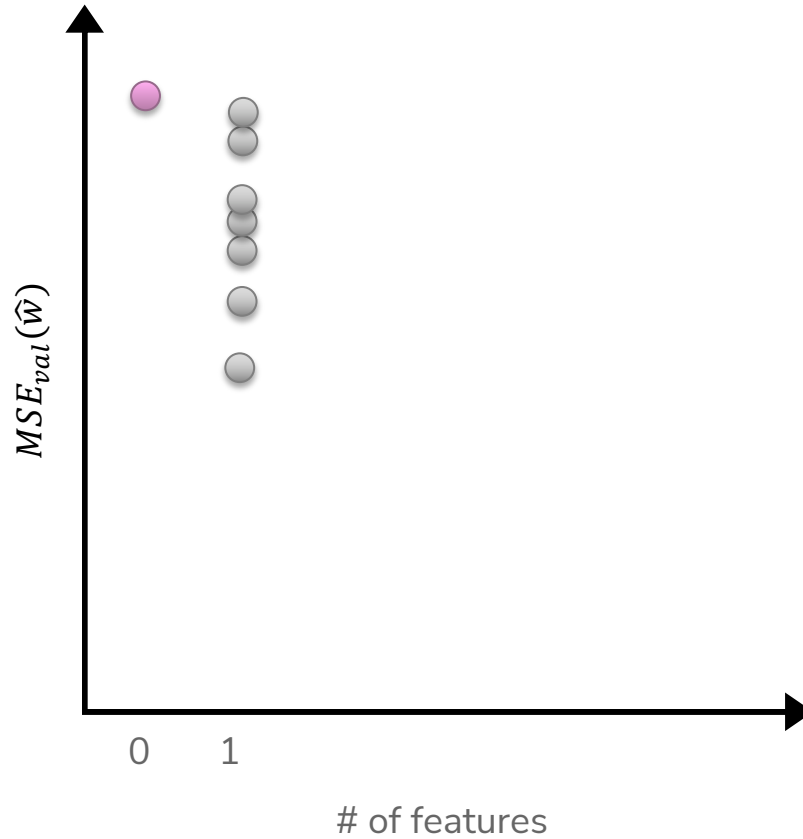
Best Model Size 1



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

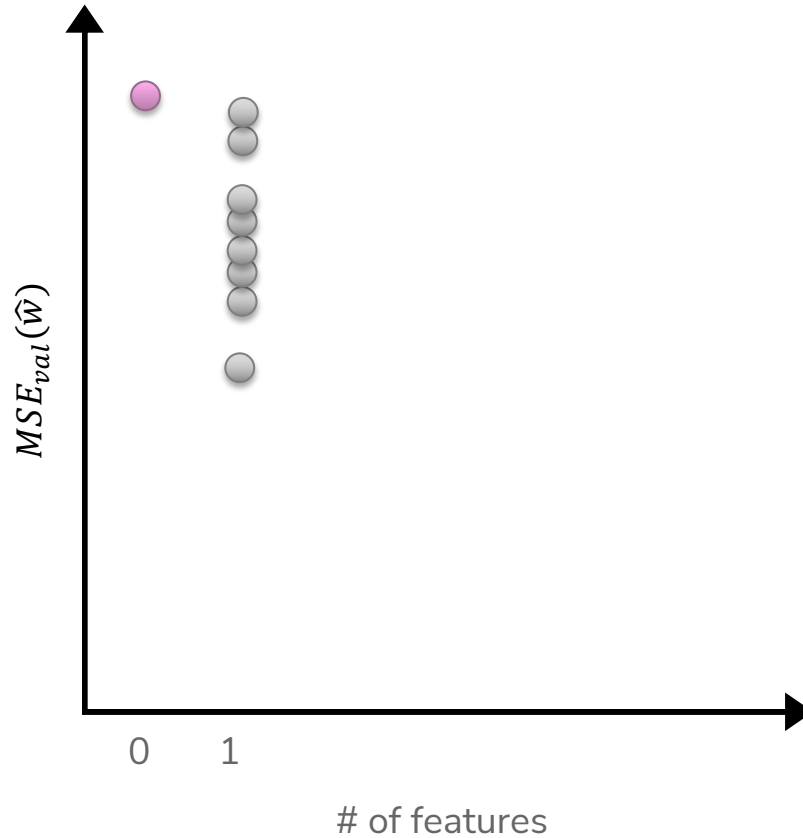
Best Model Size 1



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

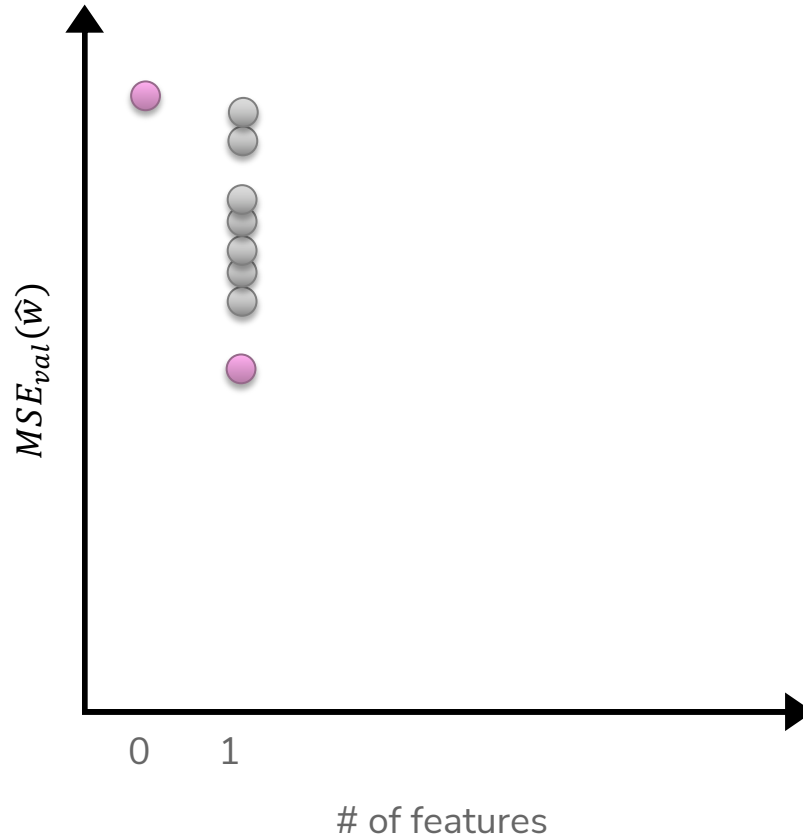
Best Model Size 1



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

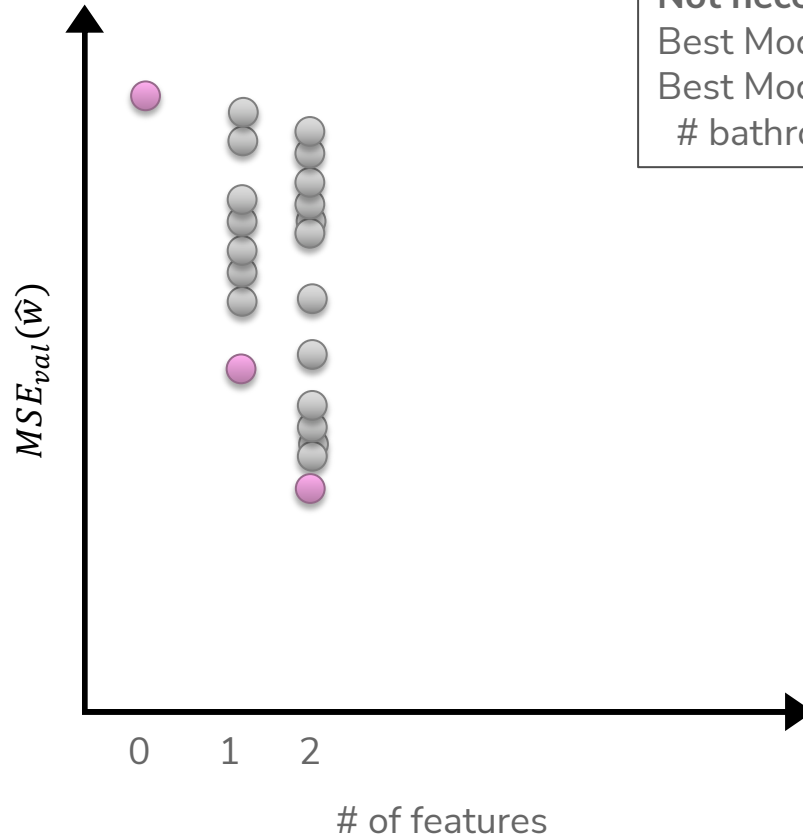
Best Model Size 1



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

Best Model Size 2



Not necessarily nested!

Best Model – Size 1: sq.ft living

Best Model – Size 2:

bathrooms & # bedrooms

Features

bathrooms

bedrooms

sq.ft. living

sq.ft lot

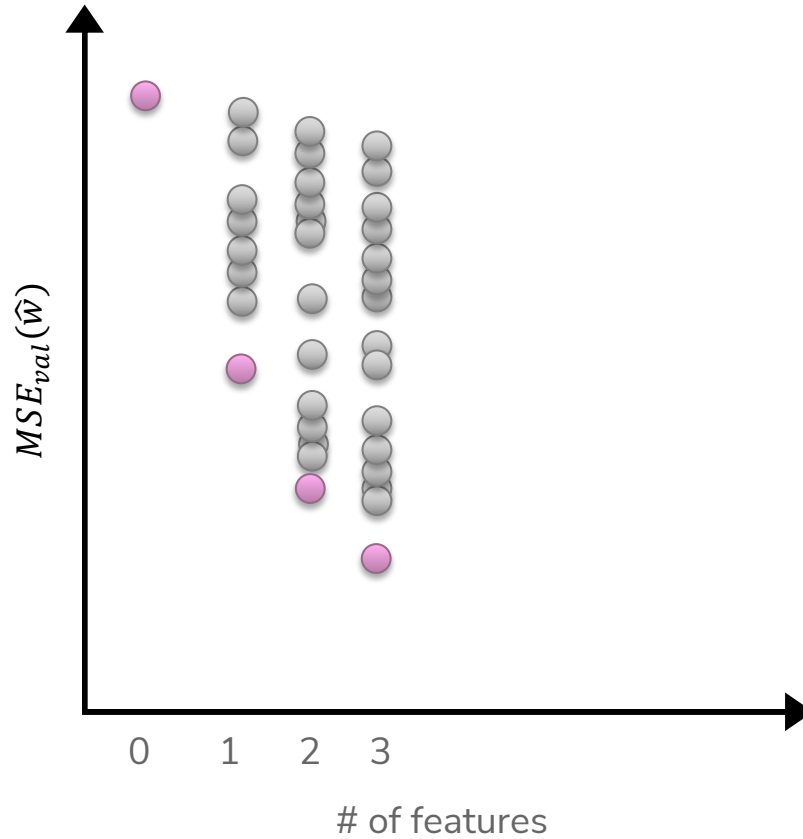
floors

year built

year renovated

waterfront

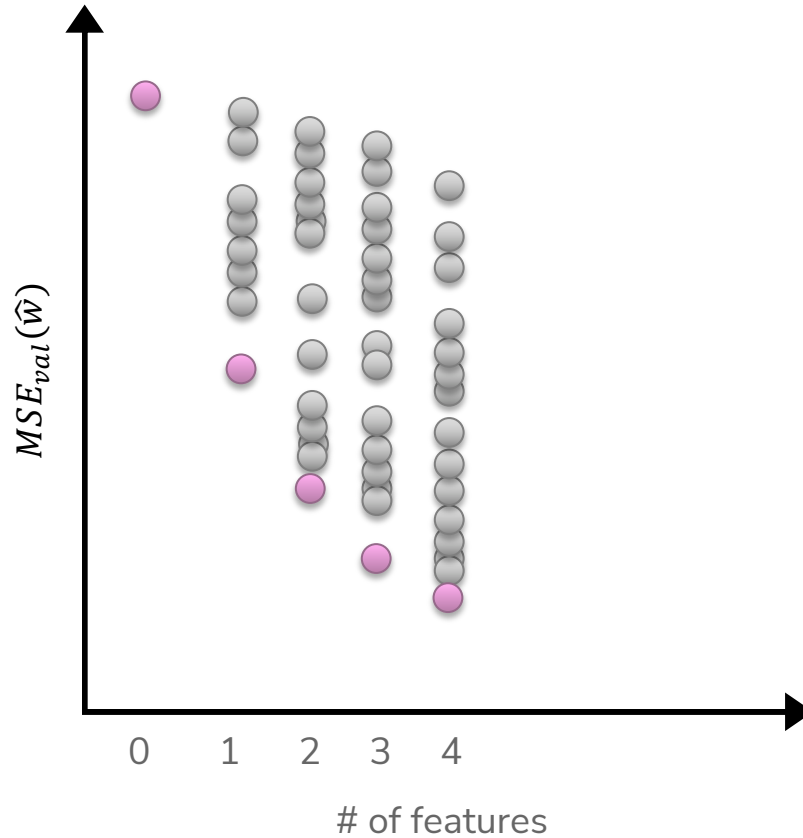
Best Model Size 3



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

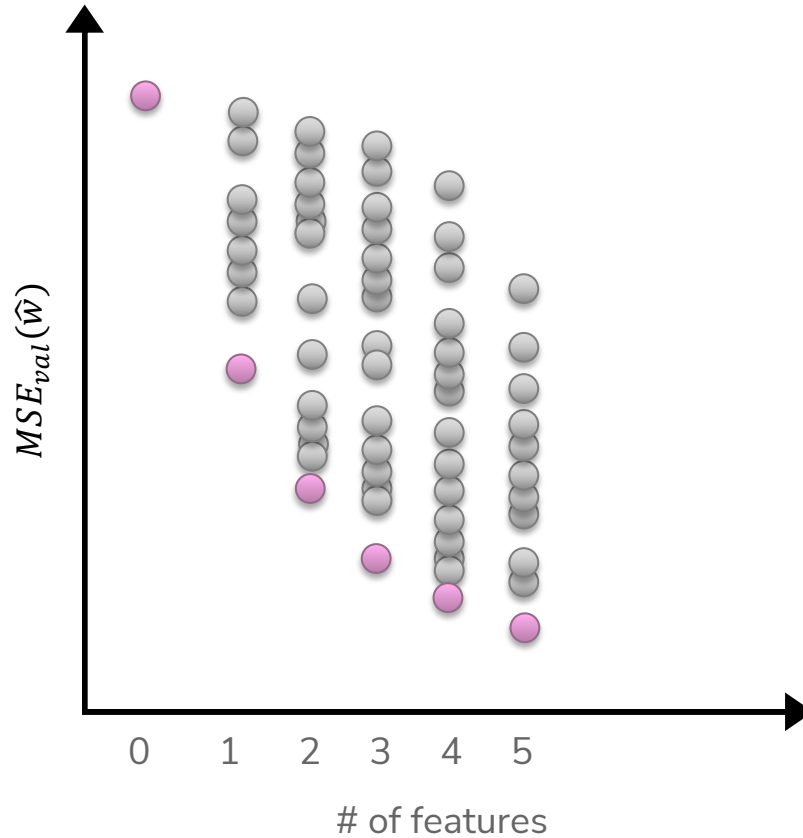
Best Model Size 4



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

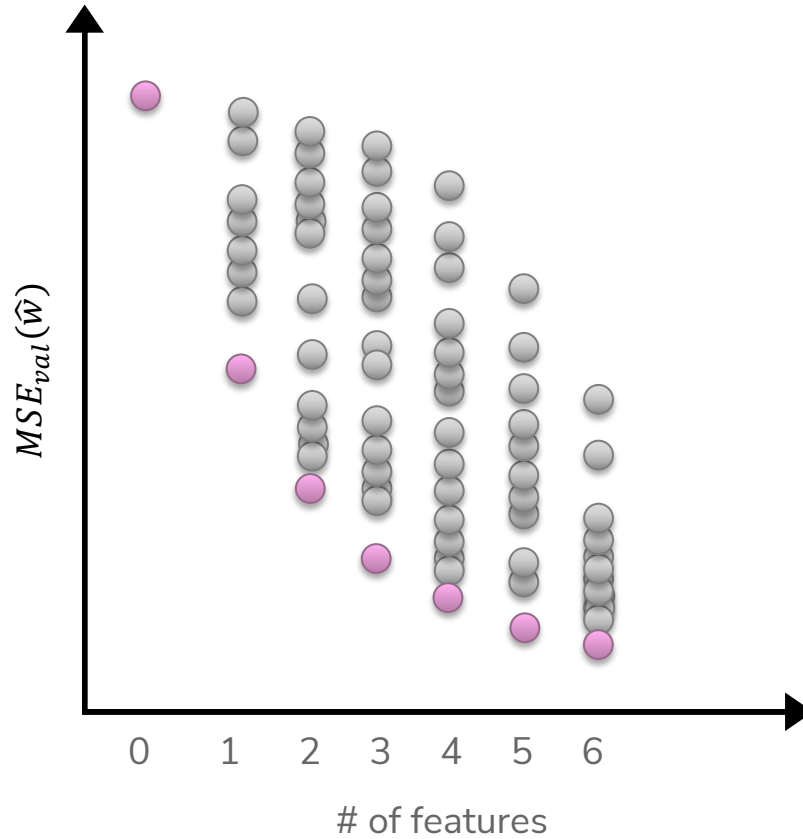
Best Model Size 5



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

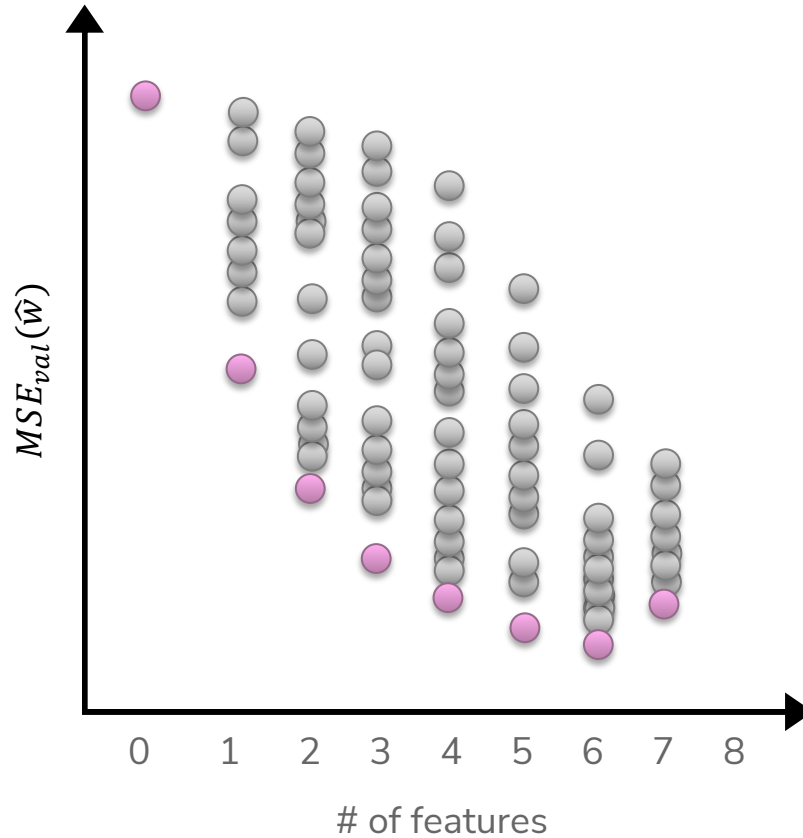
Best Model Size 6



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

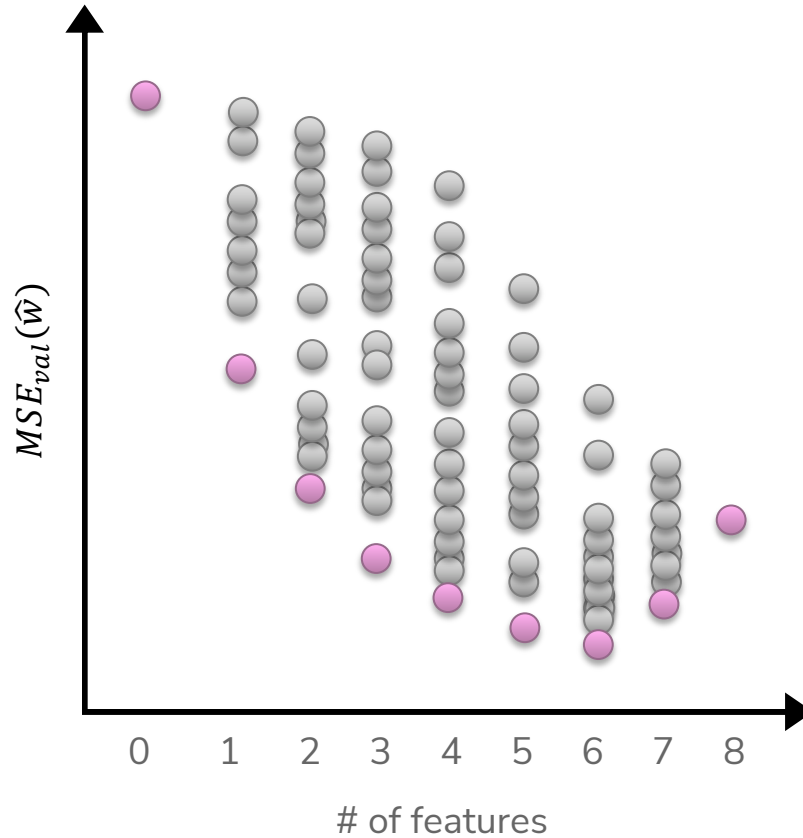
Best Model Size 7



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

Best Model Size 8



Features

- # bathrooms
- # bedrooms
- sq.ft. living
- sq.ft lot
- floors
- year built
- year renovated
- waterfront

Efficiency of All Subsets

How many models did we evaluate?

$\hat{y}_i = w_0$	[0 0 0 ... 0 0 0]
$\hat{y}_i = w_0 + w_1 h_1(x)$	[1 0 0 ... 0 0 0]
$\hat{y}_i = w_0 + w_2 h_2(x)$	[0 1 0 ... 0 0 0]
...	...
$\hat{y}_i = w_0 + w_1 h_1(x) + w_2 h_2(x)$	[1 1 0 ... 0 0 0]
...	...
$\hat{y}_i = w_0 + w_1 h_1(x) + ... + w_D h_D(x)$	[1 1 1 ... 1 1 1]

If evaluating all subsets of 8 features only took 5 seconds, then

16 features would take 21 minutes

32 features would take almost 3 years

100 features would take almost $7.5 \cdot 10^{20}$ years

- 50,000,000,000x longer than the age of the universe!

Think

1 min

We've seen that using a validation set to find the best polynomial degree (from 0 to $p - 1$) requires training p models.

Say you have a dataset with d input columns, and you're using the all subset's approach to find the best features for your model. How many models would you train?

A. d

B. $d - 1$

C. $2d$

D. 2^d

E. 2^{d+1}

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We've seen that using a validation set to find the best polynomial degree (from 0 to $p - 1$) requires training p models.

Say you have a dataset with d input columns, and you're using the all subset's approach to find the best features for your model. How many models would you train?

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B. $d - 1$

C. $2d$

D. 2^d

E. 2^{d+1}

Choose Num Features?

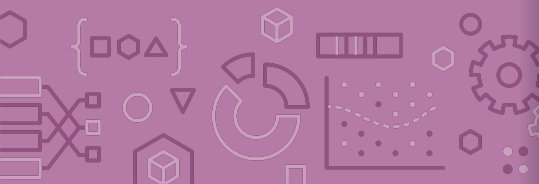
Clearly all subsets is unreasonable. How can we choose how many and which features to include?

Option 1

Greedy Algorithm

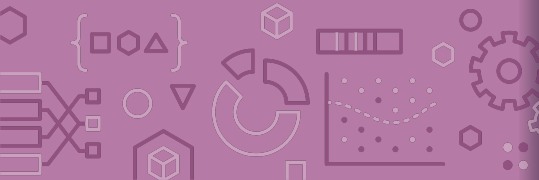
Option 2

LASSO Regression (L1 Regularization)





Brain Break



Greedy Algorithms

Greedy Algorithms

Knowing it's impossible to find exact solution, approximate it!

Forward stepwise

Start from model with no features, iteratively add features as performance improves.

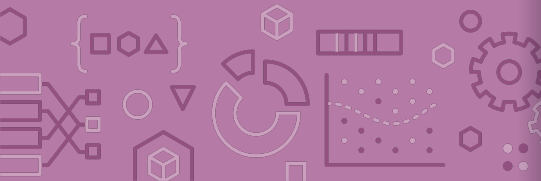
Backward stepwise

Start with a full model and iteratively remove features that are the least useful.

Combining forward and backwards steps

Do a forward greedy algorithm that eventually prunes features that are no longer as relevant

And many many more!



Forward Stepwise

(Example Greedy Algorithm)

Start by selecting number of features k

```
min_val = ∞  
 $S_0 \leftarrow \emptyset$   
for  $i \leftarrow 1..k$ :  
    Find feature  $f_i$  not in  $S_{i-1}$ , that when combined  
    with  $S_{i-1}$ , minimizes the validation loss the most.  
     $S_i \leftarrow S_{i-1} \cup \{f_i\}$   
    if val_loss( $S_i$ ) > min_val:  
        break
```

Called greedy because it makes choices that look best at the time.

Think 

1 min

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Say you want to find the optimal two-feature model, using the forward stepwise algorithm. What model would the forward stepwise algorithm choose?

Features	Val Loss
# bath	201
# bed	300
sq ft	157
year built	224

Features	Val Loss
(# bath, # bed)	120
(# bath, sq ft)	131
(# bath, year built)	190
(# bed, sq ft)	137
(# bed, year built)	209
(sq ft, year built)	145

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(sq ft, year built)	145

Option 2

Regularization

Recap: Regularization

Before, we used the quality metric that minimize loss

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

Change quality metric to balance loss with measure of overfitting

$L(w)$ is the measure of fit

$R(w)$ measures the magnitude of coefficients

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

How do we actually measure the magnitude of coefficients?



Recap: Magnitude

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

$$\hat{w} = \underset{w}{\operatorname{argmin}} MSE(w) + \lambda R(w)$$

Sum?

$$R(w) = w_0 + w_1 + \dots + w_d$$

Doesn't work because the weights can cancel out (e.g. $w_0 = 1000$, $w_1 = -1000$) which so $R(w)$ doesn't reflect the magnitudes of the weights

Sum of absolute values?

$$R(w) = |w_0| + |w_1| + \dots + |w_d| = \|w\|_1$$

It works! We're using L1-norm, for L1-regularization (LASSO)

Sum of squares?

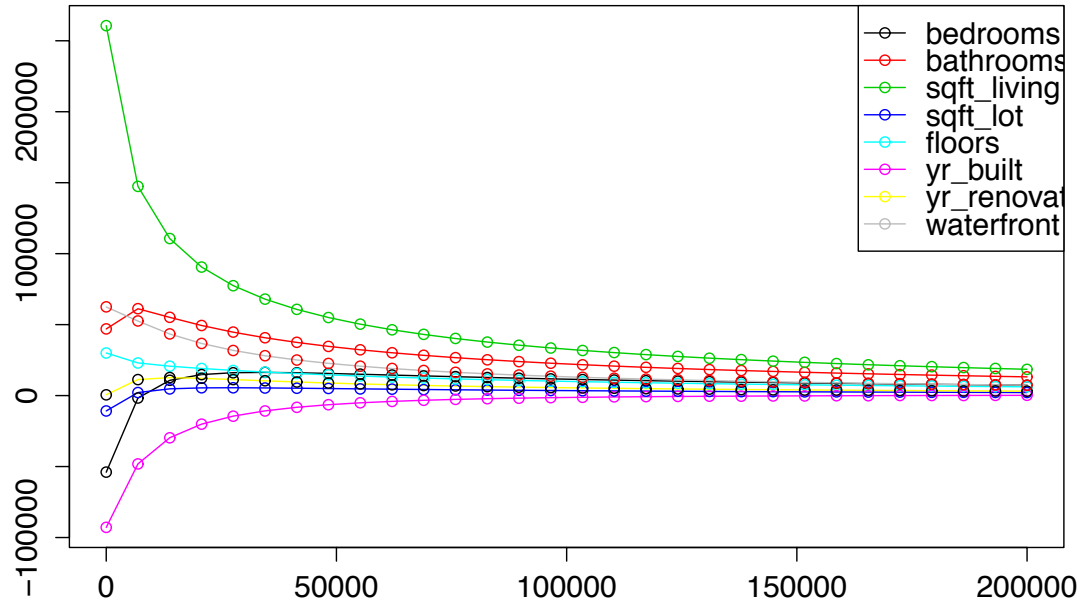
$$R(w) = |w_0|^2 + |w_1|^2 + \dots + |w_d|^2 = w_0^2 + w_1^2 + \dots + w_d^2 = \|w\|_2^2$$

It works! We're using L2-norm, for L2-regularization (Ridge Regression)

Note: Definition of p-Norm: $\|w\|_p^p = |w_0|^p + |w_1|^p + \dots + |w_d|^p$

Ridge for Feature Selection

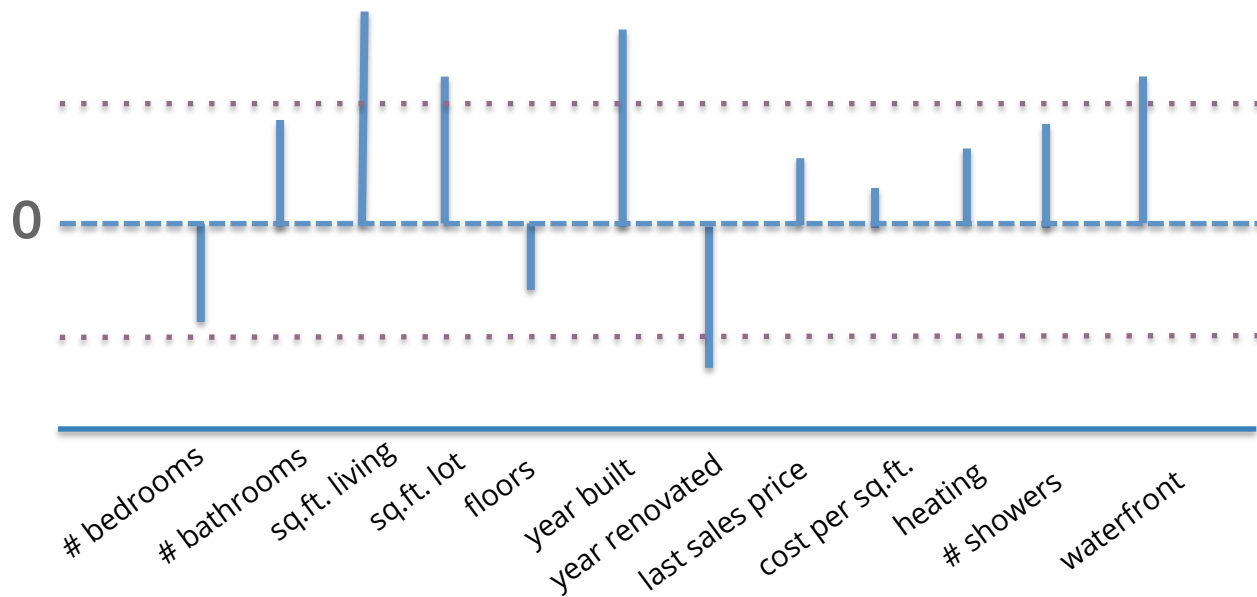
We saw that Ridge Regression shrinks coefficients, but they don't become 0. What if we remove weights that are sufficiently small?



Ridge for Feature Selection

Instead of searching over a **discrete** set of solutions, use regularization to reduce coefficient of unhelpful features.

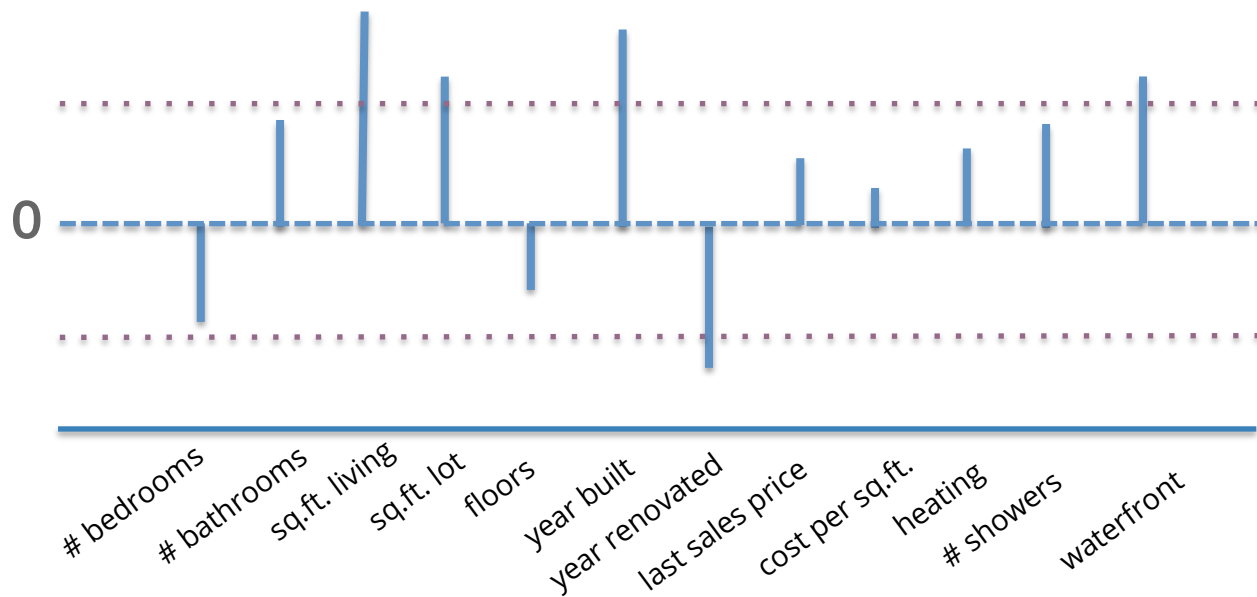
Start with a full model, and then “shrink” ridge coefficients near 0.
Non-zero coefficients would be considered selected as important.



Ridge for Feature Selection

Look at two related features `#bathrooms` and `# showers`.

Our model ended up not choosing any features about bathrooms!

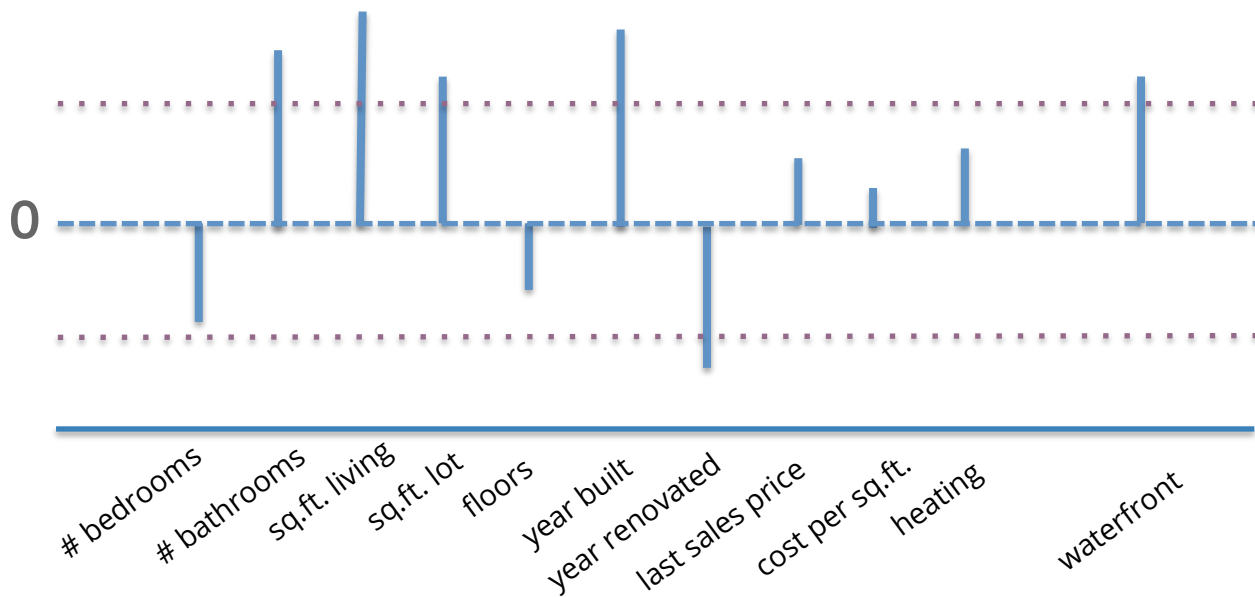


Ridge for Feature Selection

What if we had originally removed the # showers feature?

The coefficient for # bathrooms would be larger since it wasn't "split up" amongst two correlated features

Instead, it would be nice if there were a regularizer that favors sparse solutions in the first place to account for this...



LASSO Regression

Change quality metric to minimize

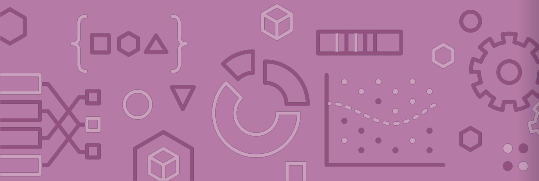
$$\hat{w} = \underset{w}{\operatorname{argmin}} MSE(w) + \lambda \|w\|_1$$

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

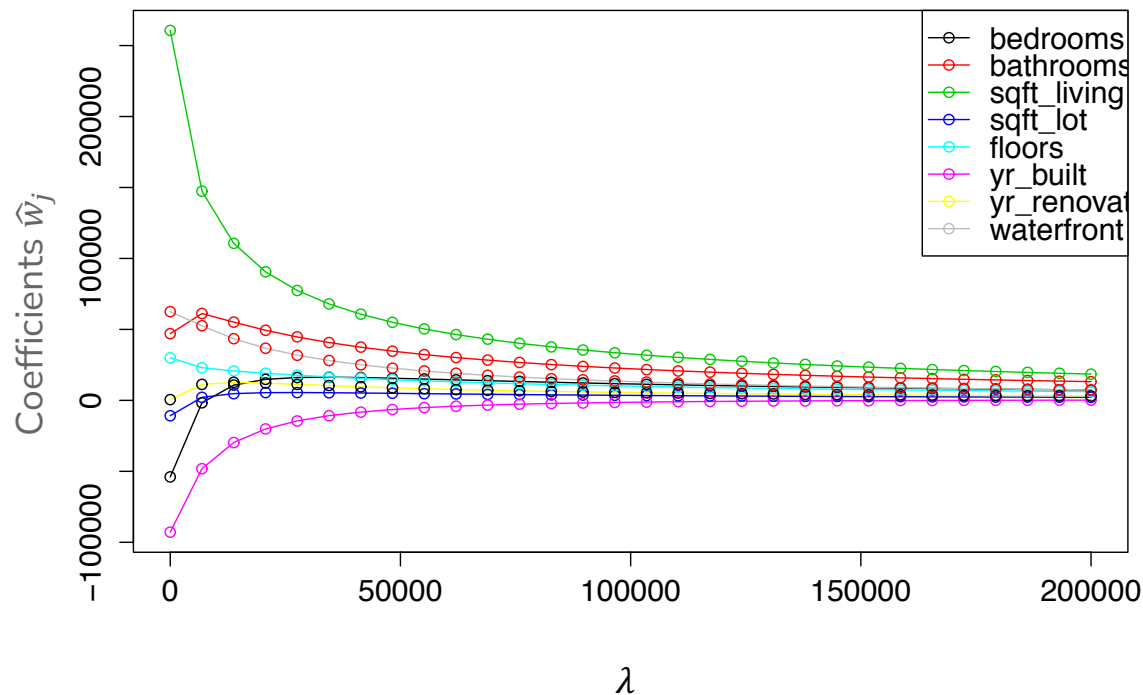
What if $\lambda = 0$?

What if $\lambda = \infty$?

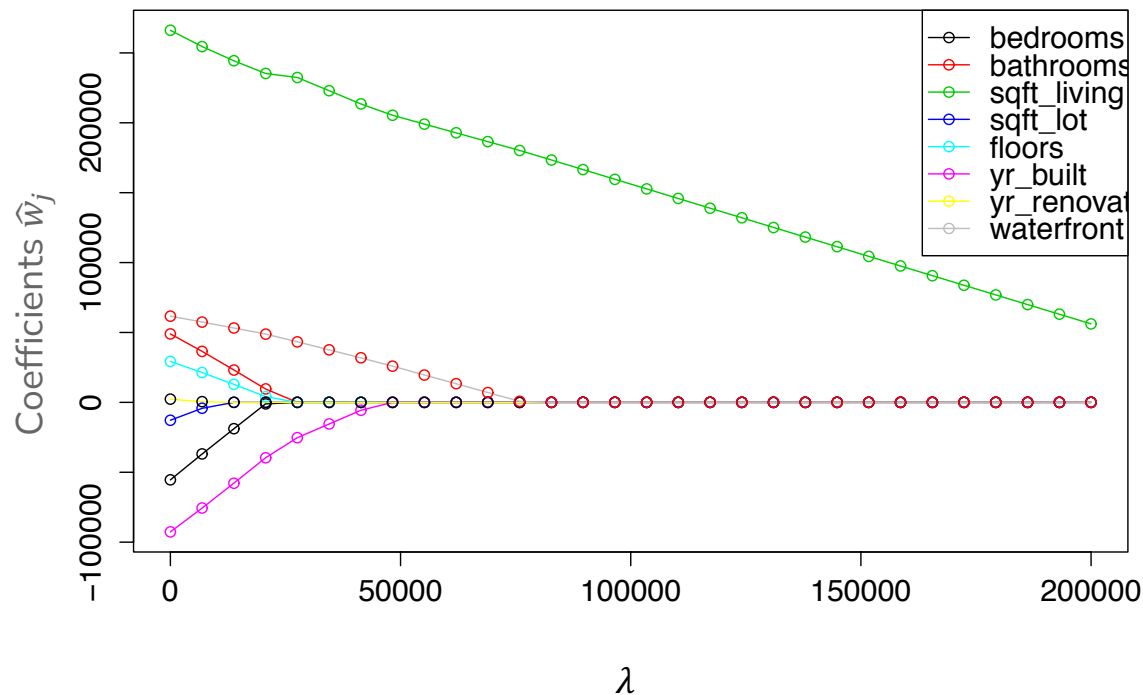
λ in between?



Ridge (L2) Coefficient Paths

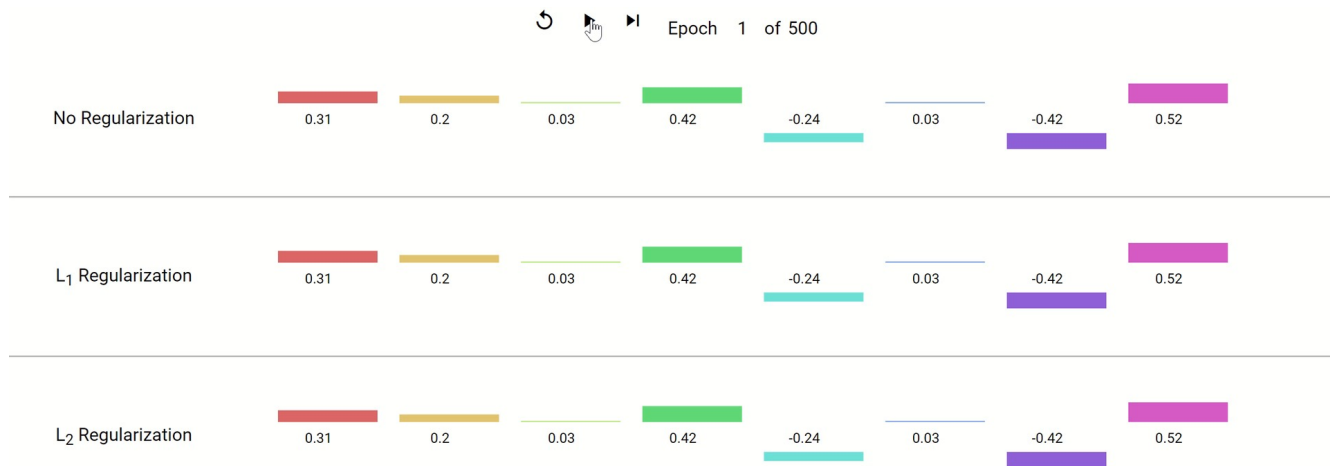


LASSO (L1) Coefficient Paths



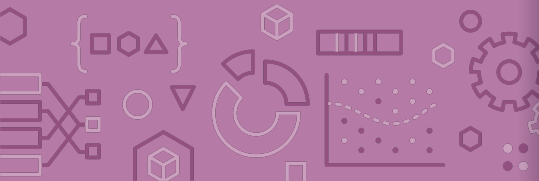
Coefficient Paths – Another View

Example from Google's [Machine Learning Crash Course](#)

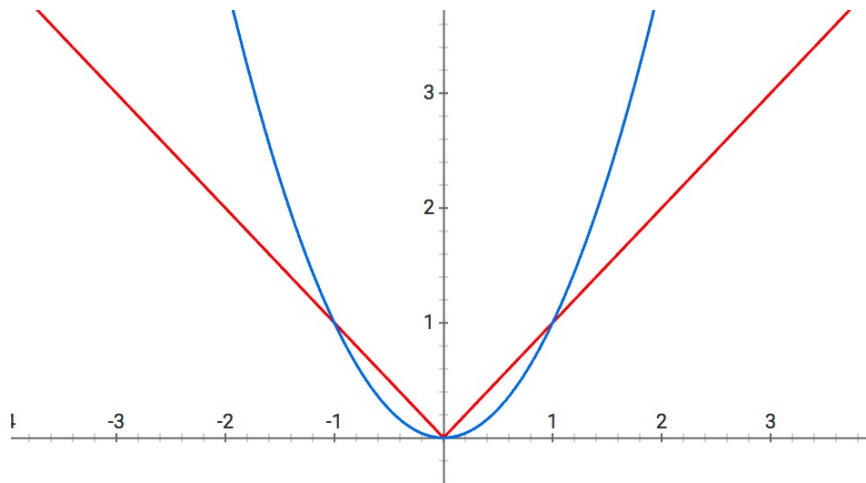


Demo

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



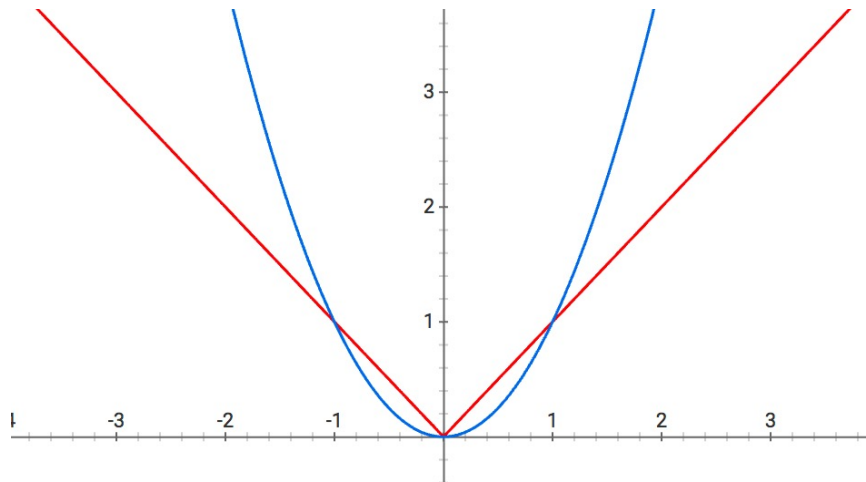
Why might the shape of the L1 penalty cause more sparsity than the L2 penalty?



Sparsity

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.

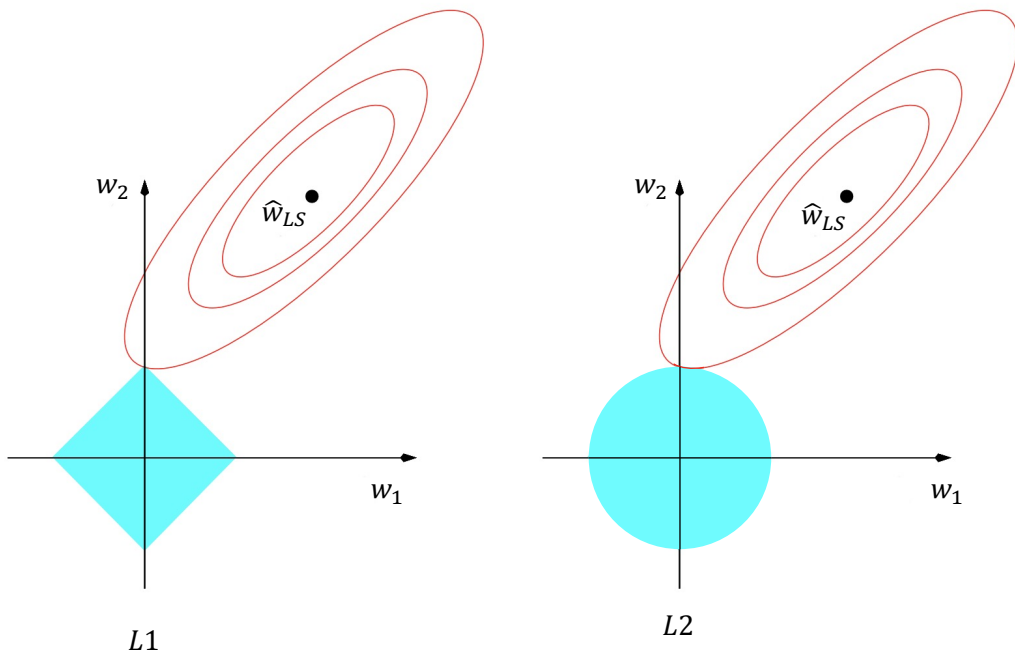
This has to do with the shape of the norm



When w_j is small, w_j^2 is VERY small!

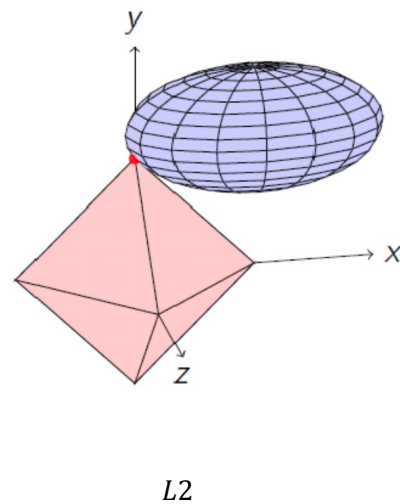
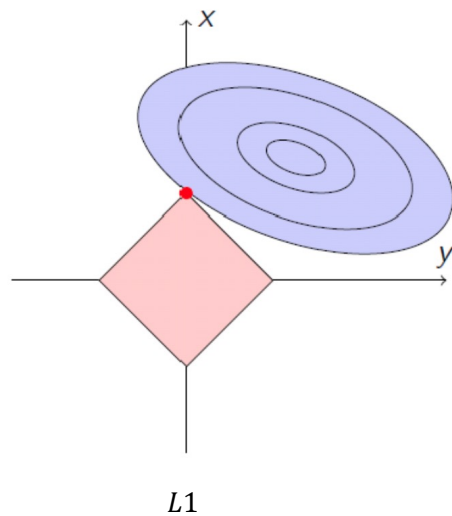
Sparsity Geometry

Another way to visualize why LASSO prefers sparse solutions



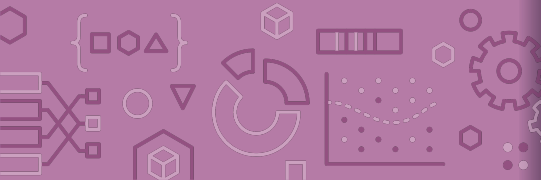
The L1 ball has spikes (places where some coefficients are 0)

Sparsity Geometry





Brain Break



Think 

1 min

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

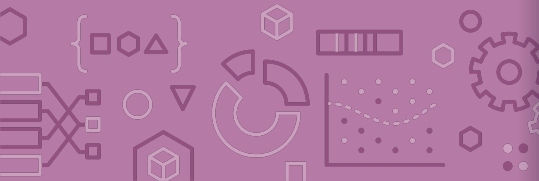
- a) Pick the λ that has the smallest $MSE(\hat{w})$ on the **validation set**
- b) Pick the λ that has the smallest $MSE(\hat{w}) + \lambda \|\hat{w}\|_2^2$ on the **validation set**
- c) Pick the λ that results in the most zero coefficients
- d) Pick the λ that results in the fewest zero coefficients
- 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 algorithm

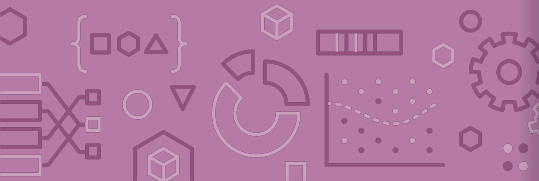


LASSO in Practice

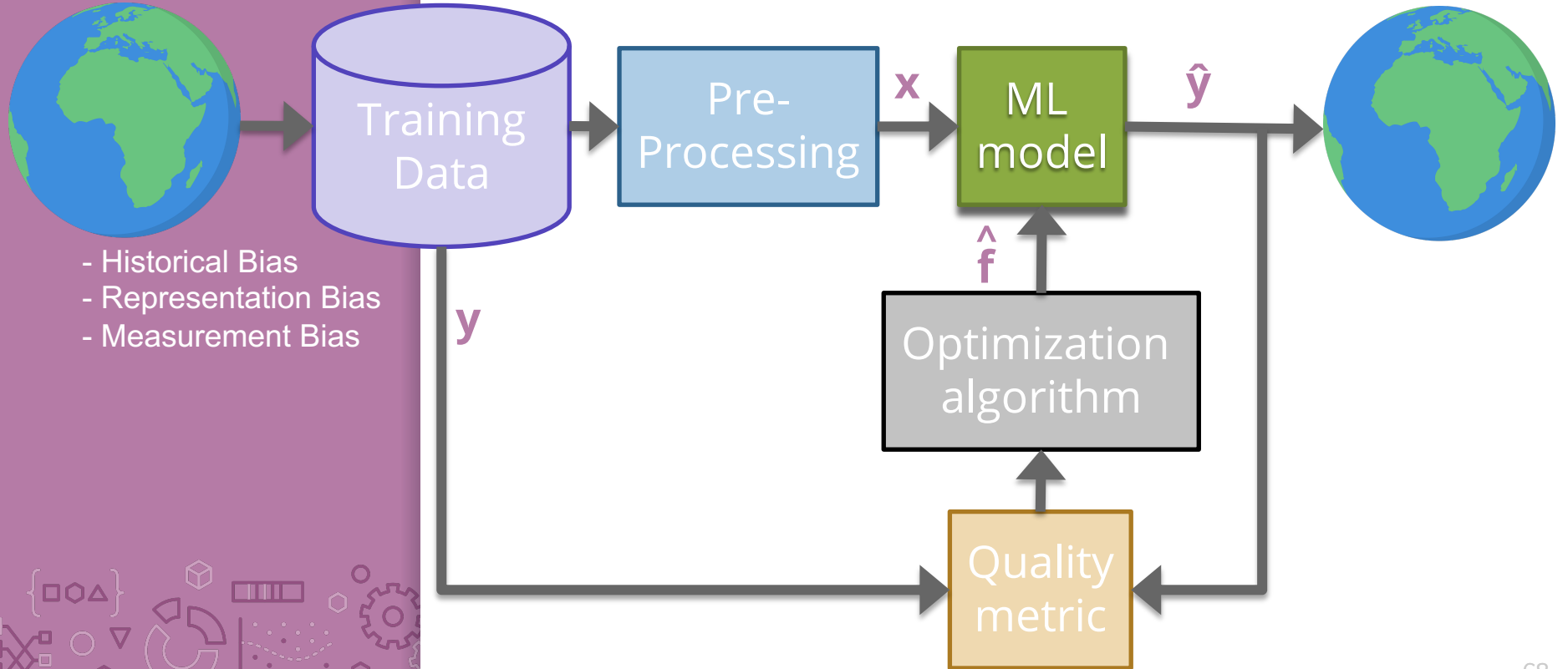
A very common usage of LASSO is in feature selection. If you have a model with potentially many features you want to explore, you can use LASSO on a model with all the features and choose the appropriate λ to get the right complexity.

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



De-biasing LASSO

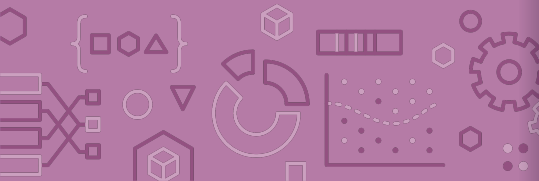
LASSO (and Ridge) adds bias to the Least Squares solution (this was intended to avoid the variance that leads to overfitting)

Recall Bias-Variance Tradeoff

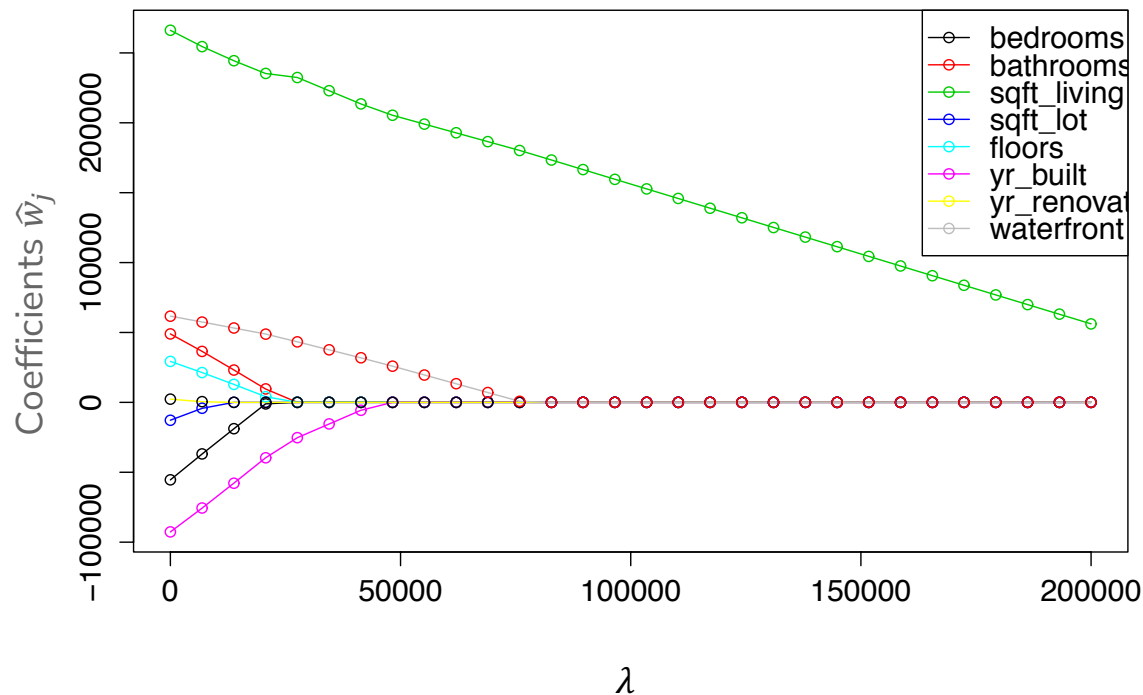
It's possible to try to remove the bias from the LASSO solution using the following steps

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

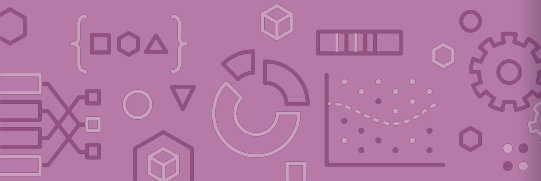


LASSO (L1) Coefficient Paths



(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 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 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!

Think 

1 min

pollev.com/cs416

Suppose you wanted to try out the following models:

LASSO with hyperparameter choices $\lambda \in [0.01, 1, 10]$

Ridge with hyperparameter choices $\lambda \in [0.05, 5, 50]$

Of the 6 models you will try, how do you pick the best predictor learned?

- a) Pick the predictor that has the smallest $MSE(\hat{w})$ on the **validation set**
- b) Pick the predictor that has the smallest $MSE(\hat{w}) + \lambda \|\hat{w}\|_2^2$ on the **validation set**
- c) Pick the predictor that has the smallest $MSE(\hat{w}) + \lambda \|\hat{w}\|_1$ on the **validation set**
- d) None of the above

A Big Grain of Salt

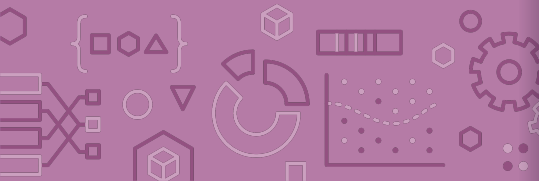
Be careful when interpreting the results of feature selection or feature importance in Machine Learning!

- 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

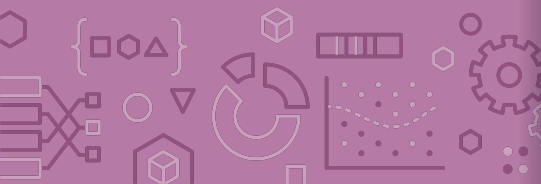
- More computationally efficient as a model (due to the sparse solutions, so you have to compute less dot products)

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: Using regularization to do feature selection

Ideas:

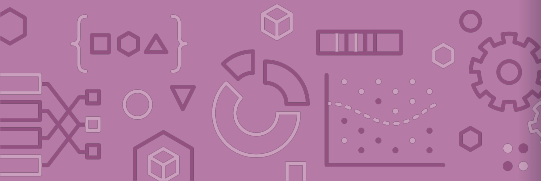
Describe “all subsets” approach to feature selection and why it’s impractical to implement.

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)



Poll Everywhere

Think

5 mins pair
5 mins share

What is a problem relevant to your field / interests that you'd want to use (or are using) machine learning to solve?

Discuss in groups of ~3.

