Lecture 5
LASSO Regularization and Feature Selection

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING

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Learning Objectives

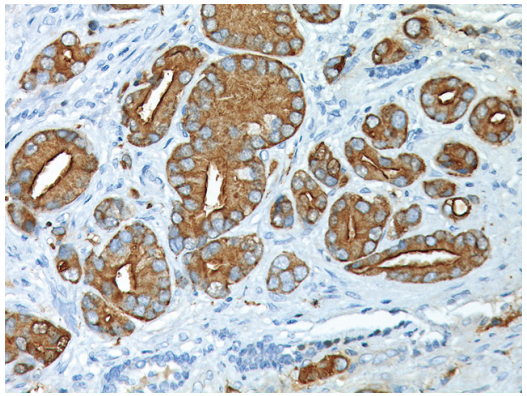
- ❑ Formulate a linear estimation problem with a regularization
- ❑ Compute an L1-regularized estimate (LASSO) using sklearn tools
- ❑ Compute the optimal regularization level using cross validation
- ❑ Interpret results from a LASSO path
- ❑ Determine final regression function from cross validation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

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

Prostate Specific Antigen Testing

- PSA levels easily tested
- High PSA believed to be associated with prostate cancer
  - Potential tool for screening
- Classic 1989 study by Thomas et al:
  - Measured PSA level of 102 men prior to prostate removal
  - Measured characteristics of prostate from samples
  - Characteristics include cancer volume, weight, …
- Data analysis:
  - What characteristics predict PSA?



Stamey, Thomas A., et al. "Prostate specific antigen in the diagnosis and treatment of adenocarcinoma of the prostate. II. Radical prostatectomy treated patients." The Journal of urology 141.5 (1989): 1076-1083.

Data

- Prostate dataset widely-used in ML classes
- Can be downloaded from many sites
- Samples = 97 patients
- 8 features of the prostate
- Target variable = lpsa (log PSA)

```
# Get data
url = 'https://web.stanford.edu/~hastie/ElemStatLearn/datasets/prostate.data'
df = pd.read_csv(url, sep='\t', header=0)
df = df.drop('Unnamed: 0', axis=1)   # skip the column of indices
```

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)

First Try: Linear Model

- Simple idea: Use linear regression

$$y \approx \hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_d x_d$$

  - y = lpsa (target PSA level)
  - $x_1, \ldots, x_d$ = prostate features (d = 8)

```
from sklearn import linear_model
from sklearn.model_selection import train_test_split
```

```
X_tr, X_ts, y_tr, y_ts = train_test_split(X,y,test_size=0.5,shuffle=True)
ntr = X_tr.shape[0]
nts = X_ts.shape[0]
print("num samples train = %d, test = %d" % (ntr, nts))
```

```
num samples train = 48, test = 49
```

- Why linear regression?
  - Easy to compute / interpret
  - Coefficients are easy to interpret
  - Larger coefficients ⇒ larger influence of feature on PSA

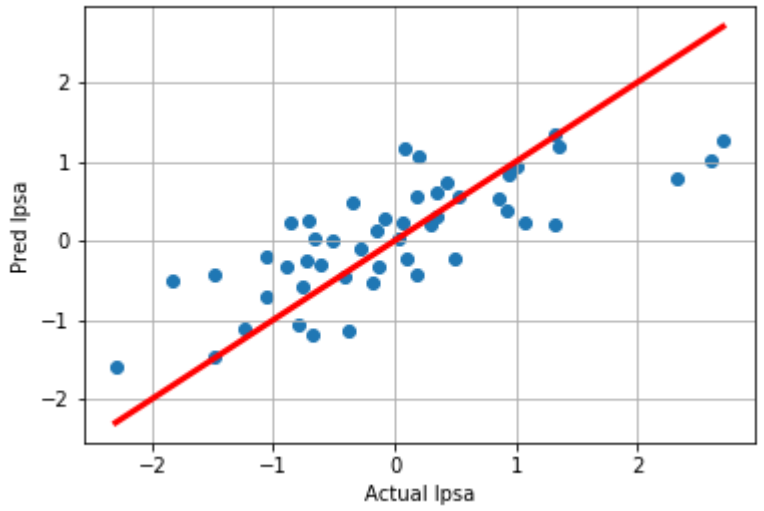
```
regr = linear_model.LinearRegression()
regr.fit(X_tr,y_tr)
```

Model Fit

- Evaluate model with cross validation
  - Train on 48 samples
  - Measure RSS on 49 samples
- We obtain reasonable fit on test data
  - $R^2 \approx 0.58$

```
y_ts_pred = regr.predict(X_ts)
rss_ts = np.mean((y_ts_pred-y_ts)**2)/(np.std(y_ts)**2)
rsq_ts = 1-rss_ts
print("Normalized test RSS = %f" % rss_ts)
print("Normalized test R^2 = %f" % rsq_ts)
```

```
Normalized test RSS = 0.419799
Normalized test R^2 = 0.580201
```

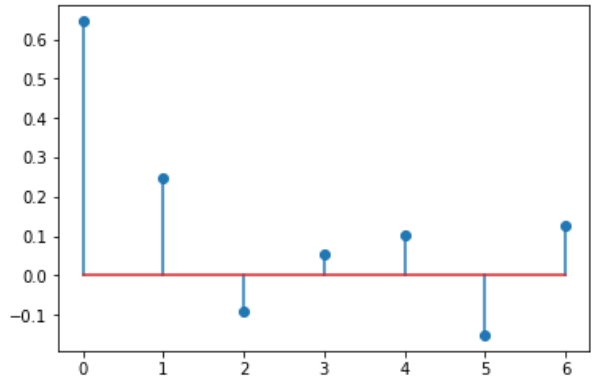


Looking at the Coefficients

- Recall that model is: $\hat{y} = b + w_1 x_1 + \cdots + w_d x_d$
- Weights w_i indicates dependence of feature i on target y
- For PSA test:
  - Highest weight on lcavol (log cancer volume)
  - But, weights on all features are non-zero
  - Hard to eliminate features
- How can we tell if some features are not significant?

```
w = regr.coef_
for name, wi in zip(names_x, w):
    print('%10s %9.4f' % (name, wi))
```

```
    lcavol    0.6457
   lweight    0.2466
       age   -0.0895
      lbph    0.0543
       svi    0.1034
       lcp   -0.1508
   gleason    0.1253
```



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- ❑ Other Model Selection Methods
- ❑ In-Class Exercise: Audio Pitch Detection

Model Selection

- Consider linear model: $y \approx \hat{y} = b + w_1 x_1 + \cdots + w_d x_d$
- Models target y as function of features $\boldsymbol{x} = (x_1, \ldots, x_d)$
- In many problems, we know only a few features are likely relevant
- This means we want $w_j = 0$ for most features
- But, we don't know a priori which features are relevant
- Model selection problem: Fit a model with a small number of features
- Mathematically:
  - Determine a subset of features $I \subseteq \{1, \ldots, d\}$ with $|I|$ small
  - Fit a model: $\hat{y} = b + w_1 x_1 + \cdots + w_d x_d$ with $w_j = 0$ for all $j \notin I$

Example 1: Medical Modeling

- PSA test:
  - We have a number of features
- But, likely that only a small number of features are relevant
- Want a method that can determine which ones matter

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

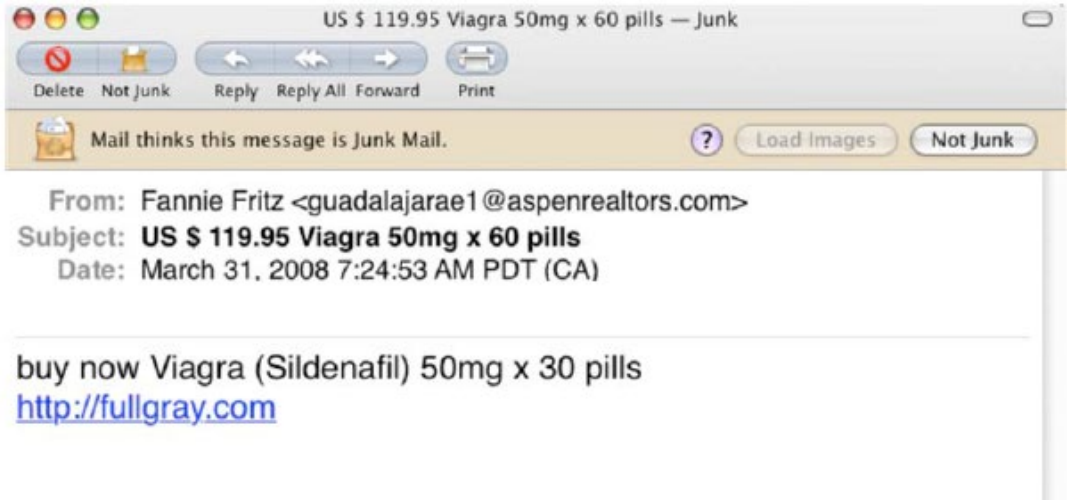
`pgg45`
: percentage Gleason scores 4 or 5

`lpsa`
: log(prostate specific antigen)

Model Selection with Limited Data

- Model selection is particularly valuable when data is limited
- Ex: Consider linear model: $\hat{y} = b + w_1 x_1 + \cdots + w_d x_d$
  - Model has $d + 1$ parameters
- From previous lecture, we need $N > d + 1$ data points $(\boldsymbol{x}_i, y_i)$
- 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 2: Spam Detection



- Classification problem:
  - Is email junk or not junk?
- Typical bag-of-word model:
  - Enumerate all words, $i = 1, \ldots, d$
  - Represent email via word count x_i = 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 3: 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

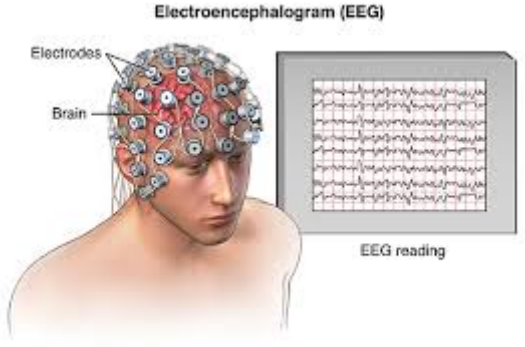
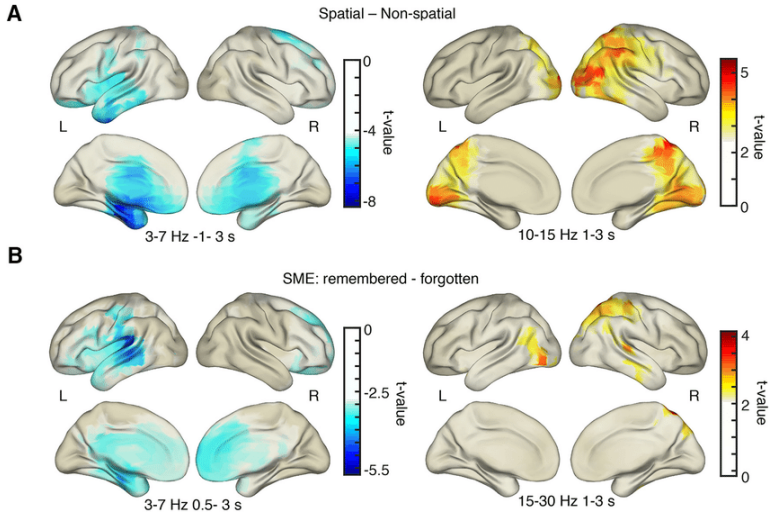
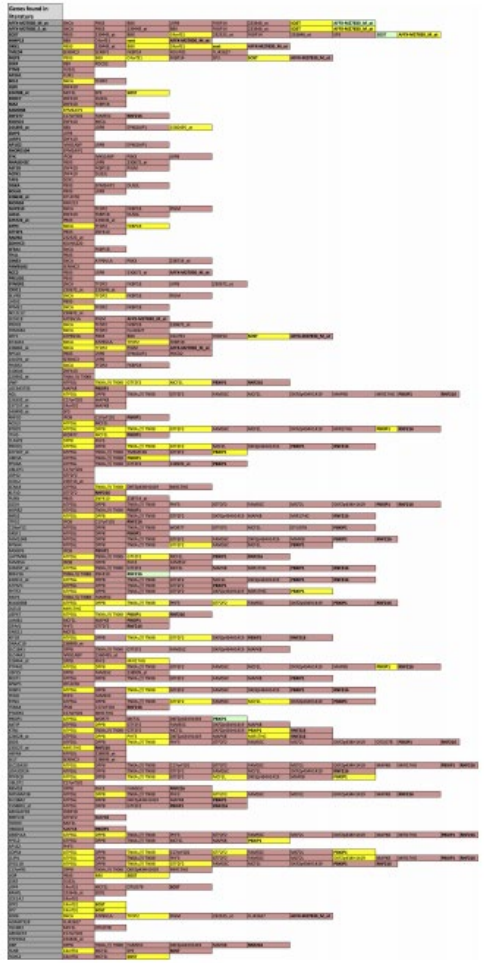


Image: mayoclinic.org



Example 4: 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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Intuition

- We know from last lecture:
  - Too many parameters ⇒ Large generalization error
- In this data set, only a few factors are likely significant
- But, we don't know which one
- Can we automatically identify them?
  - Use correlation between features and target
    - Do not always work well
  - Exhaustive search can be expansive!
- Idea: Fit model under constraint:
  - Force only a few parameters to be non-zero
- General idea of regularization:
  - Constrain the parameters with prior knowledge

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)

Regularized LS Estimation

- Standard least squares estimation (from Lecture 3):

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

- Regularized estimator:

$$\hat{\beta} = \arg\min_{\beta} J(\beta), \qquad J(\beta) = RSS(\beta) + \phi(\beta)$$

  - $RSS(\beta)$ = 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

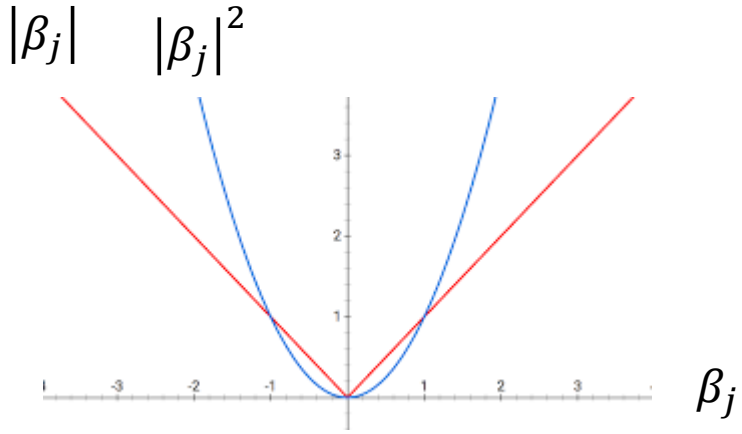
- Ridge regression (called L2)

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

- LASSO regression (called L1)

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

- Both penalize large β_j
- Level of regularization controlled by α
- Note the regularization sum
  - Does not include the intercept β_0,
  - This terms depends on the mean of the target
  - Should not be arbitrarily constrained to be small



Minimize $|\beta_j|^2$ do not penalize small non-zero coef., overly penalize large coef.
Minimize $|\beta_j|$ tend to make coefficients either 0 or large (SPARSE!)

Data Scaling

- Scaling:
  - Scale each feature and the target to have zero mean and unit variance (or STD)
  - $x_{i,j} \rightarrow (x_{i,j} - E(x_{i,j}))/\mathrm{STD}(x_{i,j})$
  - $y_i \rightarrow \big(y_i - \mathrm{E}(y_i)\big)/\mathrm{STD}(y_i)$
- 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

L1 and L2 Norm

- Assuming the data have been scaled to have zero mean and unit variance
- Ridge cost function:

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

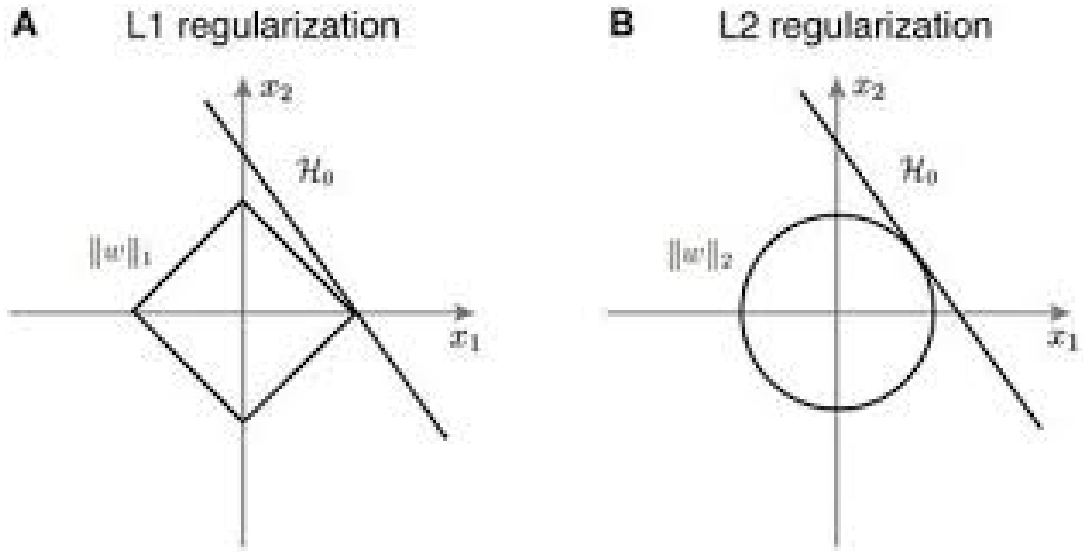
- LASSO cost function:

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

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

Ridge vs LASSO

- Optimization can be easily performed for L1 and L2 regularizers
  - Regularizer is convex
  - More on this later
- L2 tends to lead to many “small” coefficients
  - Not great for feature selection
  - Closed-form solution possible
- L1 tends to lead to more sparse solutions
  - Several coefficients are zero
  - No closed-form solution
  - Will focus this lecture on L1



Ridge Regression

- Loss function

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

- Why minimize $\|\beta\|^2$?
  - Tries to keep coefficients small
  - Only use coefficients when it reduces prediction error
- Without regularization:
  - Parameters are unrestricted
  - Models have high variance
  - Large positive and negative coefficients cancel each other for correlated features

Ridge Regression

- Solution for given regularization level
  - Easily obtainable by setting gradient to zero (HW!)

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

$$\boldsymbol{\beta}_{ridge} = (A^T A + \alpha I)^{-1} A^T \boldsymbol{y}$$

- How to determine the right regularization level α?
  - Through cross validation!

- Sklearn function for ridge regression:
  - http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Ridge.html

Coefficient path with ridge regression

Note that larger α does not lead to fewer non-zero coefficients, but only smaller (and mostly positive) coefficients!

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

For more on this subject, see Sec. 3.4.1.

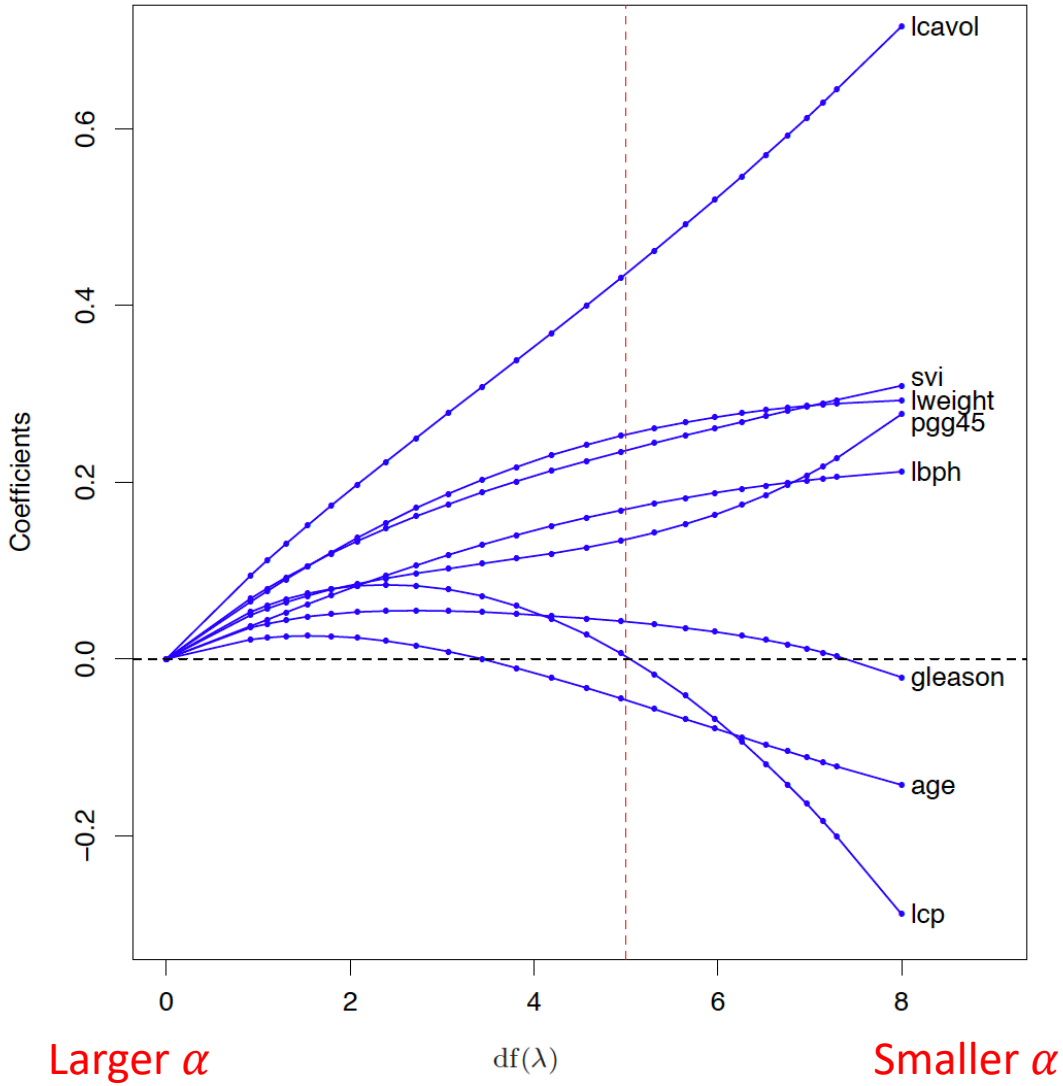


FIGURE 3.8. *Profiles of ridge coefficients for the prostate cancer example, as the tuning parameter λ is varied. Coefficients are plotted versus $\mathrm{df}(\lambda)$, the effective degrees of freedom. A vertical line is drawn at $\mathrm{df} = 5.0$, the value chosen by cross-validation.*

LASSO Regression

- LASSO cost function:

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

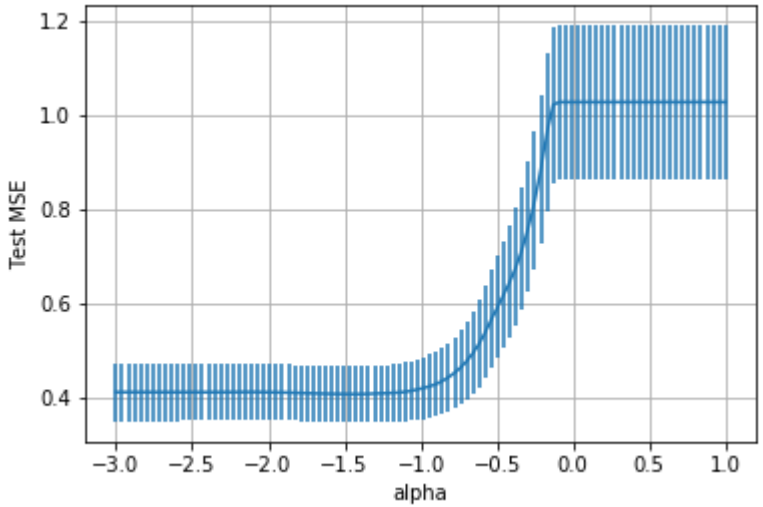
- Because derivative of $|\beta_j|$ is not continuous, there is no closed-form solution.
- However, there is a unique minimum because the cost function is convex.
- Many methods to solve iteratively
  - Least angle regression (LAR), coordinate descent, ADMM
  - Beyond the scope of this class
  - See textbook [Hastie2008] for LAR method

Selecting 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

Computing LASSO in python

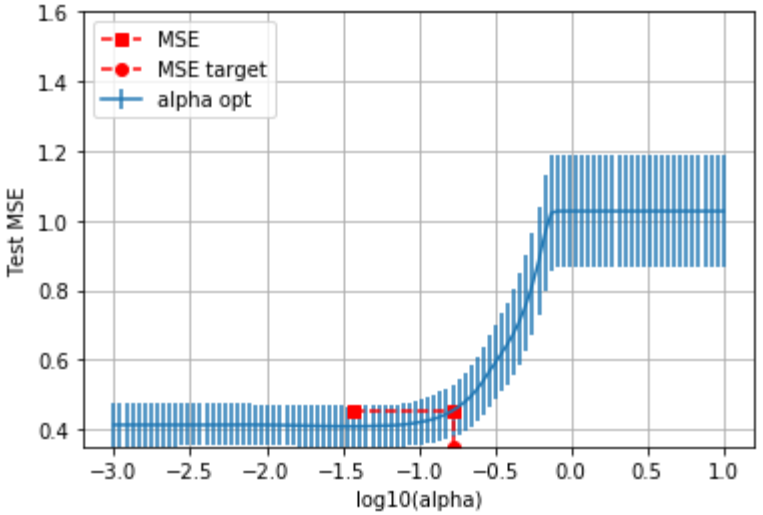
- Use sklearn Lasso method
  - Solve using coordinate descent
- Cross validation loop
  - Outer loop: Loop over folds
  - Inner loop: Loop over α
  - Measure mean and std deviation of MSE




```
# Create a k-fold cross validation object
nfold = 10
kf = sklearn.model_selection.KFold(n_splits=nfold,shuffle=True)

# Create the LASSO model.  We use the `warm start` parameter so
# This speeds up the fitting.
model = linear_model.Lasso(warm_start=True)

# Regularization values to test
nalpha = 100
alphas = np.logspace(-3,1,nalpha)

# MSE for each alpha and fold value
mse = np.zeros((nalpha,nfold))
for ifold, ind in enumerate(kf.split(X)):


    # Get the training data in the split
    Itr,Its = ind
    X_tr = X[Itr,:]
    y_tr = y[Itr]
    X_ts = X[Its,:]
    y_ts = y[Its]

    # Compute the lasso path for the split
    for ia, a in enumerate(alphas):

        # Fit the model on the training data
        model.alpha = a
        model.fit(X_tr,y_tr)

        # Compute the prediction error on the test data
        y_ts_pred = model.predict(X_ts)
        mse[ia,ifold] = np.mean((y_ts_pred-y_ts)**2)
```

Using One Standard Deviation Rule

- Use one standard deviation rule from before
  - Find α_0 with minimum mean MSE, mean_mean
  - Set $\text{mse\_tgt} = \text{mse\_mean}[\alpha_0] + \text{mse\_}se[\alpha_0]$
  - Find largest α where mse_mean[α] < mse_tgt




```
# Find the minimum MSE and MSE target
imin = np.argmin(mse_mean)
mse_tgt = mse_mean[imin] + mse_se[imin]
alpha_min = alphas[imin]

# Find the least complex model with mse_mean < mse_tgt
I = np.where(mse_mean < mse_tgt)[0]
iopt = I[-1]
alpha_opt = alphas[iopt]
print("Optimal alpha = %f" % alpha_opt)
```

Coefficients

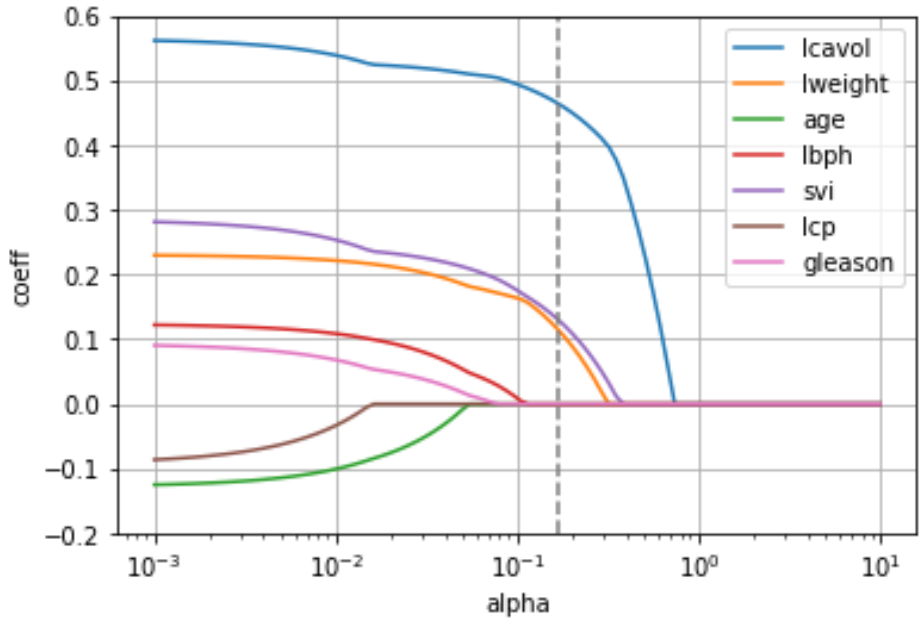
- Select α via cross-validation
- Then, find coefficients using all training data.
- Final coefficients are sparse:
  - Only three factors are non-zeros
  - Lcavol: log cancer volume
  - Lweight: Log weight
  - Svi: seminal vesicle invasion
- Use only features corresponding to non-zero coefficients for linear regression

```
model.alpha = alpha_opt
model.fit(X,y)

# Print the coefficients
for i, c in enumerate(model.coef_):
    print("%8s %f" % (names_x[i], c))
```

```
  lcavol 0.464526
 lweight 0.115832
     age 0.000000
    lbph 0.000000
     svi 0.131102
     lcp 0.000000
 gleason 0.000000
```

LASSO path

- Useful to plot coefficients as a function of α.
- Called the LASSO path
- Indicates relative importance of different factors
- For this data set:
  - lcavol most important
- Don't draw medical conclusions
  - Need more detailed significance testing
  - Complex subject for another class…



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

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Maximum Likelihood Estimate

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

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

- Maximum likelihood estimator:

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

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

- Hence

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

Bayes Estimation (MAP Estimate)

- Maximum a posterior (MAP) estimator of $\boldsymbol{\beta}$:

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

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

- Bayes Rule: $p(\boldsymbol{\beta}\,|\boldsymbol{y}, A) = p(\boldsymbol{y}|A, \boldsymbol{\beta}\,)p(\boldsymbol{\beta})/p(\boldsymbol{y}|A)$

- Hence: $\widehat{\boldsymbol{\beta}} = \arg\max_{\beta} p(y|A, \boldsymbol{\beta}\,)p(\boldsymbol{\beta})$ (because $\boldsymbol{y}$ and A are fixed)
  - Likelihood: $p(y|A, \boldsymbol{\beta}\,)$ How well $\boldsymbol{\beta}$ matches data
  - Prior: $p(\boldsymbol{\beta}\,)$: How well $\boldsymbol{\beta}$ agrees with prior knowledge about its distribution (constraints)

- More in probability class…

Bayes Estimation with Logarithms

- Often easier to use logarithms:

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

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

- Hence

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

- 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:

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

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

$$p(\beta_j) = \tfrac{1}{2\pi\sigma} exp(-{\beta_j}^2/2\gamma^2),\ -\log p(\beta_j) = {\beta_j}^2/2\gamma^2 + constants$$

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

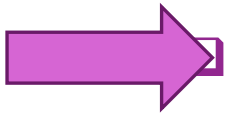
- Assuming β_j are i.i.d. Laplacian with zero mean:

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

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

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



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.

$$ftest = \frac{r^2}{1-r^2}(\text{nsample-2})$$

- Mutual information between a feature and the target

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

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

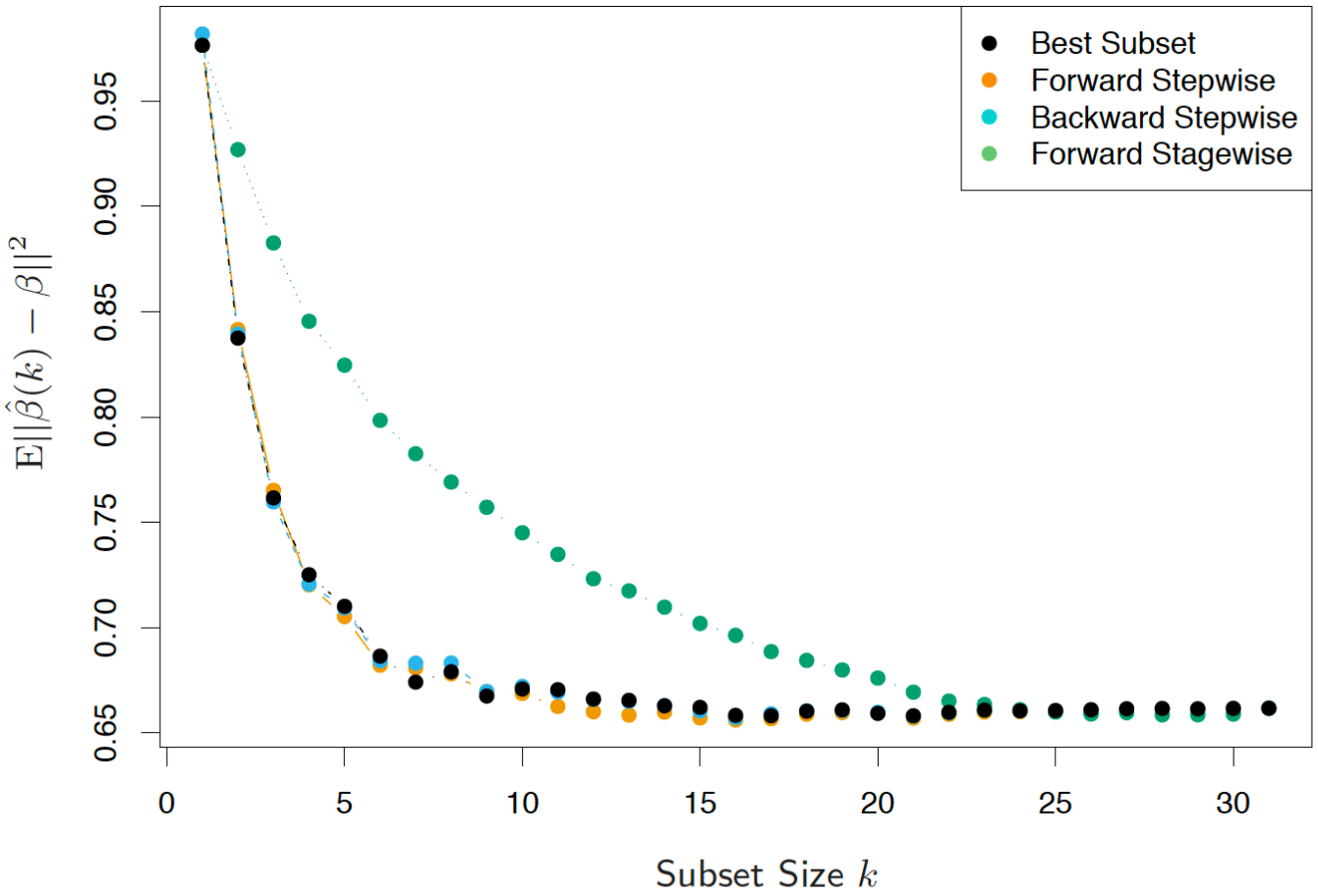


FIGURE 3.6. *Comparison of four subset-selection techniques on a simulated linear regression problem* $Y = X^T\beta + \varepsilon$. *There are* $N = 300$ *observations on* $p = 31$ *standard Gaussian variables, with pairwise correlations all equal to* 0.85. *For* 10 *of the variables, the coefficients 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.

Going through demo comparing different feature selection methods

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>>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!

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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