Ch 6.3: Dimension Reduction

Lecture 13 - CMSE 381

Michigan State University
::
Dept of Computational Mathematics, Science & Engineering

Weds, March 11, 2024

Announcements

Last time:

- Shrinkage: Ridge and Lasso

This lecture:

- PCA / PCR
- PLS

Section 1

Last time

Find β to minimize:

Least Squares:

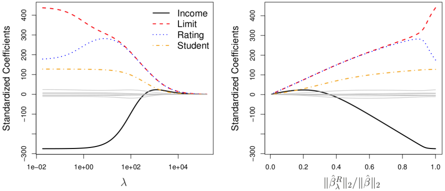
$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

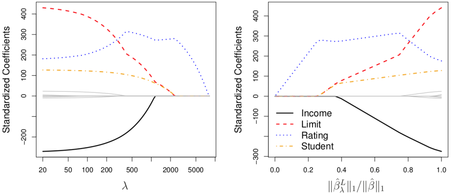
Ridge:

$$RSS + \sum_{j=1}^{p} \beta_j^2$$

The Lasso:

$$RSS + \sum_{j=1}^{p} |\beta_j|$$





Also, find best choice of λ or s using CV

Section 2

Dimension Reduction

Linear transformation of predictors

Original Predictors:

$$X_1, \cdots, X_p$$

New Predictors:

$$Z_1, \cdots, Z_M$$

$$Z_m = \sum_{j=1}^{p} \varphi_{jm} X_j$$

- The goal is for $M \ll p$
- Need to figure out good φ to do this

Two examples

Two dimensions down to 1.....

- $$Z_1 = X_1 + 3 \cdot X_2$$
- Matrix version:
$$\begin{pmatrix} Z_1 \end{pmatrix} = \begin{pmatrix} X_1 & X_2 \end{pmatrix} \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$
- Example data:

X_1	X_2	Z_1
0	1	4
3	4	17
1	1	4
-1	0	-1

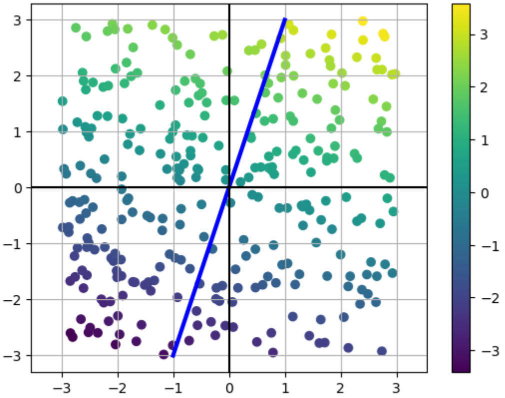
an example with just three dimensions down to two

- $\varphi = \begin{pmatrix} 1 & 0 \\ 0 & 1/2 \\ 0 & 1/2 \end{pmatrix}$

$$Z_1 = X_1 + 0 \cdot X_2 + 0 \cdot X_3$$
$$Z_2 = 0 \cdot X_1 + \frac{1}{2} X_2 + \frac{1}{2} X_3$$

Geometric interpretation

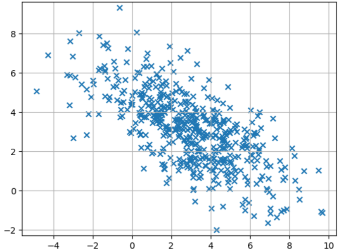
- Get the φ to unit column norm
- Example: $Z_1 = \frac{1}{\sqrt{10}} X_1 + \frac{3}{\sqrt{10}} X_2$
- The Z value is the distance from the projection of (X_1, X_2) onto the vector $(1, 3)$ to the origin.

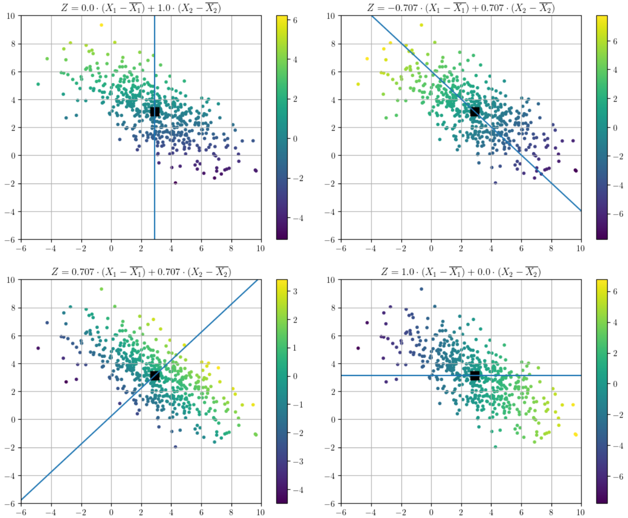


Projection onto a line

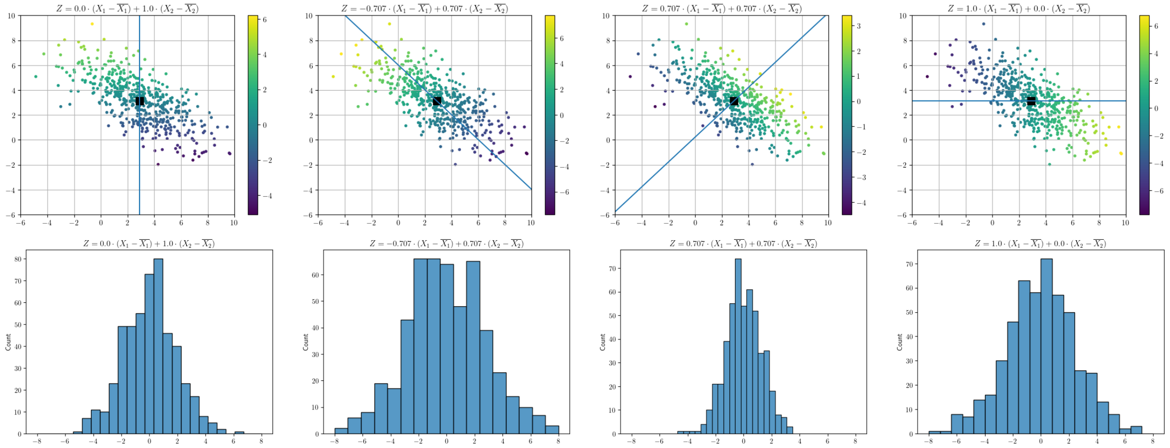
https://www.desmos.com/
calculator/cih7wy8oyg

Different projections





Histograms of Z values



The goal

- Find good φ's for some $M \ll p$
- Fit regression model on Z_i's using least squares

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \varepsilon_i$$

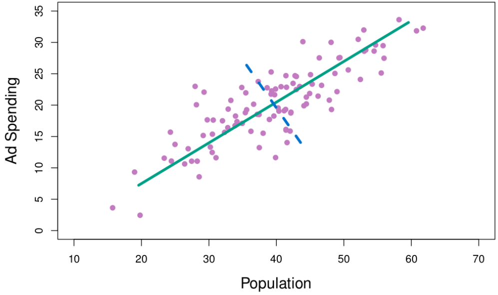
- in this notation, θs replace βs

- Dimension reduction comes from the fact that we're fitting models on a smaller number of variables
- Next two subsection: ways to find φs: PCA and partial least squares

Section 3

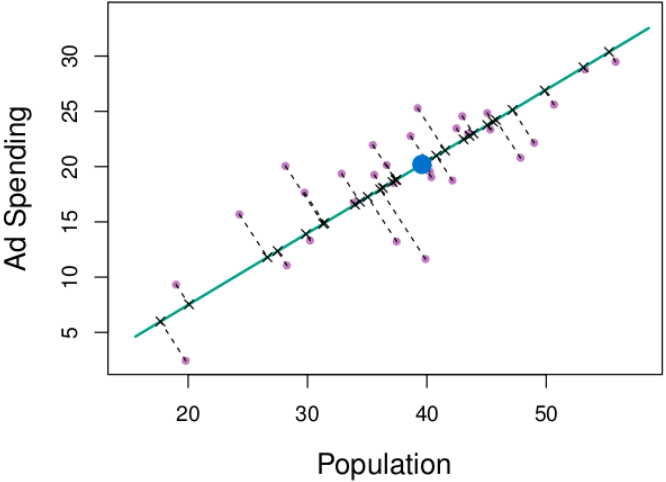
Review of PCA

An example dataset



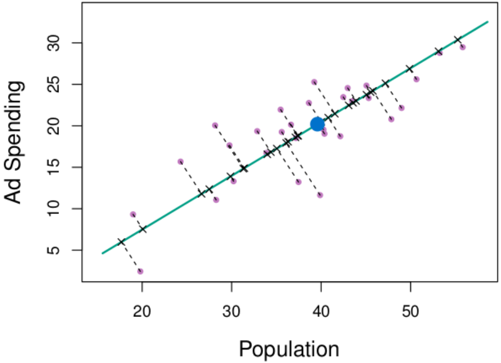
- Population size in tens of thousands of people
- Ad spending for a company in thousands of dollars
- 100 data points
- By eye: green line is the direction of most variability, calle the principal direction
- Meaning if we project observations onto the line, then the projected observations would have the largest possible variance
-

Projection onto first PC



$$Z_1 = 0.839 \cdot (\mathtt{pop} - \overline{\mathtt{pop}}) + 0.544 \cdot (\mathtt{ad} - \overline{\mathtt{ad}})$$

How to compute the first PC ?

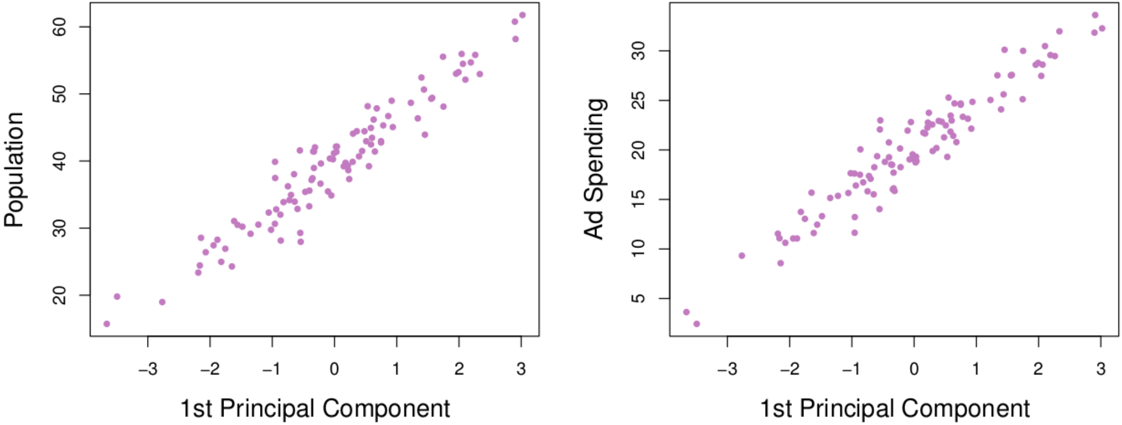


- Of every linear combo of pop and ad, this one has the highest variance
- Maximizes $\mathrm{Var}(\varphi_{1,1}(pop - \overline{pop}) + \varphi_{2,1}(ad - \overline{ad}))$
- Require $\varphi_{11}^2 + \varphi_{21}^2 = 1$, otherwise, just make φ super big to blow up variance

The other principal components

- Z_2 is linear combo of variables uncorrelated to Z_1
- Find the one that explains the most variance
- Result: requires Z_2 to be the direction that explains the most variance among all directions that are uncorrelated with Z_1
- Requires Z_k to be the direction that explains the most variance among all directions that are orthogonal or perpendicular to $Z_1, Z_2, ..., Z_{k-1}$

Principal component scores



$$z_{i1} = 0.839 \cdot (\mathtt{pop}_i - \overline{\mathtt{pop}}) + 0.544 \cdot (\mathtt{ad}_i - \overline{\mathtt{ad}})$$

Computing all PC directions together

Let X be the data matrix whose $(i, k)th$ entry is the kth predictor's value for observation i. We do the following to find the PCs.

- Centralize the data $X^c = X - \frac{1}{n}X11^T$
- Compute the SVD of X^c, $X^c = U\Sigma V^T$
- the kth PC is v_k which is the kth column of V.
- the PC scores of Z_k is $X^c v_k$.
- the PC score z_{ik} is $X_i^c v_k$, where X_i^c is the ith row of X^c.

Section 4

Principal Components Regression

So you've found your PCA coefficients

Now what?

- Do linear regression on $Z_1, \cdots, Z_M$
- Book calls this "principal components regression"
- Linear model is $y = \theta_0 + \theta_1 Z_1 + \cdots + \theta_M Z_M$

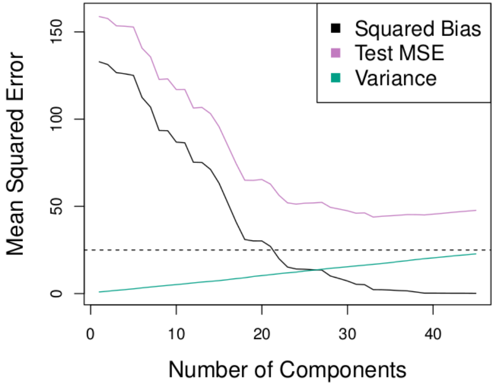
What are we assuming?

- The directions in which $X_1, \cdots, X_p$ have the most variation are the directions that are associated with Y
- If assumption holds, then fitting on Z_i better than fitting on X_i since fewer variables lessens chance of overfitting

Doing better

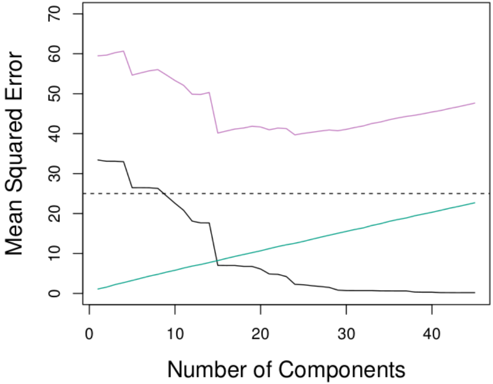
Example with simulated data: $n = 50$ observations of $p = 45$ predictors
Y is a function of 2 predictors

- Right side is usual least squares estimate
- Typical U shape for Test MSE
- PCR with good choice of number of components improvement over plain least squares



Doing better

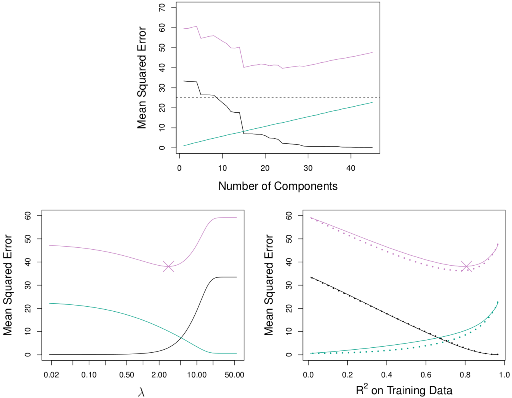
Example with simulated data: $n = 50$ observations of $p = 45$ predictors
Y is a function of all predictors



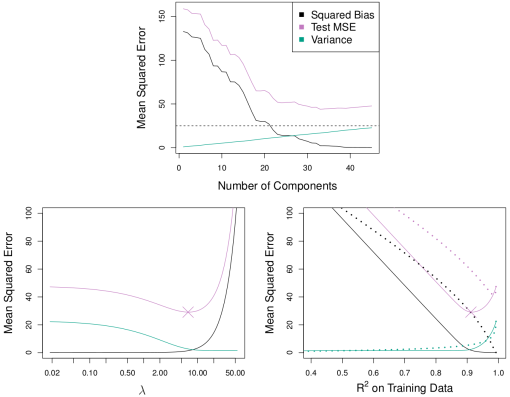
- Right side is usual least squares estimate
- Even better improvement using PCR than previous
- note the change in y-axis values

Comparison to results on shrinkage

Y is a function of all predictors



Y is a function of 2 predictors



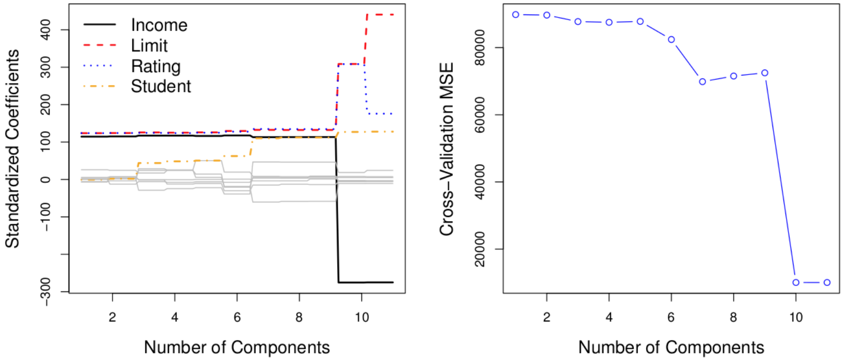
Shrinkage does better

What is missing?

Why the PCR result is worse than Lasso on the above example?

- A critical assumption for PCR to work is that, the directions in which $X_1, \cdots, X_p$ have the most variation are the directions that are associated with Y
- If assumption holds, then fitting on Z_i better than fitting on X_i since fewer variables lessens chance of overfitting

Picking M



- Credit data set
- Major drop in MSE at 10 compoentns, so barely a savings with the original 11 variables

Properties of PCR

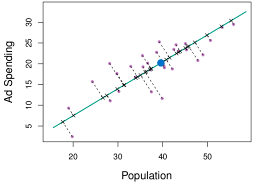
- Note better in previous example because lots of PCs needed
- It does better when info contained in the first few PCs
- Number of PCs to use can be picked with CV
- Standardization needed to make sure big data values don't skew the results

- Not a feature selection method because we don't get a subset of features, we get a collection of linear combos of features

Summary

PCA

- Unsupervised dimensionality reduction
- Choose component Z_1 in the direction of most variance using only X_i's information
- Choose Z_2 and beyond by the same method after "getting rid" of info in the directions already explained



PCR

- Do PCA on input data
- Do Linear Regression on chosen number of PCs.
- Warning: Lose interpretability of the coefficients.

Section 5

Partial Least Squares (PLS)

Supervised alternative

PCR: dimension reduction is Non-supervised

- No input from the Y values before learning the PCs.
- No guarantee that directions that explain Xs help to predict the Ys

Partial Least Squares (PLS):

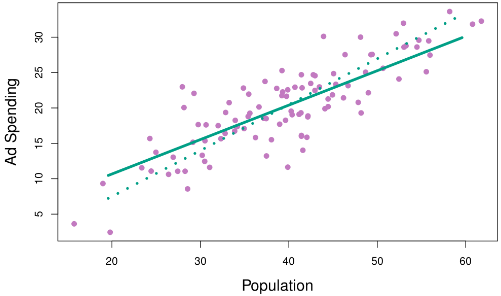
- Identify new features $Z_1, \cdots, Z_M$ linear combos of original where quality measure involves Y
- Fit linear model using least squares on these M features

First direction Z_1 for Partial Least Squares (PLS)

- Set φ_{j1} equal to the coefficient from simple linear regression of Y onto X_j
  This means we do p linear regressions, not that we take the multivariable linear regression coefficients
- The first direction is

$$Z_1 = \sum_{j=1}^{p} \varphi_{j1} X_j$$

- PLS places highest weight on variables most strongly related to the response
- In example, PLS chooses direction less change in ad direction than pop relative to PCA



Ex. Prediction of Y =Sales (not shown) on X_1 =Population and X_2 =Ad Spending

- Solid green: First PLS direction
- Dashed: First PC direction

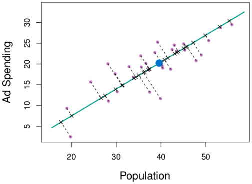
Second (and more) PLS directions

- Regress each variable on Z_1 and take residuals *This is the remaining info not explained by first PLS direction*
- Compute Z_2 using *orthogonalized data* same as for Z_1
- Number M can be picked using CV after standardizing predictors

PCR vs PLS

PCR

- Unsupervised dimensionality reduction + linear regression
- Choose component Z_1 in the direction of most variance using only X_i's information
- Choose Z_2 and beyond by the same method after "getting rid" of info in the directions already explained



PLS

- Supervised dimensionality reduction
- Choose component Z_1 by using simple regression coefficients of each X_i onto Y
- Choose Z_2 and beyond by the same method after "getting rid" of info in the directions already explained
- better suited than PCR for prediction tasks.