# CSE/STAT 416

Regularization – LASSO Regression

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Adapted from Hunter Schafer's Slides



#### 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.

## **I** Poll Everywhere

Think &

30 sec



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?



 $\min f(x)$ 

returns the minimum value of f(x)

argmin f(x) xreturns the value of xfor which f(x) attains its minimum

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



#### Cross-Validation



# This should be randomized!

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 12;1

moderate [i]



#### Ridge Regression

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

Change quality metric to minimize

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

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



 $\lambda$  in between?

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

## **I** Poll Everywhere

X Minutes

How does  $\lambda$  affect the bias and variance of the model? For each underlined section, select "Low" or "High" appropriately.

When  $\lambda = 0 \implies (omple \times$ 

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

When  $\lambda = \infty$   $\implies$  Simple

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



#### Choosing $\lambda$



The process for selecting  $\lambda$  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

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

2

Compute validation error

 $\checkmark$  validation\_error =  $MSE_{val}(\widehat{w}_{ridge(\lambda)})$ 

Track  $\lambda$  with smallest *validation\_error* 

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

#### Scaling Features

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

$$\tilde{h}_j(x_i) = \frac{h_j(x_i) - \mu_j(x_1, \dots, x_N)}{\sigma_j(x_1, \dots, x_N)} \qquad \begin{array}{c} \text{For feature j} \\ \text{Mj mean} \end{array}$$

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*:

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

**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!

# **I** Poll Everywhere

Think 원

1 min



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

Overfitting / Underfitting Train Set / Test Set Bias Variance Regularization



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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).  $\widehat{w}$  could have  $10^{11}$  coefficients. Evaluating  $\widehat{y} = \widehat{w}^T h(x)$  would be very slow!

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

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

## Sparsity: Housing



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

Lot size Single Family Year built Last sold price Last sale price/sqft Finished sqft Unfinished sqft Finished basement sqft # floors Flooring types Parking type Parking amount Cooling Heating Exterior materials Roof type Structure style

Dishwasher Garbage disposal Microwave Range / Oven Refrigerator Washer Dryer Laundry location Heating type letted Tub Deck Fenced Yard Lawn Garden Sprinkler System

•••

#### Sparsity: Reading Minds

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





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





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



















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





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



0 1 2

















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





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





## **I** Poll Everywhere

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.

for deg in [0,...,p-1]: • train model w/ degree deg on +rain set • get val error return model w/ least val error

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.* 2*d* 

#### **I** Poll Everywhere

Group 22

2 min

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*A. d B. d* − 1 *C.* 2*d* 

#### 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)

L2⇒ Ridge L1⇒LASSO







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* 



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

## **I** Poll Everywhere

1 min



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

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



2 min



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(sq ft, year built)	145

Option 2 Regularization

#### Recap: Regularization

L(w) is the mea R(w) measures ג

Before, we used the quality metric that minimize loss  $\widehat{w} = \underset{w}{\operatorname{argmin}} L(w)$ 

Change quality metric to balance loss with measure of overfitting L(w) is the measure of fit R(w) measures the magnitude of coefficients

$$\widehat{w} = \operatorname{argmin}_{w} L(w) + R(w)$$

How do we actually measure the magnitude of coefficients?

## Recap: Magnitude

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

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

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?  $\rightarrow Ll$  Regularization  $R(w) = |w_0| + |w_1| + \dots + |w_d| = ||w||_1$ 

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

Sum of squares?  $\Rightarrow$  L2 Regularization  $R(w) = |w_0|^2 + |w_1|^2 + ... + |w_d|^2 = w_0^2 + w_1^2 + ... + w_d^2 = ||w||_2^2$ 

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

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

## MUST NORMALIZE

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



Coeffi

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. Small threshhold # bedrooms rooms sq.ft. lot floors built vear built vear renovated price per sq.ft. heating waterfront vear last sales price cost per sq.ft. heating waterfront

Look at two related features #bathrooms and # showers.

Our model ended up not choosing any features about bathrooms!





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





 $\lambda$  is a tuning parameter that changes how much the model cares about the regularization term.

What if 
$$\lambda = 0$$
?  
 $\omega = \alpha r g min MSE(\omega) = \omega_{ors}$ 

What if 
$$\lambda = \infty$$
?  
 $\hat{\omega} = \operatorname{argmin} \lambda \| \omega \|_{1} = 0$ 

## Ridge (L2) Coefficient Paths



## LASSO (L1) Coefficient Paths



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#### 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?

 $\omega = [\omega_0, \omega_1]$ 



#### 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.



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

## Sparsity Geometry





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

## Sparsity Geometry











## **I** Poll Everywhere

1 min

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How should we choose the best value of  $\lambda$  for LASSO?

- (a) Pick the  $\lambda$  that has the smallest  $MSE(\hat{w})$  on the **validation set** 
  - b) Pick the  $\lambda$  that has the smallest  $MSE(\hat{w}) + \lambda ||\hat{w}||_2^2$  on the **validation set**
  - c) Pick the  $\lambda$  that results in the most zero coefficients
  - d) Pick the  $\lambda$  that results in the fewest zero coefficients
  - e) None of the above

Same as in Ridge!

#### Choosing $\lambda$

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

Exactly the same as Ridge Regression :)

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

For any hyper-parameter: Pick the hyperparameter tha has the lowest errval = MSE val (ŵ)

#### 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  $\lambda$  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



#### De-biasing LASSO



#### As you increase $\lambda$ , the resulting models have less voriance and high bigs

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



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## (De-biased) LASSO In Practice

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- 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  $\lambda$  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 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

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

Combines both to achieve best of both worlds!
## **I** Poll Everywhere

1 min

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?



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

ONLY USED IN TRAINING!

## 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: 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  $\boldsymbol{\lambda}$  is varied

Interpret LASSO coefficient path plot

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



# **I** Poll Everywhere

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.