

Unit 5


LASSO Regularization and Feature Selection

EE-UY 4563/EL-GY 9143: INTRODUCTION TO MACHINE LEARNING
PROF. SUNDEEP RANGAN (WITH MODIFICATION BY YAO WANG)

Learning Objectives

- ☐ Describe **model selection** and identify when it may be needed
- ☐ Mathematically describe linear regression with **regularization**
- ☐ Select regularizers to impose constraints such as sparsity
- ☐ Compute an L1-regularized estimate (LASSO) using sklearn tools
- ☐ Compute the optimal regularization level using cross validation
- ☐ Interpret results from a LASSO path
- ☐ Set regularizer based on a probabilistic prior
- ☐ Perform other feature selection methods

Outline

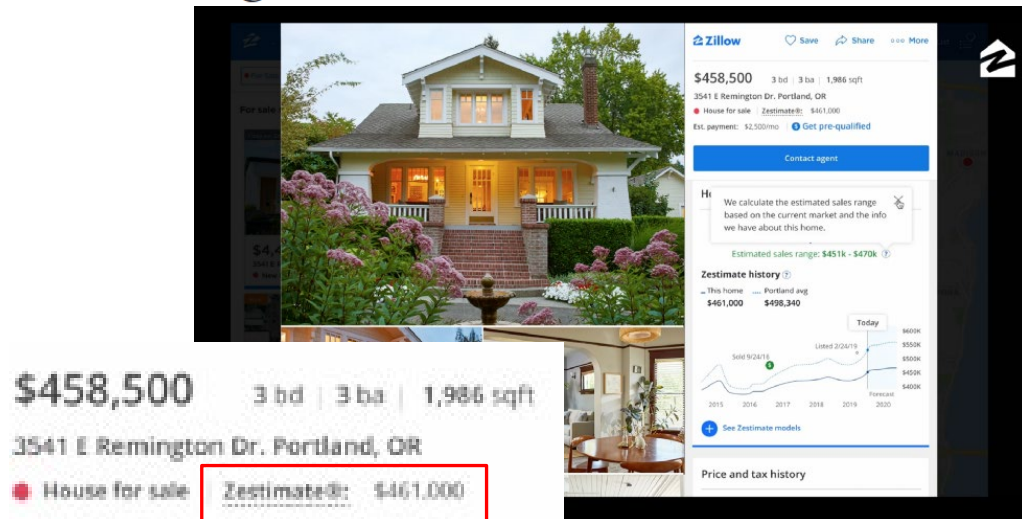
 Motivating Example: Feature selection in predicting housing prices

- ☐ Model selection and regularization
- ☐ Housing prices prediction with LASSO
- ☐ Probabilistic interpretation
- ☐ Other model selection examples
- ☐ Other model selection methods
- ☐ In-Class Exercise: Audio Pitch Detection

Predicting Housing Prices

AI, MACHINE LEARNING & RESEARCH

Introducing a new and improved Zestimate algorithm



<https://www.zillow.com/tech/introducing-a-new-and-improved-zestimate-algorithm/>

- ❑ Many services now predict house prices
- ❑ Data science enters real estate!
- ❑ Many possible variables:
 - Square meters
 - Condition
 - Zip code
 - Education quality
 - ...
- ❑ What variables *really* determine the price?



Ames, Iowa Dataset



Ames, Iowa: Alternative to the Boston Housing Data as an End of Semester Regression Project

[Dean De Cock](#)

Truman State University

Journal of Statistics Education Volume 19, Number 3(2011),
www.amstat.org/publications/jse/v19n3/decock.pdf

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Key Words: Multiple Regression; Linear Models; Assessed Value; Group Project.

Abstract

This paper presents a data set describing the sale of individual residential property in Ames, Iowa from 2006 to 2010. The data set contains 2930 observations and a large number of explanatory variables (23 nominal, 23 ordinal, 14 discrete, and 20 continuous) involved in assessing home values. I will discuss my previous use of the Boston Housing Data Set and I will suggest methods for incorporating this new data set as a final project in an undergraduate regression course.

- ❑ Ames, Iowa Dataset
 - Sales from 2006 to 2010
 - From Dean De Cock
- ❑ Alternative to Boston Housing dataset
- ❑ Many more variables to explore
 - Approximately 81 variables
 - 2930 samples

Loading the Dataset

```
1 df = pd.read_csv('housing_train.csv')
2 df.head()
```

	Id	MSSubClass	MSZoning	LotFrontage	LotArea	Street	Alley	LotShape	LandContour	Utilities	...	PoolArea	PoolQC	Fence	MiscFeature	MiscVal
0	1	60	RL	65.0	8450	Pave	NaN	Reg	Lvl	AllPub	...	0	NaN	NaN	NaN	0
1	2	20	RL	80.0	9600	Pave	NaN	Reg	Lvl	AllPub	...	0	NaN	NaN	NaN	0
2	3	60	RL	68.0	11250	Pave	NaN	IR1	Lvl	AllPub	...	0	NaN	NaN	NaN	0
3	4	70	RL	60.0	9550	Pave	NaN	IR1	Lvl	AllPub	...	0	NaN	NaN	NaN	0
4	5	60	RL	84.0	14260	Pave	NaN	IR1	Lvl	AllPub	...	0	NaN	NaN	NaN	0

5 rows × 81 columns

Issues:

- Many different types of data: Discrete and continuous
- Missing values (NaN)

Data Cleaning

```
1 nsamp, natt = df.shape
2 print('Number samples = %d' % nsamp)
3 print('Number attributes per sample = %d' % natt)
```

Number samples = 1460
Number attributes per sample = 81

```
1 df = df.dropna(axis=1)
2
3 nsamp, natt = df.shape
4 print('Number samples = %d' % nsamp)
5 print('Number attributes per sample = %d' % natt)
6
```

```
1 df = df.loc[df['SaleCondition'] == 'Normal']
2
3 nsamp, natt = df.shape
4 print('Number samples = %d' % nsamp)
5 print('Number attributes per sample = %d' % natt)
```

Number samples = 1198
Number attributes per sample = 62

❑ Original data

❑ Remove columns with NaN values

- Could use more sophisticated methods

❑ Keep only normal sales

- Recommended in De Cock paper
- Makes fitting much easier

Categorical Variables

- ❑ Data has many categorical variables
- ❑ Need to code the categorical variables to numerical values

Real valued

Categorical

	Id	MSSubClass	MSZoning	LotFrontage	LotArea	Street	Alley	LotShape	LandContour	Utilities	...	PoolArea
0	1	60	RL	65.0	8450	Pave	NaN	Reg	Lvl	AllPub	...	0
1	2	20	RL	80.0	9600	Pave	NaN	Reg	Lvl	AllPub	...	0
2	3	60	RL	68.0	11250	Pave	NaN	IR1	Lvl	AllPub	...	0
3	4	70	RL	60.0	9550	Pave	NaN	IR1	Lvl	AllPub	...	0
4	5	60	RL	84.0	14260	Pave	NaN	IR1	Lvl	AllPub	...	0

Splitting the Variables

❑ First, split the variables into categorical and real

```
# Remove the ID, month sold and sales price (it is the target)
ignore_vars = ['Id', 'MoSold', 'SalePrice']

# Find real and categorical variables
cols = df.columns
cat_vars = []
real_vars = []

for col in cols:
    if not (col in ignore_vars):
        if df.dtypes[col] == 'object':
            cat_vars.append(col)
        else:
            real_vars.append(col)
```

Categorical variables = ['MSZoning', 'Street', 'Alley', 'LotShape', 'LandContour', 'Utilities', 'LotConfig', 'LandSlope', 'Neighborhood', 'Condition1', 'Condition2', 'BldgType', 'HouseStyle', 'RoofStyle', 'RoofMatl', 'Exterior1st', 'Exterior2nd', 'MasVnrType', 'ExterQual', 'ExterCond', 'Foundation', 'BsmtQual', 'BsmtCond', 'BsmtExposure', 'BsmtFinType1', 'BsmtFinType2', 'Heating', 'HeatingQC', 'CentralAir', 'Electrical', 'KitchenQual', 'Functional', 'FireplaceQu', 'GarageType', 'GarageFinish', 'GarageQual', 'GarageCond', 'PavedDrive', 'PoolQC', 'Fence', 'MiscFeature', 'SaleType', 'SaleCondition']

Real variables = ['MSSubClass', 'LotFrontage', 'LotArea', 'OverallQual', 'OverallCond', 'YearBuilt', 'YearRemodAdd', 'MasVnrArea', 'BsmtFinSF1', 'BsmtFinSF2', 'BsmtUnfSF', 'TotalBsmtSF', '1stFlrSF', '2ndFlrSF', 'LowQualFinSF', 'GrLivArea', 'BsmtFullBath', 'BsmtHalfBath', 'FullBath', 'HalfBath', 'BedroomAbvGr', 'KitchenAbvGr', 'TotRmsAbvGrd', 'Fireplaces', 'GarageYrBlt', 'GarageCars', 'GarageArea', 'WoodDeckSF', 'OpenPorchSF', 'EnclosedPorch', '3SsnPorch', 'ScreenPorch', 'PoolArea', 'MiscVal', 'YrSold']

One Hot Coding

Original

	MSZoning	Street	LotShape	LandContour	Utilities	LotConfig
0	RL	Pave	Reg	Lvl	AllPub	Inside
1	RL	Pave	Reg	Lvl	AllPub	FR2
2	RL	Pave	IR1	Lvl	AllPub	Inside
4	RL	Pave	IR1	Lvl	AllPub	FR2
5	RL	Pave	IR1	Lvl	AllPub	Inside

One Hot coded

	MSZoning_FV	MSZoning_RH	MSZoning_RL	MSZoning_RM	Street_Pave
0	0	0	1	0	1
1	0	0	1	0	1
2	0	0	1	0	1
4	0	0	1	0	1
5	0	0	1	0	1

- ❑ Use pandas `get_dummies`
- ❑ Replaces categorical variables with one-hot coded values
 - Ex: MSZoning
 - Becomes MSZoning_FV, MSZoning_RH, ...

```
# Get the dataframes with real and categorical variables
df_real = df[real_vars]
df_cat = df[cat_vars]

# One-hot encode the categorical variables
df_cat_enc = pd.get_dummies(df_cat, drop_first=True)
```

Scaling Data

- ❑ Split data into training and test
- ❑ Scale data
 - Remove mean and variance
- ❑ Needed to compare coefficients
 - Ensures that all variables have same range
- ❑ Note: The scaling transform is
 - Fit on the training data
 - Performed on training and test

```
from sklearn.model_selection import train_test_split  
  
Xtr, Xts, ytr, yts = train_test_split(X,y,test_size=0.3)
```

```
from sklearn.preprocessing import StandardScaler  
  
# Create the scaler objects  
xscal = StandardScaler()  
yscal = StandardScaler()  
  
# Fit and transform the training data  
Xtr1 = xscal.fit_transform(Xtr)  
ytr1 = yscal.fit_transform(ytr[:,None])  
  
# Transform the test data  
Xts1 = xscal.transform(Xts)  
yts1 = yscal.transform(yts[:,None])
```

First Try: Linear Regression

```
from sklearn.linear_model import LinearRegression, Ridge
from sklearn.metrics import r2_score

# Fit
reg_ls = LinearRegression()
reg_ls.fit(Xtr1, ytr1)

# Training R^2
yhat1_tr = reg_ls.predict(Xtr1)
rsq_tr = r2_score(yhat1_tr, ytr1)
print('Training R^2 = %12.4e' % rsq_tr)

# Test R^2
yhat1_ts = reg_ls.predict(Xts1)
rsq_ts = r2_score(yts1, yhat1_ts)
print('Test R^2      = %12.4e' % rsq_ts)
```

```
Training R^2 = 9.3726e-01
Test R^2      = -1.0430e+20
```

- ❑ Simple idea:
 - Use linear regression over features
- ❑ Fits the training data very well!
 - $R^2 \approx 0.937$
- ❑ But, completely fails on the test data
 - $R^2 > 10^{20}$

Conditioning

- ❑ What went wrong?
- ❑ Recall LS solution is: $\hat{\beta} = (A^T A)^{-1} A^T y$
- ❑ Matrix $A^T A$ may be ill-conditioned
 - Eigenvalues close to zero
 - Inverse blows up
- ❑ With ill-conditioned data:
 - Training error is fine
 - But the test error blows up
- ❑ Overfits data

```
from sklearn.linear_model import LinearRegression, Ridge
from sklearn.metrics import r2_score

# Fit
reg_ls = LinearRegression()
reg_ls.fit(Xtr1, ytr1)

# Training R^2
yhat1_tr = reg_ls.predict(Xtr1)
rsq_tr = r2_score(yhat1_tr, ytr1)
print('Training R^2 = %12.4e' % rsq_tr)

# Test R^2
yhat1_ts = reg_ls.predict(Xts1)
rsq_ts = r2_score(yts1, yhat1_ts)
print('Test R^2      = %12.4e' % rsq_ts)
```

```
Training R^2 = 9.3726e-01
Test R^2      = -1.0430e+20
```

Improving Conditioning via Ridge Regression

❑ Standard LS solution: $\hat{\beta} = (A^T A)^{-1} A^T y$

❑ **Ridge Regression**: Add a conditioning term:

$$\hat{\beta} = (A^T A + cI)^{-1} A^T y$$

- c is a small positive value.
- Makes inverse well-behaved
- We will see this technique more later

❑ Get good test R^2

```
reg_ls = Ridge(alpha=1e-5)
reg_ls.fit(Xtr1, ytr1)
yhat1 = reg_ls.predict(Xts1)
rsq = r2_score(yts1, yhat1)
print('Test R^2      = %12.4e' % rsq)
```

Test R^2 = 0.904567

What Components Matter?

❑ Simple idea: Look at large coefficients

❑ We see variables that we may expect:

- Square footage
- Quality
- Zoning

❑ But there are some issues

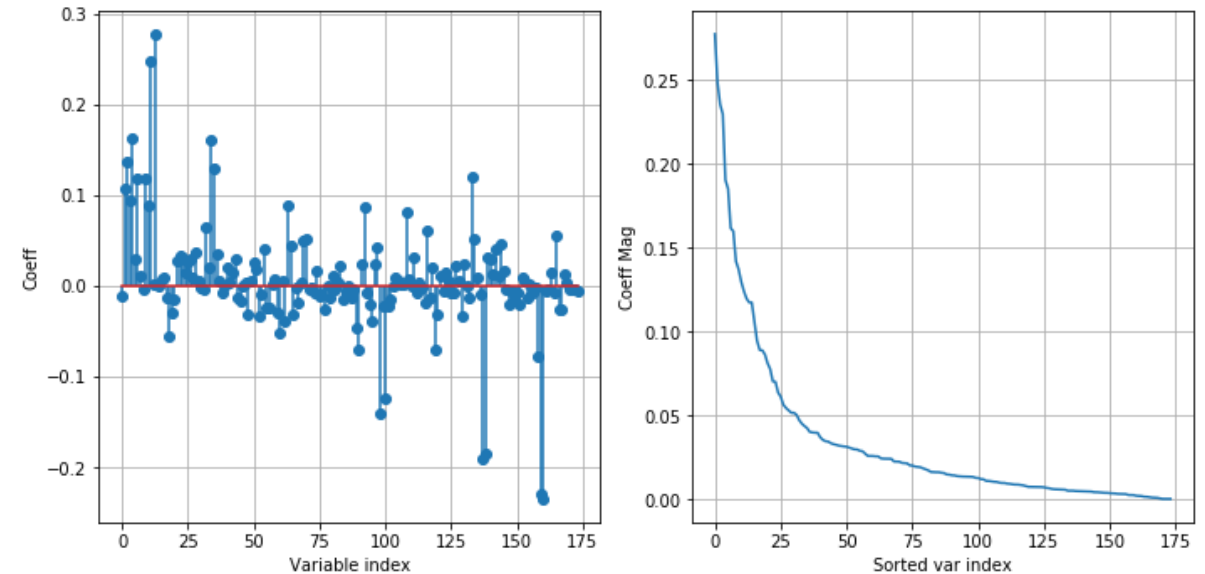
- Some variables seem highly correlated
- Ex: GrLivArea and 2ndFlrSF
- KitchenQual and OverallQual
- Do we need both?

```
1 coeff_ls = reg_ls.coef_.ravel()
2 nprint = 10
3 I = np.argsort(np.abs(coeff_ls))
4 I = np.flipud(I)
5 for i in range(nprint):
6     j = I[i]
7     print('%20s %f' % (xnames[j], coeff_ls[j]))
```


```
GrLivArea 0.277146
2ndFlrSF 0.248113
KitchenQual_TA -0.235208
KitchenQual_Gd -0.229472
ExterQual_Gd -0.190125
ExterQual_TA -0.184943
YearBuilt 0.161462
MSZoning_RL 0.159591
RoofStyle_Gable -0.141669
OverallQual 0.136913
```

What Components Do *Not* Matter?

- ❑ All coefficients are far from zero
- ❑ Very few coefficients that can be removed
- ❑ Does this mean all variables matter?
- ❑ **Model or feature selection problem:**
 - *How do we find the variables that matter?*



Outline

- ☐ Motivating Example: Feature selection in predicting housing prices
-  ☐ Model selection and regularization
 - ☐ Housing prices prediction with LASSO
 - ☐ Probabilistic interpretation
 - ☐ Other model selection examples
 - ☐ Other model selection methods
- ☐ In-Class Exercise: Audio Pitch Detection

Model Selection via Sparsity

	MSZoning_FV	MSZoning_RH	MSZoning_RL	MSZoning_RM	Street_Pave	LotShape_IR2	LotShape_IR3	LotShape_Reg	LandContour_HLS
0	0	0	1	0	1	0	0	1	0
1	0	0	1	0	1	0	0	1	0
2	0	0	1	0	1	0	0	0	0
4	0	0	1	0	1	0	0	0	0
5	0	0	1	0	1	0	0	0	0

174 variables after
one-hot coding

❑ **Model selection problem:** Need to identify the parameters that *really* matter

- Help interpret results
- Improves generalization error (less parameters)

❑ **Idea:** Fit model under **sparsity constraint**:

- Linear model: $\hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$
- Feature x_j is ignored if $\beta_j = 0$
- Try to force most $\beta_j = 0 \Rightarrow$ Model only uses a few of the variables

Regularized LS Estimation

❑ **Regularization**: General method for finding constrained solutions

- E.g. solutions that are sparse

❑ Standard least squares estimation (from Lecture 3):

$$\hat{\beta} = \arg \min_{\beta} MSE(\beta), \quad MSE(\beta) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

❑ **Regularized estimator**:

$$\hat{\beta} = \arg \min_{\beta} J(\beta), \quad J(\beta) = MSE(\beta) + \phi(\beta)$$

- $MSE(\beta)$ = mean-squared prediction error from before
- $\phi(\beta)$ = regularizing function.

❑ **Concept**: Regularizer penalizes β that are “unlikely”

- Constrains estimate to smaller set of parameters

Two Common Regularizers

❑ Ridge regression (called L2)

$$\phi(\beta) = \frac{\alpha}{n} \sum_{j=1}^d |\beta_j|^2$$

❑ LASSO regression (called L1)

$$\phi(\beta) = 2\alpha \sum_{j=1}^d |\beta_j|$$

❑ Coefficient $\alpha > 0$ determines regularization level

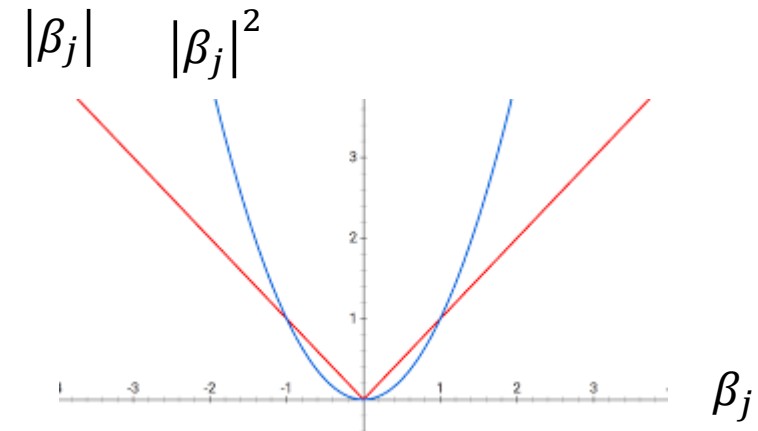
- Higher $\alpha \Rightarrow$ Higher level of regularization, more constrained
- Will show how to select α later via cross-validation
- Scaling factors adjust to match sklearn convention

❑ Both penalize large β_j : Tries to make β_j small

- Will see that L1 also promotes sparsity

❑ Convention: Do not include intercept term β_0

- In general, no reason to make this term small



L1 and L2 Norm

□ Ridge and LASSO Regularization can be written with **norms**

□ **Ridge** cost function:

$$J(\boldsymbol{\beta}) = \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \alpha \sum_{j=1}^d |\beta_j|^2 = \|\mathbf{y} - \mathbf{A}\boldsymbol{\beta}\|^2 + \alpha \|\boldsymbol{\beta}\|_2^2$$

□ **LASSO** cost function:

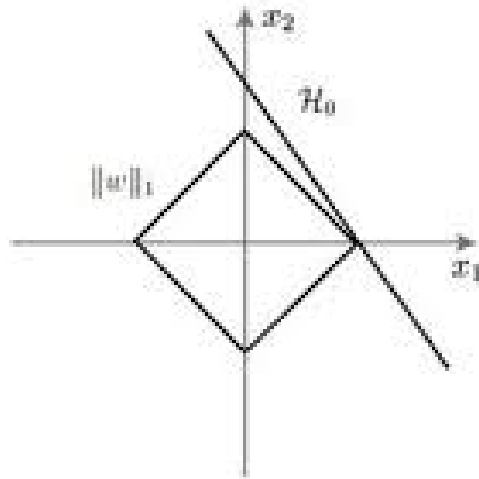
$$J(\boldsymbol{\beta}) = \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \alpha \sum_{j=1}^d |\beta_j| = \frac{1}{2n} \|\mathbf{y} - \mathbf{A}\boldsymbol{\beta}\|^2 + \alpha \|\boldsymbol{\beta}\|_1$$

◦ $\|\boldsymbol{\beta}\|_1$ = **L1 norm** (pronounced ell-1)

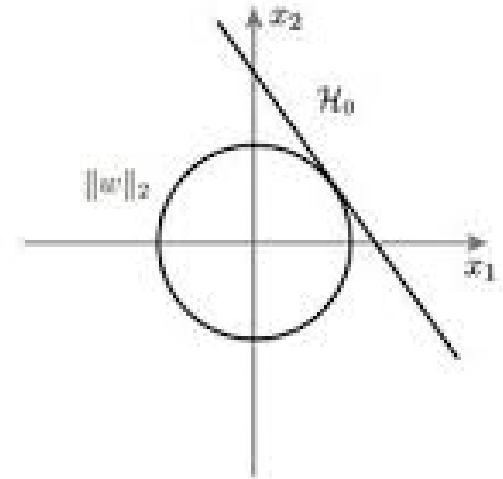
Ridge vs LASSO

- L2 tends to lead to many “small” coefficients
 - But solutions are not exactly zero
 - Not ideal for feature selection
- L1 tends to lead to more **sparse** solutions
 - Several coefficients are zero

A L1 regularization



B L2 regularization



Solving Ridge Regression

- Ridge regression problem: Find β to minimize

$$J(\beta) = \|\mathbf{y} - A\beta\|^2 + \alpha\|\beta\|^2$$

- Solution for given regularization level

$$\beta_{ridge} = (A^T A + \alpha I)^{-1} A^T \mathbf{y}$$

- Set gradient = 0
- See homework

- Sklearn function for ridge regression:

- http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Ridge.html

Solving LASSO Regression

□ LASSO cost function:

$$J(\boldsymbol{\beta}) = \frac{1}{2n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \alpha \sum_{j=1}^d |\beta_j| = \frac{1}{2n} \|\mathbf{y} - \mathbf{A}\boldsymbol{\beta}\|^2 + \alpha \|\boldsymbol{\beta}\|_1$$

□ Because derivative of $|\beta_j|$ is not continuous, there is no closed-form solution.

□ Many methods to solve iteratively

- Least angle regression (LAR), coordinate descent, ADMM
- However, the cost function is convex \Rightarrow no local minima [See Unit 7]
- Beyond the scope of this class
- See textbook [Hastie2008] for LAR method

Data Scaling

❑ Scaling: Whenever using regularization:

- Scale each feature and the target to have zero mean and unit variance (or STD)
- $x_{ij} \rightarrow (x_{i,j} - \bar{x}_j) / \text{STD}(x_{ij})$
- $y_i \rightarrow (y_i - \bar{y}) / \text{STD}(y_i)$

❑ After predictor for the scaled data are determined:

- Derive the equivalent predictor on the original data (HW!)

❑ Motivation:

- Without scaling, the regularization level depends on the data range
- With mean removal, we do not need the intercept term β_0
- So that the regularization term is simply a L2 or L1 norm of coefficient vector

Selecting the Regularization Level

- ❑ How do we select regularization level α ?
 - Higher $\alpha \Rightarrow$ More constrained / simpler model
 - Lower $\alpha \Rightarrow$ More complex model
- ❑ Similar to inverse of model order
- ❑ Find α via cross-validation

Pseudo-code

Split in training X_{tr}, y_{tr} and test X_{ts}, y_{ts} .

For α in α_{test} :

- $\hat{\beta} = \text{fit}(X_{tr}, y_{tr}, \alpha)$ // Fit on training data
- $\hat{y}_{ts} = \text{predict}(X_{ts})$ // Predict on test data
- $S[\alpha] = \text{score}(y_{ts}, \hat{y}_{ts})$ // Score on test data

$\hat{\alpha} = \text{argmax } S[\alpha]$ // Select α with highest test score

Summary

Method	Regularizer	Effect on parameters	Solution for Fitting
None	$\phi(\boldsymbol{\beta}) = 0$	Leaves parameters unconstrained	$\hat{\boldsymbol{\beta}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{y}$
Ridge	$\phi(\boldsymbol{\beta}) = \frac{\alpha}{n} \ \boldsymbol{\beta}\ _2^2$	Makes parameters small Close to zero	$\hat{\boldsymbol{\beta}} = (\mathbf{A}^T \mathbf{A} + \alpha \mathbf{I})^{-1} \mathbf{A}^T \mathbf{y}$
LASSO	$\phi(\boldsymbol{\beta}) = 2\alpha \ \boldsymbol{\beta}\ _1$	Makes parameters sparse. Many coefficients exactly zero	No analytic solution. Need to run an optimizer

❑ Regularized least squares

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} J(\boldsymbol{\beta}), \quad J(\boldsymbol{\beta}) = \frac{1}{n} \|\mathbf{y} - \mathbf{A}\boldsymbol{\beta}\|^2 + \phi(\boldsymbol{\beta})$$

❑ Whatever you choose for the regularizer:

- Scale data before training
- Select regularization level with cross-validation

In-Class Exercise

Question

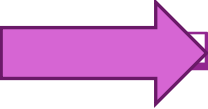
We wish to fit a linear model of the form,

$$\hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p,$$

for a problem with $p = 100$ variables. Suggest regularizers $\phi(\boldsymbol{\beta})$ to impose the following constraints:

- (a) All the coefficients $\beta_j, j = 1, \dots, p$ should be close to zero, but not necessarily exactly zero.
- (b) Most of the coefficients $\beta_j, j = 1, \dots, p$ should be exactly zero
- (c) Among the first fifty coefficients, $\beta_j, j = 1, \dots, 50$, most coefficients should be zero. But, the other coefficients should be unconstrained.

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LASSO Regression in Python

❑ Sklearn built in Lasso class

❑ Easy to use

- Set alpha
- Fit on training data
- Predict and score on test

Test $R^2 = 0.899122$

```
1 from sklearn.linear_model import Lasso
2 from warnings import simplefilter
3 from sklearn.exceptions import ConvergenceWarning
4 simplefilter("ignore", category=ConvergenceWarning)
5
6 # Select alpha
7 alpha = 3e-3
8
9 # Create Lasso object and fit on training data
10 reg = Lasso(alpha=alpha)
11 reg.fit(Xtr1, ytr1)
12
13 # Predict and score on test
14 yhat1 = reg.predict(Xts1)
15 rsq = r2_score(yts1, yhat1)
16
17 print('Test  $R^2 =$  %f' % rsq)
```

Optimizing Alpha via Cross Validation

- ❑ In each fold we:
 - Split data into training and test
 - Fit the scale on the training
 - Transform training and test
 - For each alpha:
 - Fit training and score on test
- ❑ Note: Scaling is redone on each fold
 - Ensures scaling is part of the training

```
10 # Run the cross-validation
11 rsq = np.zeros((nalpha, nfold))
12 for ifold, ind in enumerate(kf.split(X)):
13
14     # Get the training data in the split
15     Itr, Its = ind
16     Xtr = X[Itr, :]
17     ytr = y[Itr]
18     Xts = X[Its, :]
19     yts = y[Its]
20
21     # Fit and transform the data
22     Xtr1 = xscal.fit_transform(Xtr)
23     Xts1 = xscal.transform(Xts)
24     ytr1 = yscal.fit_transform(ytr[:, None])
25     yts1 = yscal.transform(yts[:, None])
26
27     for i, alpha in enumerate(alphas):
28
29         # Fit on the training data
30         reg = Lasso(alpha=alpha)
31         reg.fit(Xtr1, ytr1)
32
33         # Score on the test data
34         yhat1 = reg.predict(Xts1)
35         rsq[i, ifold] = r2_score(yts1, yhat1)
36
37     print('Fold = %d' % ifold)
38
39 # Compute mean and SE
40 rsq_lasso_mean = np.mean(rsq, axis=1)
41 rsq_lasso_se = np.std(rsq, axis=1) / np.sqrt(nfold-1)
```

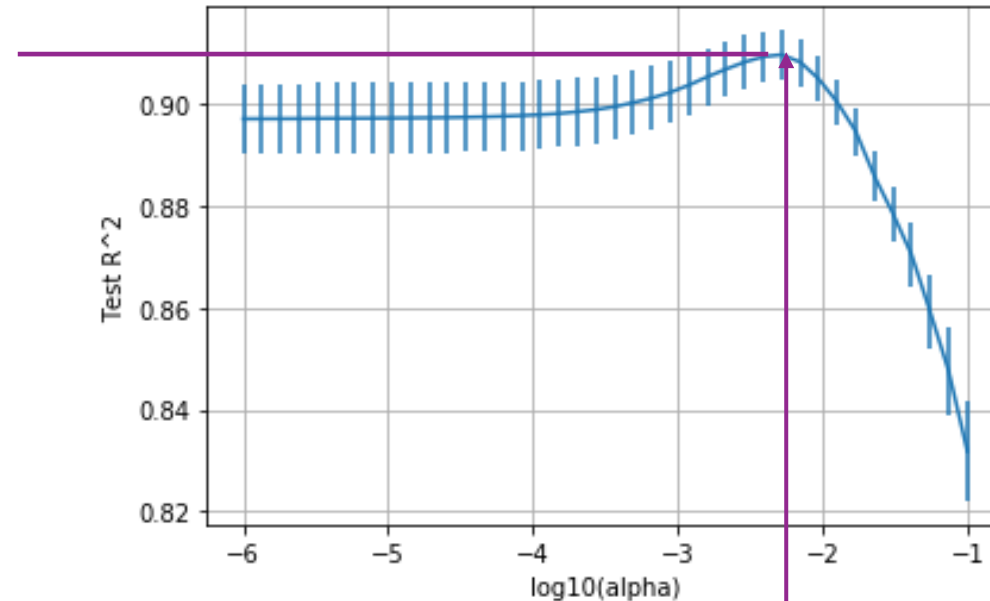
Cross Validation: Normal Rule

Max mean test R^2

□ Select alpha to maximize mean test R^2

- Normal rule
- Lower values of $\alpha \Rightarrow$ overfit
- Higher values of $\alpha \Rightarrow$ underfit

Alpha optimal (normal rule) = $5.2233e-03$
Mean test R^2 (normal rule) = 0.910



Under-regularized
Overfit

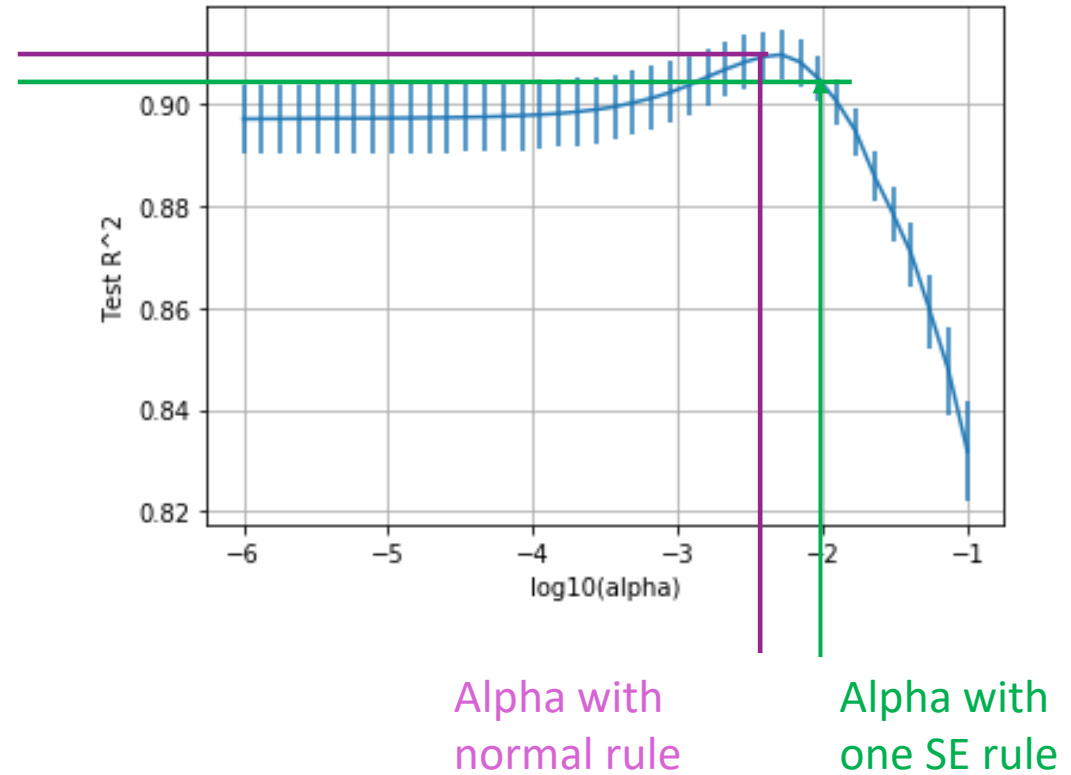
Optimal Alpha
(normal rule)

Over-regularized
Underfit

Cross Validation: One SE Rule

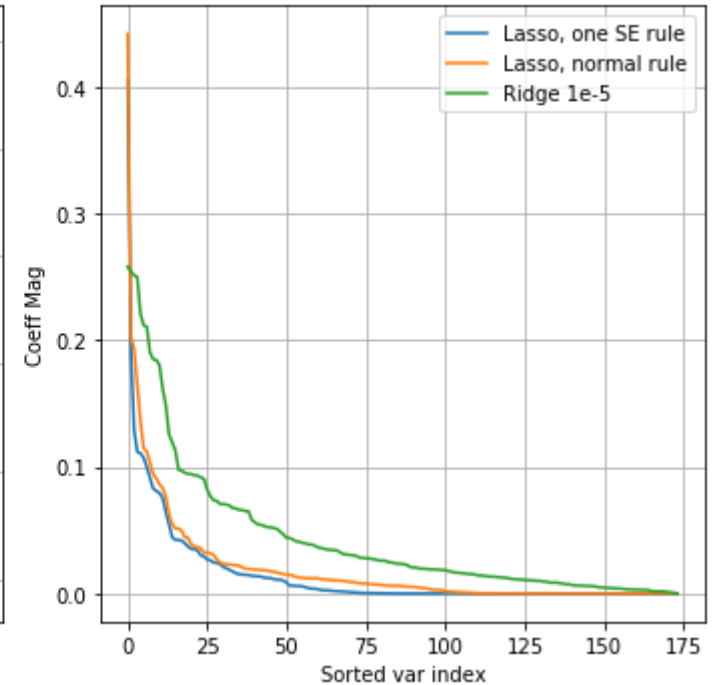
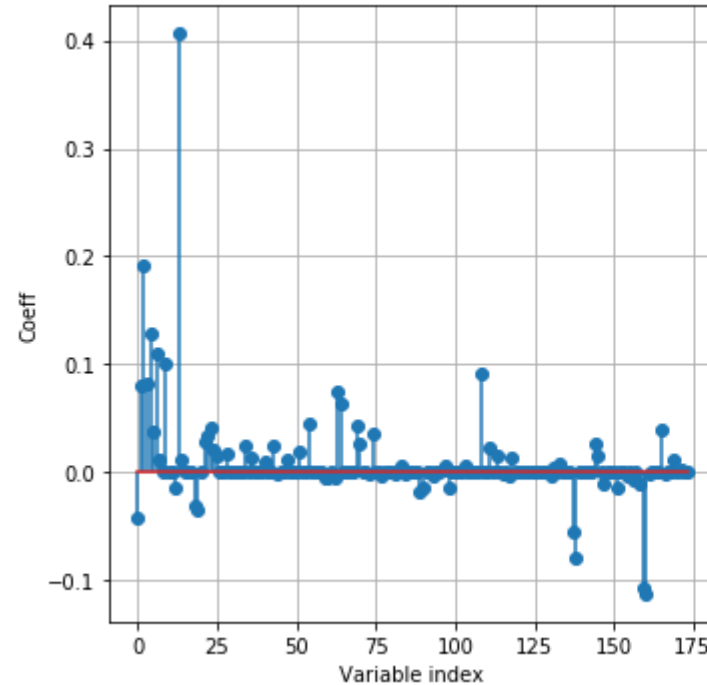
Max mean test R^2
Max mean test R^2 -one SE

- Can also use one SE rule:
 - Selects a higher regularized model
 - More sparse solution



Sparsity in the Coefficients

- Adding L1 regularization:
 - Makes coefficient smaller
 - Many coefficients approx. 0



Most Important Variables

❑ Right table: Variables with 10 large coefficient magnitudes

❑ Minimally regularized (Ridge) has:

- Variables that are highly correlated
- Ex: GrLivArea and 2ndFlrSF
- Several large variables

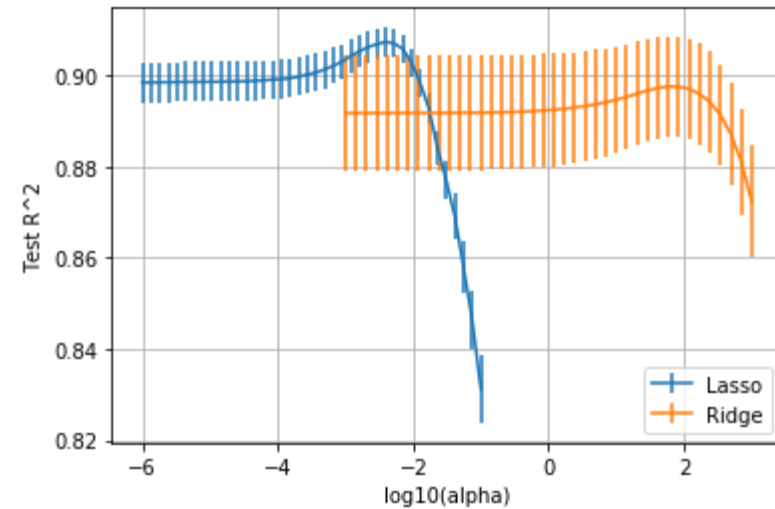
❑ Lasso:

- Reduces correlated variables
- Selects GrLivArea alone
- Gives the variables more importance

Ridge		Lasso	
GrLivArea	0.29	GrLivArea	0.42
2ndFlrSF	0.26	OverallQual	0.18
KitchenQual_Gd	-0.21	KitchenQual_TA	-0.17
KitchenQual_TA	-0.20	KitchenQual_Gd	-0.16
LotArea	0.18	YearBuilt	0.13
YearBuilt	0.16	BsmtFinSF1	0.12
OverallQual	0.16	Neighborhood_NoRidge	0.09
ExterQual_Gd	-0.15	OverallCond	0.09
Exterior2nd_VinylSd	0.15	TotalBsmtSF	0.09
ExterQual_TA	-0.15	LotArea	0.08

Ridge Vs. Lasso

- ❑ Can optimize alpha for both regularizer
- ❑ Optimal mean test R^2 is better for LASSO
- ❑ Offers better feature selection

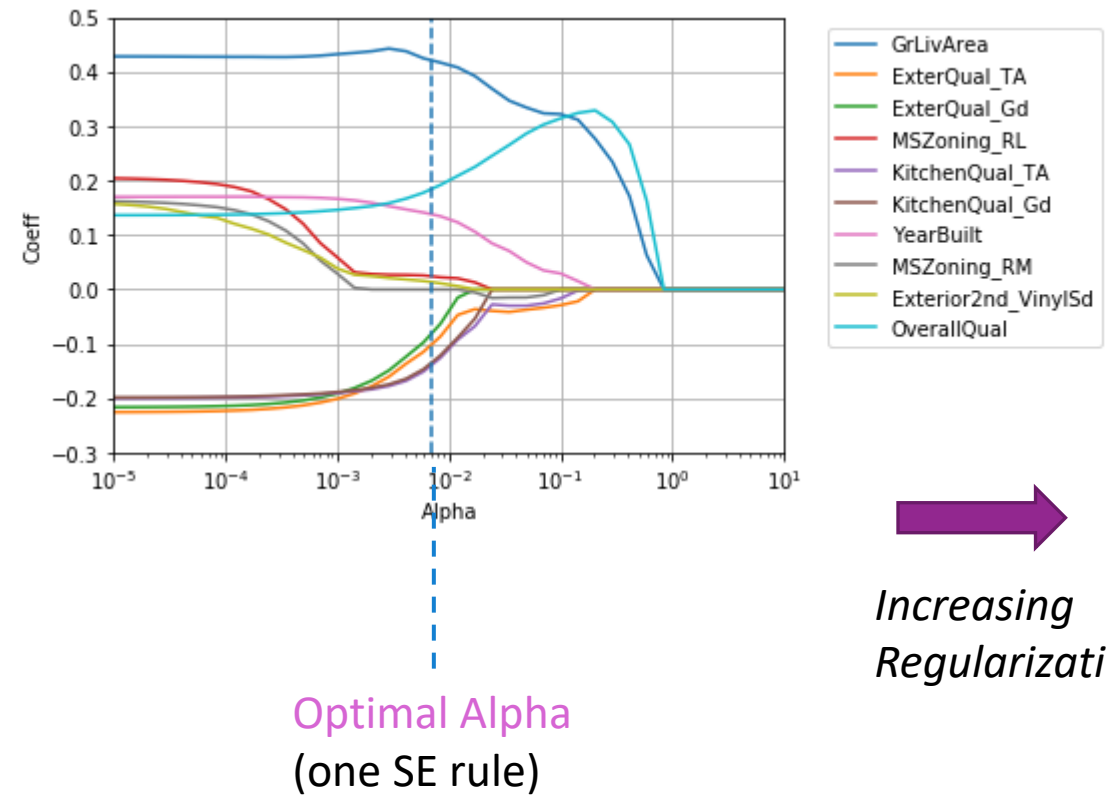


Optimal R^2 Lasso: 0.907283

Optimal R^2 Ridge: 0.897498

Lasso Path


- Plot of coefficients vs. alpha
- For large alpha:
 - All coefficients are zero
- As alpha is decreased:
 - One coefficient is activated at a time
 - Indicates an ordering of importance



Finding the Final Regressor

- ❑ Select features from cross-validation
- ❑ Re-run ordinary (un-regularized) regression on reduced features
- ❑ Use K –fold validation
- ❑ K -folds yield K weights and biases
- ❑ Take mean of the weights and biases for the final parameter estimate
- ❑ Take mean of the test MSE for the estimate of the test MSE

Outline

- ❑ Motivating Example: Feature selection in predicting housing prices
- ❑ Model selection and regularization
- ❑ Housing prices prediction with LASSO
- ❑ Probabilistic interpretation
- ❑ Other model selection examples
- ❑ Other model selection methods
- ❑ In-Class Exercise: Audio Pitch Detection

Maximum Likelihood Estimate

- Suppose that true data generated from probabilistic model with Gaussian noise:

$$\mathbf{y} = A\boldsymbol{\beta} + \mathbf{w}, \quad w_i \sim N(0, \sigma^2)$$

- Maximum likelihood estimator:

$$\hat{\boldsymbol{\beta}} = \arg \max_{\boldsymbol{\beta}} p(\mathbf{y}|A, \boldsymbol{\beta}) = \arg \min_{\boldsymbol{\beta}} [-\ln p(\mathbf{y}|A, \boldsymbol{\beta})]$$

- Gaussian density for noise in \mathbf{y} : $\ln p(\mathbf{y}|A, \boldsymbol{\beta}) = -\frac{1}{2\sigma^2} \|\mathbf{y} - A\boldsymbol{\beta}\|^2$

- Hence

$$\hat{\boldsymbol{\beta}} = \arg \max_{\boldsymbol{\beta}} p(\mathbf{y}|A, \boldsymbol{\beta}) = \arg \min_{\boldsymbol{\beta}} [\|\mathbf{y} - A\boldsymbol{\beta}\|^2] = \text{Least Squares Solution}$$

Bayes Estimation (MAP Estimate)

□ Maximum a posterior (MAP) estimator of β :

$$\hat{\beta} = \arg \max_{\beta} p(\beta | y, A)$$

- $\hat{\beta}$ = Most likely parameter value given evidence y, A

□ Bayes Rule: $p(\beta | y, A) = p(y|A, \beta)p(\beta)/p(y|A)$

□ Hence: $\hat{\beta} = \arg \max_{\beta} p(y|A, \beta)p(\beta)$ (because y and A are fixed)

- Likelihood: $p(y|A, \beta)$ How well β matches data
- Prior: $p(\beta)$: How well β agrees with prior knowledge about its distribution (constraints)

□ More in probability class...

Bayes Estimation with Logarithms

- Often easier to use logarithms:

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= \arg \max_{\boldsymbol{\beta}} p(\mathbf{y} | A, \boldsymbol{\beta}) p(\boldsymbol{\beta}) = \arg \min_{\boldsymbol{\beta}} [-\ln p(\mathbf{y} | A, \boldsymbol{\beta}) p(\boldsymbol{\beta})] \\ &= \arg \min_{\boldsymbol{\beta}} [-\ln p(\mathbf{y} | A, \boldsymbol{\beta}) - \ln p(\boldsymbol{\beta})]\end{aligned}$$

- Gaussian density for noise in \mathbf{y} : $\ln p(\mathbf{y} | A, \boldsymbol{\beta}) = -\frac{1}{2\sigma^2} \|\mathbf{y} - A\boldsymbol{\beta}\|^2$

- Hence

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\frac{1}{2\sigma^2} \|\mathbf{y} - A\boldsymbol{\beta}\|^2 - \ln p(\boldsymbol{\beta}) \right] = \arg \min_{\boldsymbol{\beta}} [\|\mathbf{y} - A\boldsymbol{\beta}\|^2 + \phi(\boldsymbol{\beta})]$$

- **Conclusion:** MAP estimate = regularized LS with $\phi(\boldsymbol{\beta}) = -2\sigma^2 \ln p(\boldsymbol{\beta})$
 - Penalize $\boldsymbol{\beta}$ proportional to $-\ln p(\boldsymbol{\beta})$: Less likely $\boldsymbol{\beta}$ penalized more

Ridge and Lasso as Bayesian Estimators

□ Bayesian Estimator:

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\frac{1}{2\sigma^2} \|\mathbf{y} - A \boldsymbol{\beta}\|^2 - \ln p(\boldsymbol{\beta}) \right]$$

□ Assuming β_j are i.i.d. Gaussian with zero mean:

$$p(\beta_j) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\beta_j^2 / 2\sigma^2), \quad -\log p(\beta_j) = \beta_j^2 / 2\sigma^2 + \text{constants}$$


$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\|\mathbf{y} - A \boldsymbol{\beta}\|^2 + \frac{\sigma^2}{\gamma^2} \|\boldsymbol{\beta}\|^2 \right] = \text{Ridge Regression!}$$

□ Assuming β_j are i.i.d. Laplacian with zero mean:

$$p(\beta_j) = \frac{1}{2\sigma} \exp(-|\beta_j|/\sigma), \quad -\log p(\beta_j) = |\beta_j|/\sigma + \text{constant}$$

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left[\|\mathbf{y} - A \boldsymbol{\beta}\|^2 + \frac{2\sigma^2}{\gamma} \|\boldsymbol{\beta}\|_1 \right] = \text{Lasso Regression!}$$

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Example 1: Medical Modeling

- ❑ Ex: Prostate specific antigen (PSA) test
 - Many years ago, PSA level was being consider for cancer screening
 - Question: Is a PSA test good for cancer?
 - Obtain features of prostate and correlate with PSA level
 - Determine if cancer volume is a relevant feature
 - See demo 1 on github site
 - Also in text

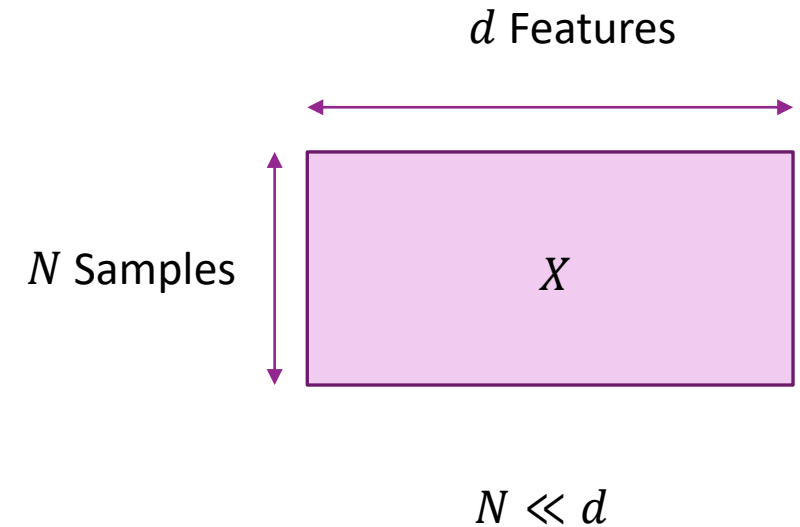


The data frame has the following components:

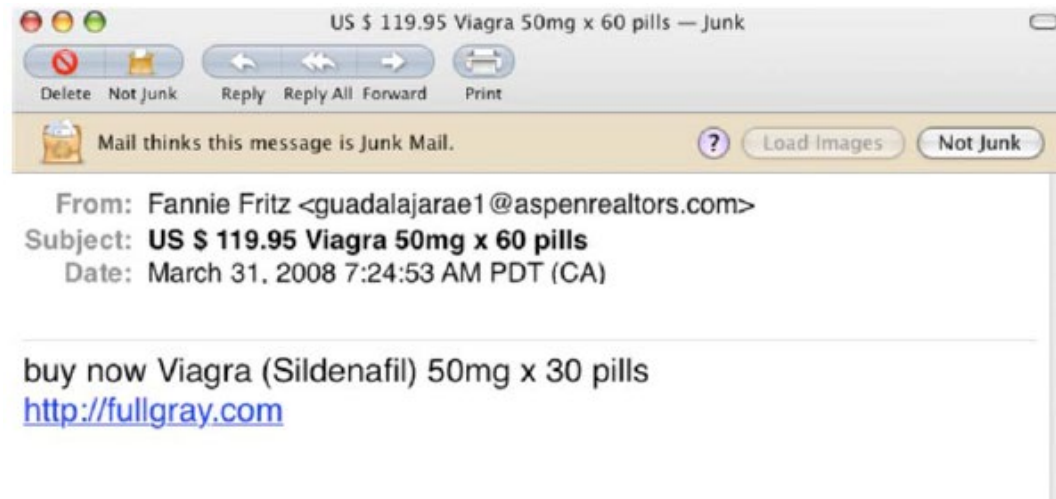
```
lcavol      log(cancer volume)
lweight     log(prostate weight)
age         age
lbph        log(benign prostatic hyperplasia amount)
svi         seminal vesicle invasion
lcp         log(capsular penetration)
gleason     Gleason score
pgg45       percentage Gleason scores 4 or 5
lpsa        log(prostate specific antigen)
```

Ex 2: Model Selection with Limited Data

- ❑ Model selection is particularly valuable when data is limited
- ❑ Ex: Consider linear model: $\hat{y} = b + w_1x_1 + \dots + w_dx_d$
 - Model has $d + 1$ parameters
- ❑ From previous lecture, we need $N > d + 1$ data points (x_i, y_i)
- ❑ In many cases we have $N \ll d$
 - Examples below
 - Many few data points than features
 - Classic linear fit will not work
- ❑ But, suppose we can restrict to $K \ll N$ non-zero parameters
 - Then, we can find a good fit on those parameters
- ❑ Challenge: How do we find a small number K of relevant features



Example 3: Spam Detection



❑ Classification problem:

- Is email junk or not junk?

❑ Typical bag-of-words model:

- Enumerate all words, $i = 1, \dots, d$
- Represent email via word count $x_i = \text{num instances of word } i$

❑ Model selection:

- d = vocabulary size is typically very large
- But, only a few words are likely relevant
- Want to find $K \ll d$ relevant words

Example 4: EEG

- ❑ EEG: Electroencephalography
- ❑ Measure brain activity from electrodes on scalp
- ❑ Source localization problem:
 - Find brain region responsible for evoked response
- ❑ Problem:
 - Many possible brain regions
Typically use $d > 10,000$ voxels
 - But, limited number of measurements:
100s of electrodes
 - Cannot fit a model from all brain regions
- ❑ Model selection:
 - We know that responses are likely from a small brain region
 - Find a small number of voxels that explain response
 - See lab!

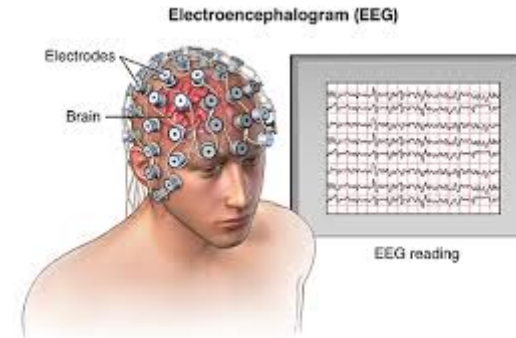
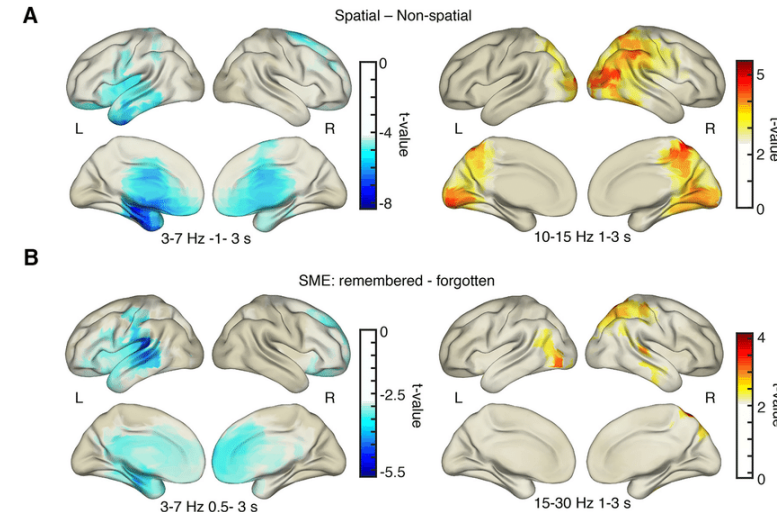
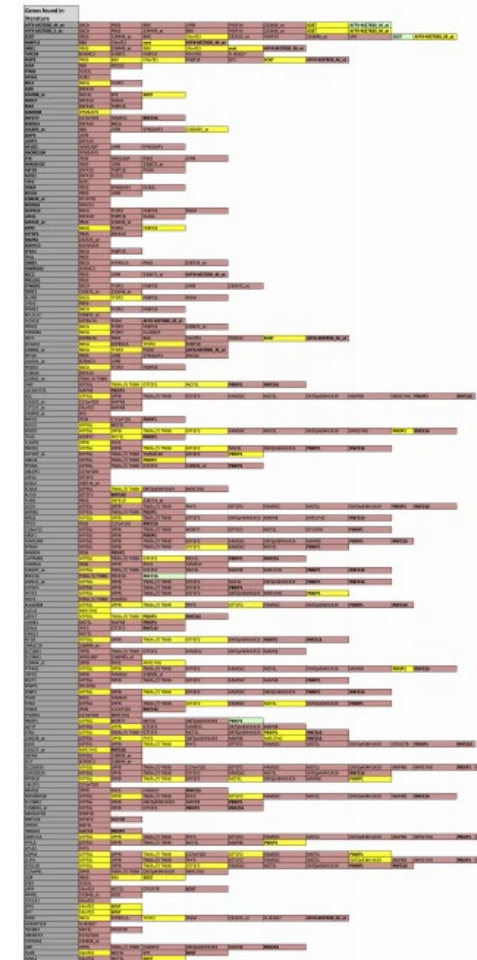


Image: mayoclinic.org




Example 5: DNA MicroArray Data

- ❑ Basic genetic problem
 - Which genes determine some characteristic (i.e. phenotype)?
- ❑ DNA microarrays:
 - Measure “expression” levels of large numbers of genes
 - Expression levels = amount of protein produced by gene
- ❑ Data modeling:
 - Fit phenotype to expression levels
 - Usually have large numbers of genes ($d \sim 1000$)
 - But, small number of data points ($n \sim 100$)
 - We know only a small number of genes are responsible
 - So, we can use model selection



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Other feature selection methods

❑ Filtering method:

- Rank the features based on their correlation or mutual information with the target and possibly the redundancy among the features
- Simple but not very good

❑ Wrapper method:

- For each candidate feature subset, apply a chosen classifier/regressor, evaluate the cross validation accuracy. Go through all possible feature subsets, or test the subsets in some greedy way
- Computationally expensive

❑ Embedded method:

- Some regression/classification method naturally lead to feature ranking and selection

❑ What is available in Python:

- http://scikit-learn.org/stable/modules/feature_selection.html

Filtering method

- ❑ Rank the features based on their correlation with the target
 - Can use other metrics: Correlation, F-test, mutual information, ...
- ❑ Also should consider the redundancy (correlation) among chosen features
 - **Minimal Redundancy Maximum Relevance (mRMR)**
 - Peng, H.C., Long, F., and Ding, C., "Feature selection based on mutual information: criteria of max-dependency, max-relevance, and min-redundancy," IEEE Transactions on Pattern Analysis and Machine Intelligence, Vol. 27, No. 8, pp. 1226–1238, 2005.
 - <http://home.penglab.com/proj/mRMR/>
 - <https://www.mathworks.com/matlabcentral/fileexchange/14916-minimum-redundancy-maximum-relevance-feature-selection>

Ranking metrics

❑ Correlation coefficient between a feature and the target

❑ F-test: test the significance of using one feature vs. not using any (use the mean of y only. Essentially measure the difference in the MSE when using only the mean value of y vs. using a single feature.

$$f_{test} = \frac{r^2}{1-r^2}(n_{sample}-2)$$

❑ Mutual information between a feature and the target

$$I(X, Y) = \iint p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dx dy$$

Embedded Method

- ❑ Results from some regression/classification methods allow feature selection
 - Linear regression: based on coefficient magnitude
 - Neural net: based on weight magnitude
 - Decision tree: based on tree level
 - Can add regularization terms on the coefficients/weights to encourage sparsity
 - LASSO regression
- ❑ Recursive feature elimination
 - Starting with all features, remove one feature that has the lowest importance (e.g. smallest coefficient magnitude)
 - Recursive feature elimination in sklearn
 - http://scikit-learn.org/stable/auto_examples/feature_selection/plot_rfe_digits.html#sphx-glr-auto-examples-feature-selection-plot-rfe-digits-py
 - http://scikit-learn.org/stable/auto_examples/feature_selection/plot_rfe_with_cross_validation.html#sphx-glr-auto-examples-feature-selection-plot-rfe-with-cross-validation-py

Wrapper method

- ❑ For each candidate feature subset, apply a chosen classifier/regressor, evaluate the cross validation accuracy. Go through all possible feature subsets, or test the subsets in some greedy way
 - Exhaustive search
 - Genetic algorithm
 - Forward stepwise
 - Backward stepwise

Exhaustive search for feature selection

- ❑ Suppose you want to consider feature subset of size up to p
- ❑ For all possible feature subsets of size 1 to p :
 - use cross validation to find mean RSS mean and standard deviation
- ❑ Choose the subset with the minimal RSS mean,
 - Or use the one standard error rule.
- ❑ When the number of features is large, may not be computationally feasible
- ❑ Fast search algorithms:
 - Genetic algorithm

Greedy feature selection

❑ Forward-Stepwise Selection

- Select one feature from all features that provides the lowest RSS with cross validation
- Select one new feature from all remaining features, so that previously chosen features plus the new feature provides the lowest RSS
- Repeat until the maximum feature number is reached, or when the RSS starts to increase

❑ Backward-Stepwise

- First use all features and find the RSS (using cross validation)
- Remove one feature and find the new RSS. Go through all possible features to remove.
- Find the one that leads to the least RSS increase. Remove this feature.
- Repeat the above, remove one from the remaining features, to find the next most important feature.

❑ Except exhaustive search, can all lead to suboptimal solution

Comparison of feature selection methods

Figure from [Hastie2008]: Hastie, Tibshirani, Friedman, The elements of statistical learning.

For more on this subject, see Sec. 3.3

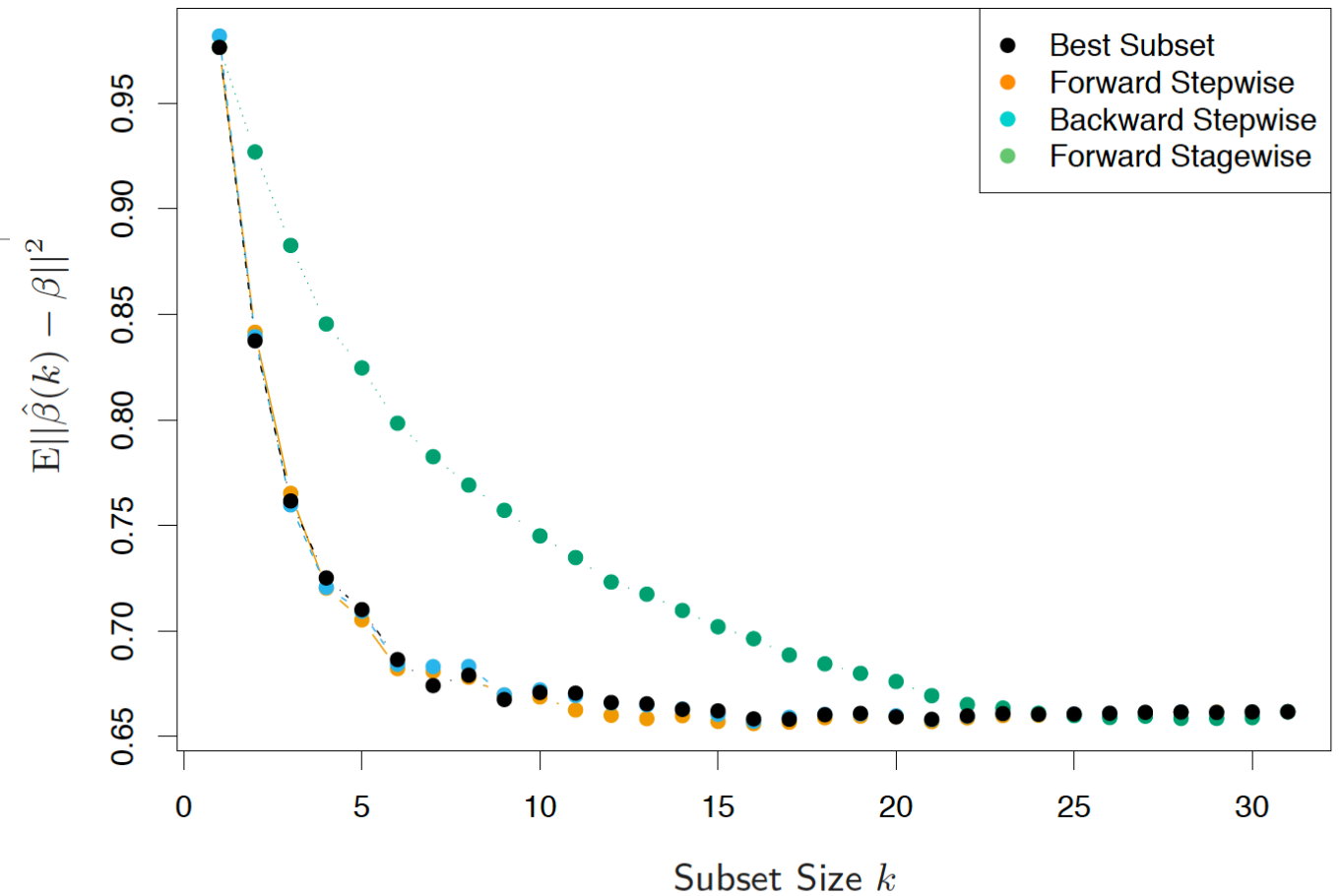


FIGURE 3.6. Comparison of four subset-selection techniques on a simulated linear regression problem $Y = X^T \beta + \varepsilon$. There are $N = 300$ observations on $p = 31$ standard Gaussian variables, with pairwise correlations all equal to 0.85. For 10 of the variables, the coefficients are drawn at random from a $N(0, 0.4)$ distribution; the rest are zero. The noise $\varepsilon \sim N(0, 6.25)$, resulting in a signal-to-noise ratio of 0.64. Results are averaged over 50 simulations. Shown is the mean-squared error of the estimated coefficient $\hat{\beta}(k)$ at each step from the true β .

More about cross validation

❑ Why do we use cross validation?

- To estimate the test error when there are insufficient training data so that we can partition the total data to a **large** training set and a **large** test set.
- Whether a dataset is large depends on the number of parameters of the model to be trained.
- Ideally the number of samples should be $>100x$ of the number of parameters, but at least $10x$.

❑ When you have sufficient training data, you can just use a certain percentage (e.g. 50%) for training and remaining for testing. The error on the testing set would be a reliable estimate of the test error.


❑ Two ways of using cross validation

- When the “best” model class, model order, and feature set are known:
 - Use CV to estimate the test error
- Use CV to determine the appropriate model class, model order and feature subset
 - For each candidate model class, model order, and feature subset, evaluate CV error
 - Determine which candidate yields the least CV error.

More about cross validation

- ❑ How to use the multiple estimated models from multiple trials?
 - Apply each on a test sample and take the average (for regression) or majority (for classification) of results
 - For linear regression, equivalent to average the model coefficients
- ❑ When your data is limited, you may want to go beyond K-folds
 - Ex: 5-fold means that you partition the data to 5 parts in some way, each part has 20% of data, and only do 5 fold training and testing
 - When your data is small, the average CV error is still very sensitive to how the data is partitioned to 5 parts. If you use random shuffling, you will get different result each time.
 - Instead, you could do L trials ($L \gg 5$) of random sampling, each time using 80% for training and 20% for testing
- ❑ How to handle limited data in machine learning is still a challenging topic!

Outline

- ❑ Motivating Example: Predicting prostate cancer from a PSA test
- ❑ Model Selection
- ❑ Model Selection from LASSO regularization
- ❑ Probabilistic interpretation
- ❑ Other Model Selection Methods
- ❑ In-Class Exercise: Audio Pitch Detection

In Class Exercise

☐ https://github.com/sdrangan/introml/blob/master/unit05_lasso/lasso_in_class.ipynb

LASSO Regression In-Class Exercise

In this exercise, we will see how to use LASSO for pitch detection in audio.

We load the following packages.

```
import numpy as np
import matplotlib.pyplot as plt
import pickle
```

Load the data

The data is taken from a sample of about 20~ms of audio from a viola. I have already pre-processed the data. You can load it with following command. The value t is the time (in seconds) and y is the sample of audio (this is a mono recording).

```
fn_src = 'https://raw.githubusercontent.com/sdrangan/introml/master/unit05_lasso/viola_sample.p'
fn_dst = 'viola_sample.p'

import os
from six.moves import urllib

if os.path.isfile(fn_dst):
```

What You Should Know to Do

- ☐ Formulate a linear estimation problem with a regularization
- ☐ Compute an L1-regularized estimate (LASSO) using sklearn tools
- ☐ Compute the optimal regularization level using cross validation
- ☐ Interpret results from a LASSO path
- ☐ Determine final regression function from cross validation
- ☐ Set regularizer based on a probabilistic prior
- ☐ Perform other feature selection methods