Unit 3 Dimensionality Reduction Techniques

(1) Principal Components Regression (PCR)

October 30, 2019 (*) Explain most of variability

1. Introduction

Using the smaller # of predictors.

(Find a tool to find representation of a data that contains as much of the

coefficients < OLS estimates which have relatively low bias and low variability varia especially when the relationship between the response and predictors is linear and n >> p

if n is <u>NOT</u> much larger than p,

- OLS fit can have high variance > may result in over-fitting and poor estimates.
- many predictors have no or little effects on the respone.

 O irrelevant variable leads to unnecessary complexity

 B harder to see the effect of the important variables.
- i. It is better to remove the irrelevant variables from the model.

How?

- O variable selection < stepwise best-subset.
 - : Identify a subset of the p-predictors that we believe to be related to the response; then fit a model using DLS on the reduced set.
- Dimension Reduction < PCR (principal component regression)
 PLS (Partial Least squares)
 - : Involves projecting the p-predictors into a M-dimensional subspace, where M<p, and fit the linear regression model using M projections as predictors.
- 3 Shumkage (Regulation) < Ridge Lasso
 - Involves shirinking the estimated wefferents toward 'D' relative to the OLS estimates, has the effect of reducing variance and performs variable selection.

2. Performing Principal Components Regression (PCR)

3.2.1 Principal Components Analysis (PCA): summanize the information in the predictors into a smaller set of variables and then try to predict Y > Imear combinations of the original Assume we have a data set where p-variables are observed. vaviables. X; ith observation of p-dimensional vector X. Plot 1A Plot 1B *PCA assumes that 80 -40 the directions w/ the largest variances (djp x predictor p) 40 are the 'most' important. most important directorio. data are presented in the : 1st principal direction. X-T coordinate system. calong which the samples show Low redundancy the largest variation, PCA is useful when High redundancy the variables within the dataset are highly (Lowelated). "redundancy" .. Due to this redundancy. PCA can be used to reduce the original variables Into a smaller number of new variables (= PG) O identify hidden pattern in a data set. explaining most of the 3 reduce the dimensionnality Variance in the original variables of the data by removing. 2 the noise and redundancy

in the data

3 identify correlated variables

> Regression technique based on principal component analysis

3.2.2 Assumption of PCR

- the directions in which the predictors show the most variation are the exact directions associated w/ the response variable. The amectrons in which x1, ..., xp show the most variation are the direction that are associated of other Xs.

→ on one hand, this assumption is NOT guaranteed to hold 1000% of the time, but, even though the assumption is not completely time it can be a good 3.2.3 Advantages and Disadvantages approximation and yield interesting results.

Advantages

1) Dimensionality reduction

By using PCR, you can easily perform dimensionality reduction a high dimensional dataset, and then fit a linear regression model to a smaller Set of variables, while at the same time keep most of the variability of the original predictors.

⇒ use only some of the puncipal components. Help to reduce the model complexity

2) Avoiding multicollinearity

A significant benefit of PCR is that by using the PCs, if there is some degree of multicollinearity between the variables in data ser, this procedures should be able to avoid this problem since performing PCA on the raw data produces linear combinations of the predictors that are uncorrelated,

3) Overfitting mitigation

If all the assumptions underlying PCR hold, then fitting a least squares model to the principal components will lead to better results than fitting a least squares models to the original data since the most of the variation and information related to the dependent variable is condensend in 3 the principal components and by estimating less coefficients you can reduce the risk of overfitting.

o Disadvantages

- O PCR + a feature selectron method
 - : each of the calculated principal components is a linear combinatorn of the original variables
 - : Hard to explain what is affecting what.
- 13 The directions that best represent each predictor are obtained in an unsupervised way.
 - : The dependent variable is NOT used to identify each principal component direction.
 - in the directions found from PCR are not be the optimal directions to use when making predictions on the dependent variable.

3. Performing PCR in R

Men's Decathlon Athletes In 2012

We will use the demo data set "decathlon2" from the *factoextra* package. The data used here describes athletes' performance during two sporting events (Desctar and OlympicG). It contains 27 individuals (athletes) described by 13 variables.

Variable Name	Description
X100m	Points scored in 100 metres
Long.jump	Points scored in long jump
Shot.put	Points scored in shot put
High.jump	Points scored in high jump
X400m	Points scored in 400 metres
X110m.hurdle	Points scored in 110 metres hurdles
Discus	Points scored in discus throw
Pole.vault	Points scored in polt vault
Javeline	Points scored in javelin throw
X1500m	Points scored in 1500 metres
Rank	Final Ranking in 2012
Points	Total scores
Competition	Name of athletic competition in 2012

R packages:

Several functions from different packages are available in the R software for computing PCA/PCR:

- prcomp() and princomp() [built-in R stats package],
- *PCA()* [FactoMineR package],
- dudi.pca() [ade4 package],
- and *epPCA()* [*ExPosition* package]

Performing PCA

```
PCA(X, scale.unit = TRUE, ncp = 5, graph = TRUE)
```

Results

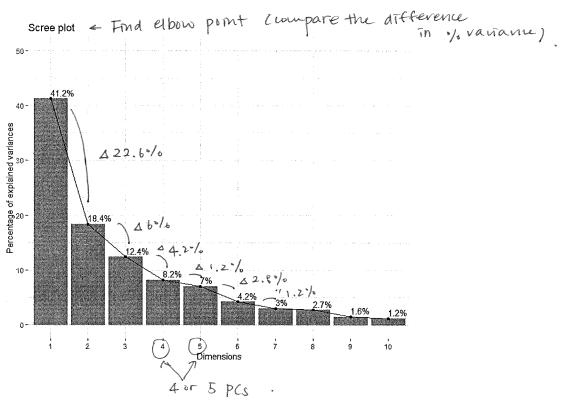
```
## **Results for the Principal Component Analysis (PCA)**
## The analysis was performed on 23 individuals, described by 10 variables
## *The results are available in the following objects:
##
井井
                         description
      name
## 1
      "$eig"
                         "eigenvalues"
     "$var"
                         "results for the variables"
## 2
     "$var$coord"
"$var$cor"
"$var$cos2"
                        "coord. for the variables"
## 3
## 4
                         "correlations variables - dimensions"
## 5
                         "cos2 for the variables"
      "$var$contrib"
                         "contributions of the variables"
## 6
                         "results for the individuals"
## 7
     "$ind"
## 8 "$ind$coord"
                         "coord. for the individuals"
## 9 "$ind$cos2"
                         "cos2 for the individuals"
## 10 "$ind$contrib"
                         "contributions of the individuals"
## 11 "$call"
                         "summary statistics"
## 12 "$call$centre"
                      "mean of the variables"
## 13 "$call$ecart.type" "standard error of the variables"
## 14 "$call$row.w"
                        "weights for the individuals"
## 15 "$call$col.w"
                         "weights for the variables"
```

measurement to show the amount of variance retarned by each pc

1) Eigenvalues/Variances

##		aireavalue	vantance pencent	cumulative.variance.percent
		-	·	cumuractive. variance. percent
##	Dim.1	4.124	41.24	(41.2) 41% of variance
##	Dim.2	1.839	18.39	41.2 41% of variance 59.6 explaned
##	Dim.3	1.239	12.39	[72.8] by
##	Dim.4	0.819	8.19	/ 80.2 1st pc.
##	Dim.5	0.702	7.02	/ 87.2
##	Dim.6	0.423	4.23	/ 91.5
##	Dim.7	0.303	3.03	94.5
##	Dim.8	0.274	2.74	72% of 97.2
##	Dim.9	0.155	1.55	Vayance 98.8
##	Dim.10	0.122	1.22	explained 100.0
ree r	olot			by 3 PCs (PLI, PC2, and PC3)

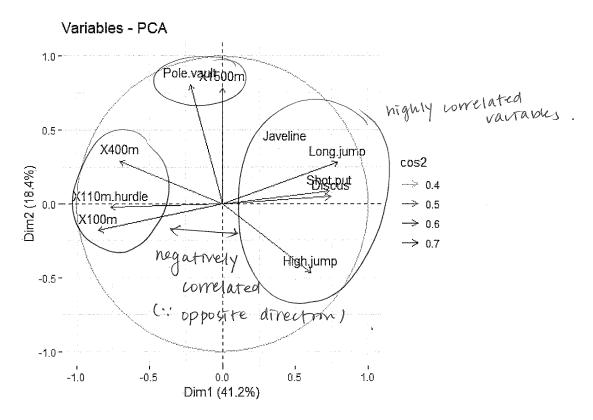
2) Scree plot



3) Result of variables

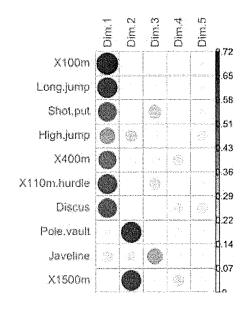
##	Principal Con	ponent Analysis Results for variables
##	==========	
##	Name	Description
##	1 "\$coord"	"Coordinates for the variables"
##	2 "\$cor"	"Correlations between variables and dimensions"
##	3 "\$cos2"	"Cos2 for the variables"
##	4 "Scontrib"	"contributions of the variables"

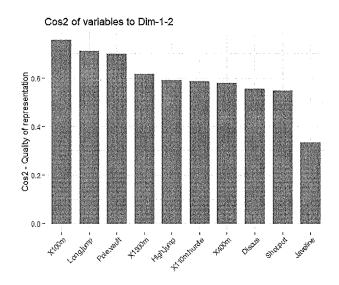
4) Correlation Circle



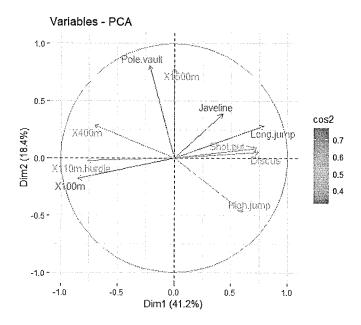
5) Quality of representation

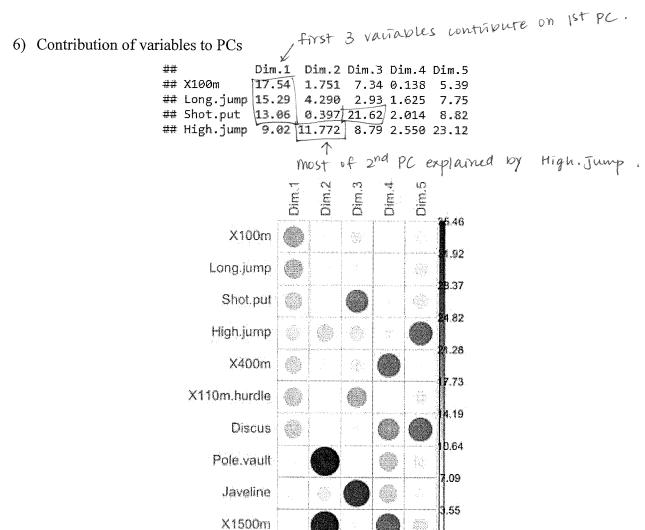
Dim.1 Dim.2 Dim.3 Dim.4 Dim.5 ## X100m 0.724 0.03218 0.0909 0.00113 0.0378 ## Long.jump 0.631 0.07888 0.0363 0.01331 0.0544 ## Shot.put 0.539 0.00729 0.2679 0.01650 0.0619 ## High.jump 0.372 0.21642 0.1090 0.02089 0.1622

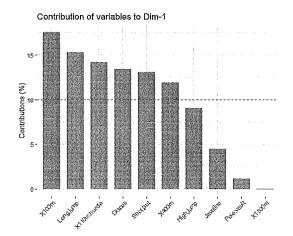


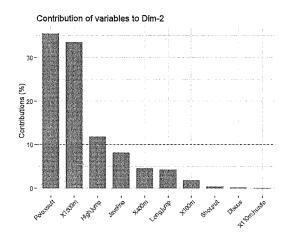


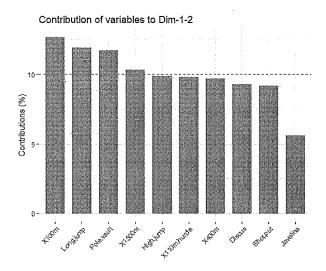
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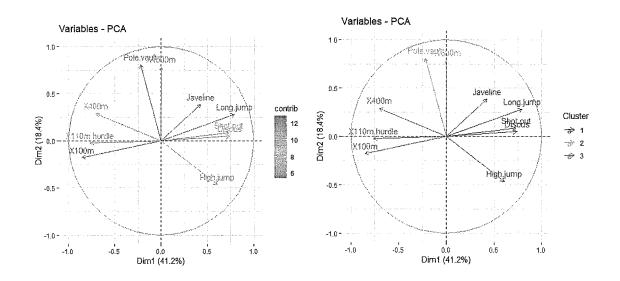


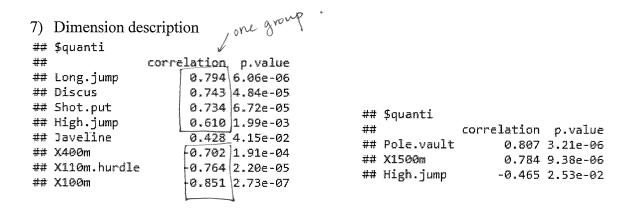




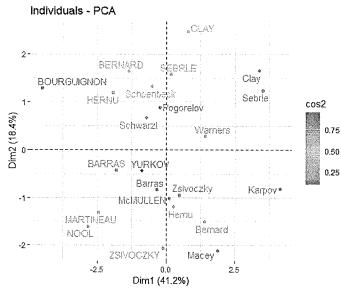


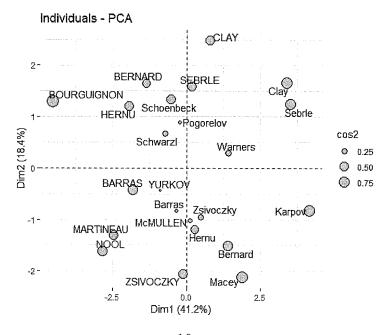


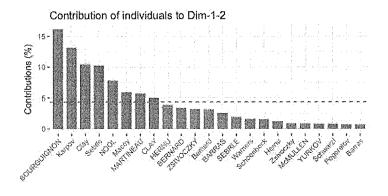




8) Graph individuals

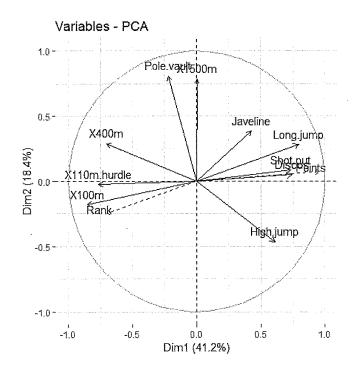


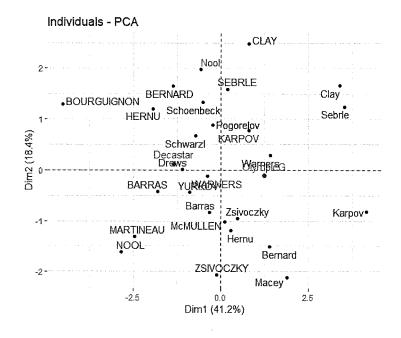


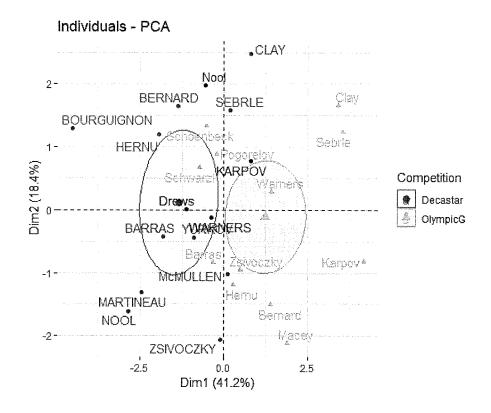


9) Specification in PCA

```
## $coord
           Dim.1
                   Dim.2 Dim.3
                                  Dim.4
          -0.701 -0.2452 -0.183 0.0558 -0.0738
## Rank
                  0.0777
                          0.158 -0.1662 -0.0311
           0.964
##
## $cor
           Dim.1
                                  Dim.4
##
                   Dim.2 Dim.3
                                          Dim.5
          -0.701 -0.2452 -0.183
                                0.0558 -0.0738
## Rank
## Points 0.964
                         0.158 -0.1662 -0.0311
##
## $cos2
##
          Dim.1
                  Dim.2 Dim.3
                                 Dim.4
          0.492 0.06012 0.0336 0.00311 0.00545
## Points 0.929 0.00603 0.0250 0.02763 0.00097
```







Unit 3. Dimensionality Reduction Techniques

· 1.1 1

(2) Partial Least Squares (PLS) Regression

dimensional reduction Technique W/ some similarities

1. Introduction

to puncipu component regression. Famone" outcome * Unit 3 presents regression methods based on dimension reduction techniques, Which can be very useful when you have a large data set with multiple

correlated predictor variables.

* All the dimension reduction methods work by first summarizing the original predictors into few new variables called principal components (PCs), which are then used as predictors to fit the linear regression model.

* Generally recommend to standardize each predictor to make them comparable.

PCR

- Offirst applies Principal Component Analysis on the data set to summarize the original predictor variables into few new variables.
- @ These PCs are then used to build the linear regression model. # of PCs to incorporate in the model is chosen by cross-Validation (CV).
- @ Suitable when the data set contains highly correlated predictors
- @ No guarantee that the selected principal components are associated w/ outcome.

... the PCs to incorporate in the model

IS NOT supervised by the outcomes.

a Alternative PCR : (PLS) Identifies linear combinations and divections that best represent the predictors. Partial least squares regression is a form of regression that involves the development of components of the original variables in a supervised way.

> the dependent variable is used to help create the new components form the original variables.

.. help to explain both the independent and dependent variables in the model.

2. Performing Partial Least Squares (PLS) Regression

response).

- 1 The weights of the first linear combination (Z) is defined the regression of I onto each of the x's
 - ⇒ Large weights are going to placed on the X-variables most related to Y in the univariate case (most strongly related to the
- @ Regress each X variable onto 21 and compute residuals
- 3 repeat step! using the residuals from 3 m place of X.
- 1 iterate.

As always, the choice of where to stop (i.e., how many z-variables to use should be done by comparing the out-of-sample predictive CVs of testing set. performance.

(MSE IT RMSE)

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3. Advantages and Disadvantages

- o Advantages
 - Identifying new features in a supervised way
 - Althempting to find directions that help explain both response and predictors
 - Reduce the bras. > more prediztive accuracy.
 - Rednu (control) the collinearity > much lower risk of chall correlation.
 - * Bias: the difference between the expected prediction of the model and the correct value which we are trying to predict.

Bias - variance trade off.

*overfitting

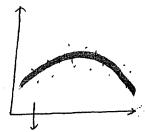
· complex mody

· perfectly predict the value > low

small # of Xs poorly predict values a High bias.

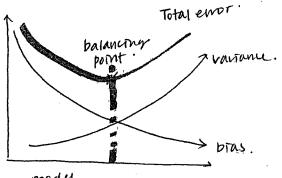
- o Disadvantages
 - * variance: the variability of model prediction for a given data point. - Potentially increase the variance.
 - Argher visk of overlooking 'real' correlations.
 - Sensitivity to the relative scaling of the predictor variables. = cannot apply for complex mixture sample. 1 in different scale

* good balanced model



relatively small if of predictors. controll variance

· follow the data pattern -> reduce the bias.



model complexity.

4. Performing PLS in R: Using the Labor Supply Data

Income data
The Labor Supply Data is a cross-sectional data containing 753 observations with 18 predictors.

Variables	Descriptions
work	participation in 1975
hoursw	wife's hours of work in 1975
child6	number of children less than 6 years old in household
child618	number of children between ages 6 and 18 in household
agew	wife's age
educw	wife's educational attainment, in years
hearnw	wife's average hourly earnings, in 1975 dollars
wagew	wife's wage reported at the time of the 1976 interview (not= 1975 estimated
_	wage)
hoursh	husband's hours worked in 1975
ageh	husband's age
educh	husband's educational attainment, in years
wageh .	husbad's wage, in 1975 dollars
income	family income, in 1975 dollars
educwm	wife's mother's educational attainment, in years
educwf	wife's father's educational attainment, in years
unemprate	unemployment rate in county of residence, in percentage points
city	lives in large city (SMSA)
experience	actual years of wife's previous labor market experience
city experience	lives in large city (SMSA)

Source: Mroz, T. (1987) "The sensitivity of an empirical model of married women's hours of work to economic and statistical assumptions", *Econometrica*, 55, 765-799.1976 Panel Study of Income Dynamics.

o 50/50 Split dataset

Set. Reed ! In order to assure reduplization.

scale =T; standardize the scale

75.51

75.51

1) Perform PLS

Data: X dimension: 392 17 Y dimension: 392 1

1

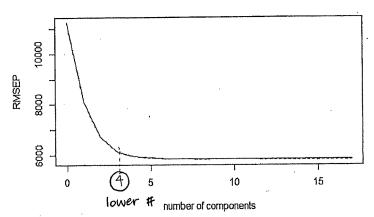
Fit method: kernelpls

Number of components considered: (17) : # of predictors = 17.

VALIDATION: RMSEP	Smaller Smaller
Cross-validated using 10 random segments.	
(Intercept) 1 comps 2 comps 3 comps 4 comps 5 comps 6 c	comps 7 comps 8 comps 9 comps
CV 11218 8121 6701 6127 5952 5886	5857 5853 5849 5854
	5842 5837 5833 5837
	16 comps 17 comps
CV 5853 5853 5852 5852 5852 5852	5852 5852 San
adjcv 5836 5836 5835 5835 5835 5835	5835 5835
delana a in di inventore illi	a & ITH DUDINGMENT M PVF.
TRAINING: % variance explained After 3 or 4 components. there	re is little improvement in PVE.
1 comps 2 comps 3 comps 4 comps 5 comps 6 comps 7 comp	ps 8 comps 9'comps 10 comps
x 17.04 26.64 37.18 49.16 59.63 64.63 69.1	13 72.82 76.06 78.59

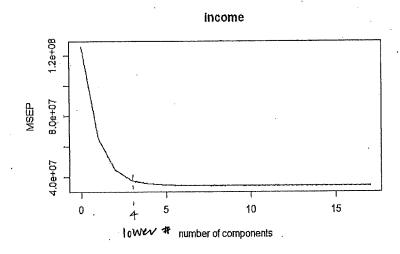
17.04 26.64 37.18 49.16 64.63 69.1372.82 72,75 74,16 74.87 75.25 75.44 75.49 income 49.26 66.63 13 comps 14 comps 15 comps 16 comps 17 comps 11 comps 12 comps 92.14 94.88 97.62 100.00 85.52 89.55 81.79, 75.52 75.52 75.52 income 75.52 75.52 75.52 75.52

2) Plot the root mean squared error (Default) income

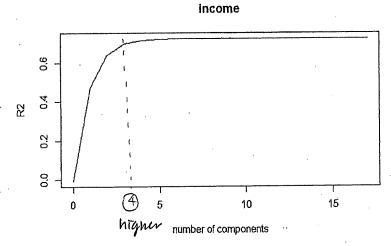


* still 5 or more compone are considerable. bias-variance trade off.

3) Plot the cross validation MSE

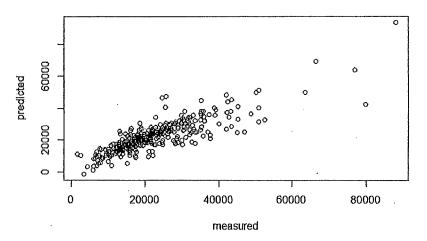


4) Plot the R^2

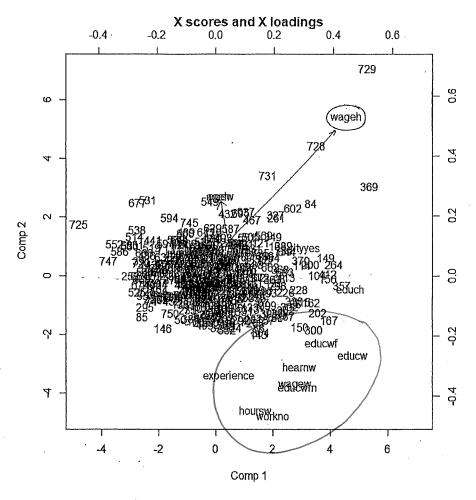


5) Plot the predicted vs measured values

income, 17 comps, validation



5) Biplot



6) OLS

Call:

Im(formula = income ~ ., data = Mroz, subset = train)

Residuals:

Min 1Q Median 3Q Max -20131 -2923 -1065 1670 36246

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.946e+04
                                   -6.036 3.81e-09 ***
                        3.224e+03
                                  -4,651 4.59e-06 ***
                        1.037e+03
            -4.823e+03
workno
                                   7.712 1.14e-13 ***
                        5.517e-01
             4.255e+00
hoursw
                                   -0.943 0.346258
chî 1d6
            -6.313e+02
                        6.694e+02
                                    2.052 0.040841 *
             4.847e+02
                        2.362e+02
child618
                                    3.424 0.000686 ***
             2,782e+02
                        8.124e+01
agew
             1.268e+02
                        1.889e+02
                                    0.671 0.502513
educw
             6.401e+02
                        1.420e+02
                                    4.507 8.79e-06 ***
hearnw
                                   1.070 0.285187
             1.945e+02
                        1.818e+02
wagew
                                   11.288 < 2e-16 ***
             6.030e+00
                        5.342e-01
hoursh
                                   -1.222 0.222488
            -9.433e+01
                        7.720e+01
ageh
                                    1.303 0.193437
             1.784e+02
                        1.369e+02
educh
                                   25.264 < 2e-16 ***
                        8.714e+01
wageh
             2,202e+03
educwm
            -4.394e+01
                        1,128e+02
                                   -0.390 \ 0.697024
                        1.053e+02
                                    1,322 0.186873
educwf
             1.392e+02
                        9.780e+01 -1.694 0.091055.
unemprate
            -1.657e+02
            -3,475e+02
                        6.686e+02 -0.520 0.603496
cityyes
                        4.490e+01 -2.737 0.006488 **
            -1.229e+02
experience
```

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1

Residual standard error: 5668 on 374 degrees of freedom Multiple R-squared: 0.7552, Adjusted R-squared: 0.744 F-statistic: 67.85 on 17 and 374 DF, p-value: < 2.2e-16

7) Comparing models

PLS OLS₂ PCR OLS1 57839715 MSE E Bias 63386682 59432814 '1ን Variance 3 # of Independent Best! varrables. FWI modu All predictors after dropping N.S effects. Variance V· (17→8). but, model bins b

7

Unit 3 Dimensionality Reduction Techniques

(3) Ridge and LASSO Regression November 6, 2019

1. A large number of predictors

Potential multicollinearity problem; predictors are nightly correlated. SE of B; is smaller than they should be. 1 overfitting problem for training set of data; Perfectly fit the training data set Poorly predict unknown values. Sample (n) using to fit Tramma set models for (70%) Testing (validation) finding the set best model (no%). refit the Best Model w/ many predictors using a test set. o produce predicted model model variances 1. Best Model @ compare predicted values to actual values. - High R2

- SMAII MYE.

- Large F.

- Small BIC.

O"OLS" fails to find the unique solution to minimize $\frac{n}{ij}(SSE_i)^2$.

unbrased estimator.

Solution. O variable selection

@ Dimentronal reduction; PCR or PLS (Based on PCA)

3 shinkage models

- Ridge

- Lasso

- Elastiz Net Regression.

2. Overview of the Shrinkage Methods

Under the assumptions, the coefficients estimated by "OLS" are unpiased and of all unbiased linear techniques also has the lowest variance $(\delta^2) \Rightarrow MVUE$ (Minimum variance unbiased Estimator) $MSE(=\delta^2) = \delta^2 + Model Bias^2 + Model Variance ... X. Best$

- O we can effectively reduce "Total MSE" by controlling Model Bias & Model variance. * Bias-variance trade off.
- D Introducing Small amount of Bias.
 → Substantial drop in the variance.
 -X. Goal is to get a model w/ smaller MSE as a 2nd optron.
- -: Shirnkage Model = Penalized regression model = Regularization. regression model
 - imposes a penalty to the model for too many prediztors.
 - This results in shrinking the coefficients of the less contributive variables toward zero.

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3. Ridge Regression

when $\sharp p \uparrow$, $s.s.R = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ under estimated.

Sig. of β_i over-estimated.

insignificant effect \rightarrow significant.

insignificant effect \rightarrow significant.

where β_i insignificant effect β_i is superiorized.

Here β_i to control the magnitude of coefficient. δ_i is δ_i or δ_i or

controll the magnitude of coefficient.

- o Choosing 2 (Tuning Parameter)
 - A controls the magnitute of coeffricients.
 - " the degree of regularization.
 - As I do, we obtain the least squares solution

 1 $\lambda = 0$, we are back to the regular regression model using ols.

- As $\lambda \uparrow \infty$, we obtain $\beta_{\lambda=\infty}^{Ridge} \approx 0$ j close to Zero"

Not equal to 0

In R, choosing the best 1.

- O Plot the components of all By against A
- Ochoose of for which the coefficients are not rapidly changing and have "sensible" sign.
- 3 Fit the model w/ best it using training set.
- Prefit the model using a testing set.

 Laculate C.V.

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4. LASSO Regression (Least Absolute Shirinkage and Selecti Operator).

S.S.R.
$$=\sum_{t=1}^{n}(y_{t}-\hat{y}_{t})^{2}+\lambda\sum_{j=1}^{p}|\beta_{j}|$$

Large
$$\lambda \Rightarrow less important \beta = 0$$

 $(\lambda \rightarrow \infty)$

Summary

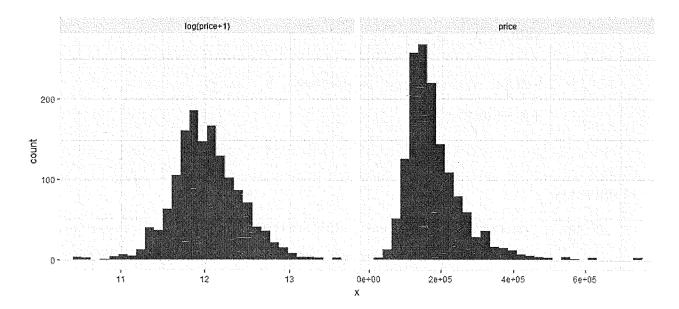
Ridge: variables w/ minor contribution have their coefficients close to Zevo. However, all the variables are incorporated in the model.

Lasso: the weffrients of some less contributive variables are forced to be exactly zero. Only most sig. variables are kept in the final model the

Flastiz net regression: combination of Ridge and Lasso. Some of coefficient toward to zero set some coefficients to exactly zero.

5. Performing Ridge and LASSO in R Data: Boston Housing Dataset

> dim(train) [1] 1460 81



```
# test out Ridge regression model

max, min decendre

lambdas <- seq(1,0,-0.001) < i > > > 0 > 0 < .

# train model

set.seed(123) # for reproducibility

model_ridge <- train(x=X_train,y=y,

method="glmnet", < Generalied Linear model,

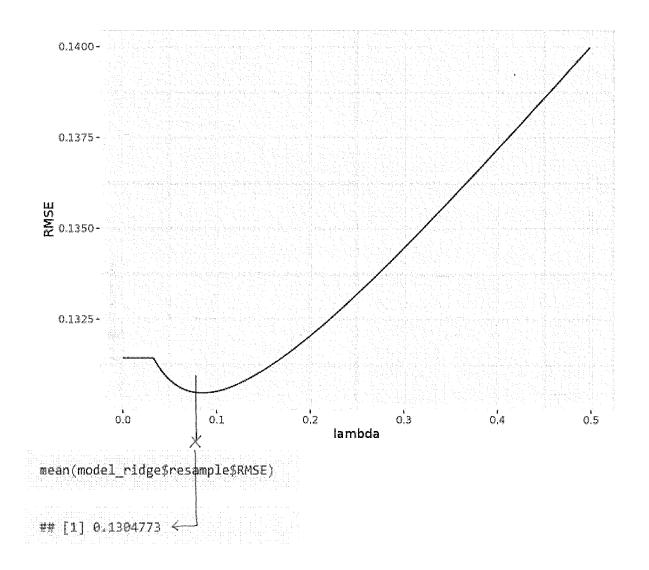
metric="RMSE", < choose the best model based on MCE.

maximize=FALSE,

trControl=CARET.TRAIN.CTRL,

tuneGrid=expand.grid(alpha=0) # Ridge regression

lambda=lambdas))
```



```
## glmnet
##
## 1460 samples
##
   288 predictor
群群
## No pre-processing
## Resampling: Cross-Validated (5 fold, repeated 5 times)
## Summary of sample sizes: 1169, 1168, 1168, 1167, 1168, 1168, ...
## Resampling results across tuning parameters:
##
拼拼
     lambda 🗀
              RMSE
                        Rsquared
     0.00010 0.1334558 0.8890952
計計
##
     0.00050 0.1296718 0.8945323
##
     0.00075 0.1284374 0.8963014
     0.00100 0.1275134 0.8976080
##
##
     0.00200 0.1251501 0.9609834
##
     0.00300 0.1240240 0.9026627
##
     0.00400 0.1238925 0.9029669(
##
     0.00500 0.1242215 0.9026495
     0.00600 0.1247290 0.9021018
##
##
     0.00700 0.1253763 0.9013804
##
     0.00800 0.1262039 0.9004245
##
     0.00900 0.1272133 0.8992018
     0.01000 0.1283448 0.8977959
##
##
     0.05000 0.1731301 0.8406120
##
     0.10000 0.2154212 0.7968063
##
     1.00000 0.3990550
                              NaN
##
## Tuning parameter 'alpha' was held constant at a value of 1
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were alpha = 1 and lambda = 0.004.
```

mean(model_lasso\$resample\$RMSE)

```
## [1] 0.1238925
```

