Chapter 6: Linear Model Selection and Regularization (Lecture 2)

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Previous lecture

Subset selection and shrinkage methods

- Subset selection and shrinkage methods have controlled variance in two ways:
  - Using a subset of the original predictors.
  - Shrinking their coefficients towards zero.
- Those methods use the original (possibly standardized) predictors $X_1, \ldots, X_p$.

Dimension reduction methods

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- Fit least square using the transformed predictors

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, ..., n$$

- If the constants ϕ_{jm} are chosen wisely, then such dimension reduction approaches can often outperform least squares regression.
- The dimension of the problem has been reduced from p + 1 to M + 1.

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- So dimension reduction serves to constrain the coefficients of a standard linear regression
- This constrain increase the bias but is useful in situations where the variance is high
- Such as large p in relation to n

Outline

- We will cover two approaches to dimensionality reduction:
  - Principal Components
  - Partial Least Squares

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- Focus in this lecture is how it can be applied for regression.
  - That is, in a supervised setting.

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- Focus in this lecture is how it can be applied for regression.
  - That is, in a supervised setting.
- PCA is a (unsupervised) technique for reducing the dimension of a $n \times p$ data matrix X.

Principal Component Analysis (PCA)

- We want to create a $n \times M$ matrix Z, with $M < p$.
- The column Z_m of Z is the m-th principal component.

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- We want Z_1 to have the highest possible variance.
  - That is, take the direction of the data where the observations vary the most.
  - Without the constrain we could get higher variance by increasing $\boldsymbol{\phi}_j$

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- And so on ...
- We can construct up to p PCs that way.
  - In which case we have captured all the variability contained in the data
  - We have created a set of orthogonal predictors
  - But have **not** accomplished dimensionality reduction

PCA Example - Ad spending

- The population size (pop) and ad spending (ad) for 100 different cities are shown as purple circles.
- The green solid line indicates the first principal component.
- The blue dashed line indicates the second principal component.

PCA Example - Ad spending (II)

- A subset of the advertising data.
- Left: 1st PC
  - The dimension along which the data vary the most
  - The line that is closest to all n of the observations.
- Right: Rotated so that the 1st PC direction coincides with the x-axis.

PCA Example - Ad spending (III)

- Plots 1st PC scores versus population and ad spending. The relationships are strong.
- Strong relationship: the 1st PC appears to capture most of the information contained in the pop and ad predictors.

PCA Example - Ad spending (IV)

- There is little relationship between 2nd PC and predictors
- Suggesting one only needs the first principal component in order to accurately represent the pop and ad budgets.

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- Assume $\boldsymbol{\Sigma}$ to be the covariance matrix associated with $\boldsymbol{X}$.
- Since Σ is a non-negative definite matrix, it has an eigen-decomposition

$$\boldsymbol{\Sigma} = \boldsymbol{C}\boldsymbol{\Lambda}\boldsymbol{C}^{-1}$$

  - $\boldsymbol{\Lambda} = diag(\lambda_1, ..., \lambda_p)$ is a diagonal matrix of (non-negative) eigenvalues in decreasing order,
  - $\boldsymbol{C}$ is a matrix where its columns are formed by the eigenvectors of $\boldsymbol{\Sigma}$.

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- $\boldsymbol{\phi}_1$ equals the column eigenvector corresponding with the largest eigenvalue of $\boldsymbol{\Sigma}$
- The fraction of the original variance kept by the M principal component

$$R^2 = \frac{\sum_{i=1}^{M} \lambda_i}{\sum_{j=1}^{p} \lambda_j}$$

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- Singular Value Decomposition (SVD) is more numerically stable than eigendecomposition and is usually used in practice.
- How many principal components to retain will depend on the specific application.
- Plotting $(1 - R^2)$ versus the number of components helps selecting how many components to pick

Recommended exercise 10

How many principal components should we use for the Credit Dataset? Justify?

PCA - Summary

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  - Our ability to visualize data is limited to 2 or 3 dimensions.
  - Lower dimension can reduce numerical algorithms computational time.
  - Many statistical models suffer from high correlation between covariates

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- Key assumptions: A small number of principal components suffice to explain:
  1) Most of the variability in the data.
  2) The relationship with the response.
- In other words, we assume that:
  - The directions in which the predictors show the most variation are the directions that are associated with Y.

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- Key assumptions: A small number of principal components suffice to explain:
  1) Most of the variability in the data.
  2) The relationship with the response.
- The assumptions above are not guaranteed to hold in every case.
  - This is true specially for assumption 2 above.
  - Since the PCs are selected via unsupervised learning.

Example: PCR vs. Lasso and Ridge (Simulated data)

- Simulated dataset in which the first five principal components of X contain all the information about the response Y.
- Dashed line: Irreducible error (Simulated data)
- Left: Results for PCR. Right: Results for lasso (solid) and ridge regression (dotted).

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- Similar to Ridge, PCR does not perform feature selection
  - PCs are linear combination of all predictors
- PCR can be seen as discretized version of Ridge regression.
  - Ridge shrinks coefs. of the PCs by $\lambda_j^2/(\lambda_j^2 + \lambda)$
  - Higher pressure on less important PCs
  - PCR discards the $p - M$ smallest eigenvalue components.

Example: Shrinkage Factor

Example: PCR (Credit Data)

- The lowest cross-validation error occurs when there are $M = 10$ components
  - almost no dimension reduction at all
- Discretized version of Ridge

Recommended exercise 11

Apply PCR on the Credit dataset and compare the results with the methods covered in Lecture 1.

PCR (Drawback)

- Dimensionality reduction is done via an unsurpevised method (PCA)
  - No guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response.

Partial Least Squares (PLS)

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- PLS works similar to PCR
  - Dimension reduction: $Z_1, ..., Z_M$, $M < p$
  - Z_i linear combination of original predictors.
  - Apply standard linear model using $Z_1, ..., Z_M$ as predictors.

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  - Z_i linear combination of original predictors.
  - Apply standard linear model using $Z_1, ..., Z_M$ as predictors.
- But it uses the response Y in order to identify new features
  - attempts to find directions that help explain both the response and the predictors.

Partial Least Squares (Algorithm)

- $Z_1 = \sum_{i=1}^{p} \phi_{j1} X_j$
  - ϕ_{j1} is the coefficient from the simple linear regression of Y onto X_j.
  - this coefficient is proportional to the correlation between Y and X_j.
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- To obtain the second PLS direction, Z_2:
  - We regress each variable on Z_1 and take the residuals
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- We can repeat this iteration process M times to get $Z_1, ..., Z_M$.

Recommended exercise 12

Apply PLS on the Credit dataset and compare the results with the methods covered in Lecture 1 and PCR.

Partial Least Squares (Performance)

- In practice, PLS often performs no better than ridge regression or PCR.
  - Supervised dimension reduction of PLS can reduce bias.
  - It also has the potential to increase variance.

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- Ridge regression may be preferred because it shrinks smoothly, rather than in discrete steps.
- Lasso falls somewhere between ridge regression and best subset regression, and enjoys some of the properties of each.
- I would say:
  - If you only concerned with prediction accuracy, either ridge or lasso.
  - If model interpretability is desirable, lasso is prefered.

Considerations in high dimensions

High dimension

- High dimension problems: $n < p$
- More common nowadays

High dimension issues (Example)

- Standard linear regression cannot be applied.
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  - Unfortunately, the C_p, AIC, and BIC approaches are problematic (hard to estimate σ^2)

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  - Perfect fit to the data, regardless of relationship
  - Unfortunately, the C_p, AIC, and BIC approaches are problematic (hard to estimate σ^2)
- Simulated example with $n = 20$ training observations.
- features that are completely unrelated to the outcome are added to the model.

Noise predictors

- The test error tends to increase as the dimensionality of the problem
  - Unless the additional features are truly associated with the response.
- The lasso was performed with $n = 100$ observations and three values of p, the number of features.
- Of the p features, 20 were associated with the response.
- When $p = 2000$ the lasso performed poorly regardless of the amount of regularization.

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- However, adding noise features that are not truly associated with the response increases test set error.
  - Noise features exacerbating the risk of overfitting
  - Previous example shows that regularizations does not eliminate the problem
- New technologies that allow for the collection of measurements for thousands or millions of features are a double-edged sword

Interpreting results in high dimension

- In the high-dimensional setting, the multicollinearity problem is extreme
- Multicollinearity: any variable in the model can be written as a linear combination of all of the other variables in the model.

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  - We can never know exactly which variables (if any) truly are predictive of the outcome.
  - We can never identify the best coefficients for use in the regression.

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- Essentially, this means:
  - We can never know exactly which variables (if any) truly are predictive of the outcome.
  - We can never identify the best coefficients for use in the regression.
  - At most, we can hope to assign large regression coefficients to variables that are correlated with the variables that truly arec predictive of the outcome.
  - We will find one of possibly many suitable predictive models.

The end

Thank you for showing up