Principal Components Regression

Predictive Modeling & Statistical Learning

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Data set `cars2004`

Data cars2004

```
                               price engine cyl  hp city_mpg
Acura 3.5 RL 4dr               43755    3.5   6 225       18
Acura 3.5 RL w/Navigation 4dr 46100    3.5   6 225       18
Acura MDX                      36945    3.5   6 265       17
Acura NSX coupe 2dr manual S   89765    3.2   6 290       17
Acura RSX Type S 2dr           23820    2.0   4 200       24
Acura TL 4dr                   33195    3.2   6 270       20
                               hwy_mpg weight wheel length width
Acura 3.5 RL 4dr                    24   3880   115    197    72
Acura 3.5 RL w/Navigation 4dr      24   3893   115    197    72
Acura MDX                           23   4451   106    189    77
Acura NSX coupe 2dr manual S        24   3153   100    174    71
Acura RSX Type S 2dr                31   2778   101    172    68
Acura TL 4dr                        28   3575   108    186    72
```

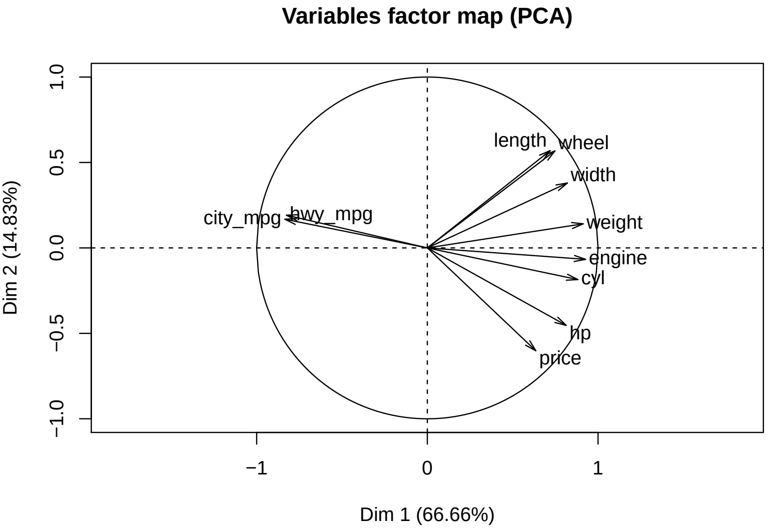
Data cars2004

```
'data.frame': 385 obs. of  10 variables:
 $ price   : int  43755 46100 ...
 $ engine  : num  3.5 3.5 ...
 $ cyl     : int  6 6 ...
 $ hp      : int  225 225 ...
 $ city_mpg: int  18 18 ...
 $ hwy_mpg : int  24 24 ...
 $ weight  : int  3880 3893 ...
 $ wheel   : int  115 115 ...
 $ length  : int  197 197 ...
 $ width   : int  72 72 ...
```

Correlation Matrix

	engine	cyl	hp	city_mpg	hwy_mpg	weight	wheel	length	width
price	0.6	0.654	0.836	-0.485	-0.469	0.476	0.204	0.210	0.314
engine		0.912	0.778	-0.706	-0.708	0.812	0.631	0.624	0.727
cyl			0.792	-0.670	-0.664	0.731	0.553	0.547	0.621
hp				-0.672	-0.652	0.631	0.396	0.381	0.500
city_mpg					0.941	-0.736	-0.481	-0.468	-0.590
hwy_mpg						-0.789	-0.455	-0.390	-0.585
weight							0.751	0.653	0.808
wheel								0.867	0.760
length									0.752

PCA


Variables factor map (PCA)
length
wheel
width
weight
engine
cyl
hp
price
city_mpg
hwy_mpg
Dim 1 (66.66%)
Dim 2 (14.83%)
−1
0
1
−1.0
−0.5
0.0
0.5
1.0

PCA: Eigenvalues

	eigenvalues	proportion	cum_prop
comp1	6.30	70.04	70.04
comp2	1.21	13.43	83.47
comp3	0.61	6.76	90.23
comp4	0.28	3.06	93.30
comp5	0.21	2.37	95.67
comp6	0.19	2.13	97.79
comp7	0.09	0.99	98.79
comp8	0.07	0.79	99.58
comp9	0.04	0.42	100.00

Predicting Price of cars

$$\texttt{price} = \beta_0 + \beta_1\,\texttt{cyl} + \beta_2\,\texttt{hp} + \ldots + \beta_9\,\texttt{width} + \varepsilon$$

```
ols_reg <- lm(price ~ ., data = cars2004)

ols_reg_sum <- summary(ols_reg)
```

OLS Regression

Regress `price` on 9 predictors

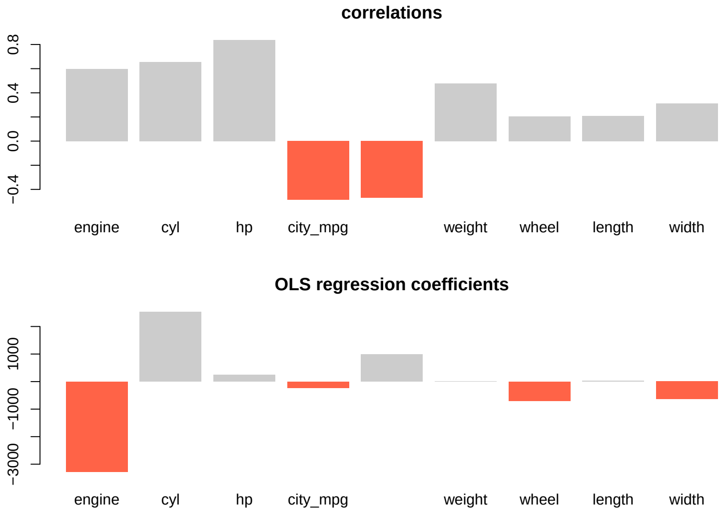
```
             Estimate  Std. Error  t value   Pr(>|t|)
(Intercept) 32536.025  17777.488   1.8302  6.802e-02
engine      -3273.053   1542.595  -2.1218  3.451e-02
cyl          2520.927    896.202   2.8129  5.168e-03
hp            246.595     13.201  18.6797  1.621e-55
city_mpg     -229.987    332.824  -0.6910  4.900e-01
hwy_mpg       979.967    345.558   2.8359  4.817e-03
weight          9.937      2.045   4.8584  1.741e-06
wheel        -695.392    172.896  -4.0220  6.980e-05
length         33.690     89.660   0.3758  7.073e-01
width        -635.382    306.344  -2.0741  3.875e-02
```

```
Call:
lm(formula = price ~ ., data = cars2004)

Residuals:
   Min     1Q Median     3Q    Max
-21534  -5411   -352   4054  92763

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 32536.025  17777.488   1.830  0.06802 .
engine      -3273.053   1542.595  -2.122  0.03451 *
cyl          2520.927    896.202   2.813  0.00517 **
hp            246.595     13.201  18.680  < 2e-16 ***
city_mpg     -229.987    332.824  -0.691  0.48998
hwy_mpg       979.967    345.558   2.836  0.00482 **
weight          9.937      2.045   4.858 1.74e-06 ***
wheel        -695.392    172.896  -4.022 6.98e-05 ***
length         33.690     89.660   0.376  0.70731
width        -635.382    306.344  -2.074  0.03875 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 10110 on 375 degrees of freedom
Multiple R-squared:  0.745,Adjusted R-squared:  0.7389
F-statistic: 121.7 on 9 and 375 DF,  p-value: < 2.2e-16
```

Correlations and OLS Coefficients

	correlation	coefficient
engine	0.5997873	-3273.05304
cyl	0.6544123	2520.92691
hp	0.8360930	246.59496
city_mpg	-0.4854130	-229.98735
hwy_mpg	-0.4694315	979.96656
weight	0.4760867	9.93652
wheel	0.2035464	-695.39157
length	0.2096682	33.69009
width	0.3135383	-635.38224

Some correlation signs don't match regression coeff. signs



correlations
0.8
0.4
0.0
−0.4
engine
cyl
hp
city_mpg
weight
wheel
length
width
OLS regression coefficients
1000
−1000
−3000
engine
cyl
hp
city_mpg
weight
wheel
length
width

Principal Components Regression (PCR)

Uses of PCA

PCA can be used to ...

- Reduce the dimensionality of a data set (i.e. reduce the number of variables)
- For data visualization and exploration purposes to obtain:
  - a map to visualize the objects in terms of their proximities, and
  - another map to visualize the variables in terms of their correlations.
- Summarize the systematic patterns of variation within observations, within variables, and between observations and variables.

Uses of PCA

When fitting a regression model:

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-\mathbf{1}}\mathbf{X}^\mathsf{T}\mathbf{y}$$

We can also use PCA as a *pre-processing* step on the predictors before fitting a regression equation.

PCA Regression Idea

Decompose the predictors data matrix $\mathbf{X}$ *into PC's, and then regress* $\mathbf{y}$ *onto the PCs*

PCA Formula Decomposition

Decompose the predictors data matrix $\mathbf{X}$ into PC's

$$\mathbf{X} = \mathbf{Z}\mathbf{V}^{\intercal}$$

where:

- $\mathbf{Z}$ is the matrix of PCs
- $\mathbf{V}$ is the matrix of loadings

Without loss of generality suppose the predictors and response are standardized.

PC Regression

Regress $\mathbf{y}$ onto the PC's:

$$\hat{\mathbf{y}} = \hat{\beta}_1 \mathbf{z_1} + \hat{\beta}_2 \mathbf{z_2} + \cdots + \hat{\beta}_p \mathbf{z_p}$$

where:

- $\mathbf{z_j}$ is the j-th PC
- $\hat{\beta}_j$ is the estimate of the j-th PCR-coefficient

PC Regression

In matrix notation:

$$\hat{\mathbf{y}} = \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR}$$

The vector of PCR coefficients is obtained via OLS:

$$\hat{\boldsymbol{\beta}}_{PCR} = (\mathbf{Z}^\mathsf{T}\mathbf{Z})^{-\mathbf{1}}\mathbf{Z}^\mathsf{T}\mathbf{y}$$

PC Regression

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	0.000	515.0450	0.0000	1.0000
PC1	-4470.761	205.4021	-21.7659	0.0000
PC2	7608.419	469.1001	16.2192	0.0000
PC3	-9650.324	661.0626	-14.5982	0.0000
PC4	-1768.547	981.9554	-1.8010	0.0725
PC5	10528.146	1116.5683	9.4290	0.0000
PC6	-5593.736	1179.2391	-4.7435	0.0000
PC7	-5746.452	1723.8664	-3.3335	0.0009
PC8	-7606.196	1928.9437	-3.9432	0.0001
PC9	5473.090	2663.9282	2.0545	0.0406

PC Regression

Usually, you don't use all p PCs, but just $k < p$ of them, i.e. $\hat{\mathbf{X}} = \mathbf{Z}\mathbf{V}^\mathsf{T}$:

$$\hat{\mathbf{y}} = \hat{\beta}_1 \mathbf{z_1} + \hat{\beta}_2 \mathbf{z_2} + \cdots + \hat{\beta}_k \mathbf{z_k}$$

Regressions with few PCs

Regression with first two PCs

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	0.000	713.7648	0.0000	1
PC1	-4470.761	284.6524	-15.7060	0
PC2	7608.419	650.0930	11.7036	0

Regressions with few PCs

Regression with first two PCs

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	0.000	713.7648	0.0000	1
PC1	-4470.761	284.6524	-15.7060	0
PC2	7608.419	650.0930	11.7036	0

Regression with first three PCs

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	0.000	602.0143	0.0000	1
PC1	-4470.761	240.0858	-18.6215	0
PC2	7608.419	548.3113	13.8761	0
PC3	-9650.324	772.6881	-12.4893	0

PC Regression property

Because of uncorrelatedness, the contributions and estimated coefficient of a PC are unaffected by which other PCs are also included in the regression.

How does PCR work?

PC Regression Idea

Decompose the predictors data matrix $\mathbf{X}$ into PC's

$$\mathbf{X} = \mathbf{Z}\mathbf{V}^\mathsf{T}$$

Replace $\mathbf{X}$ with $\mathbf{Z}\mathbf{V}^\mathsf{T}$ in the fitted values:

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^\mathsf{T}\mathbf{X})^{-\mathbf{1}}\mathbf{X}^\mathsf{T}\mathbf{y}$$

OLS Regression in terms of PCs

$$
\begin{aligned}
\hat{\mathbf{y}} &= \mathbf{X}(\mathbf{X}^\intercal\mathbf{X})^{-\mathbf{1}}\mathbf{X}^\intercal\mathbf{y} \\
&= \mathbf{Z}\mathbf{V}^\intercal\left((\mathbf{Z}\mathbf{V}^\intercal)^\intercal\mathbf{Z}\mathbf{V}^\intercal\right)^{-1}(\mathbf{Z}\mathbf{V}^\intercal)^\intercal\mathbf{y} \\
&= \mathbf{Z}\mathbf{V}^\intercal\left(\mathbf{V}\mathbf{Z}^\intercal\mathbf{Z}\mathbf{V}^\intercal\right)^{-1}\mathbf{V}\mathbf{Z}^\intercal\mathbf{y} \\
&= \mathbf{Z}\mathbf{V}^\intercal(\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\intercal)^{-1}\mathbf{V}\mathbf{Z}^\intercal\mathbf{y} \\
&= \mathbf{Z}\mathbf{V}^\intercal(\mathbf{V}\boldsymbol{\Lambda}^{-1}\mathbf{V}^\intercal)\mathbf{V}\mathbf{Z}^\intercal\mathbf{y} \\
&= \mathbf{Z}\boldsymbol{\Lambda}^{-1}\mathbf{Z}^\intercal\mathbf{y} \\
&= \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR}
\end{aligned}
$$

OLS and PCR coefficients

Relationship between OLS coefficients and PCR coefficients

$$
\begin{aligned}
\hat{\mathbf{y}} &= \mathbf{X}\hat{\boldsymbol{\beta}}_{OLS} \\
&= \mathbf{Z}\mathbf{V}^{\mathsf{T}}\hat{\boldsymbol{\beta}}_{OLS} \\
&= \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR}
\end{aligned}
$$

OLS and PCR coefficients

Relationship between OLS coefficients and PCR coefficients

$$\begin{aligned}\hat{\mathbf{y}} &= \mathbf{X}\hat{\boldsymbol{\beta}}_{OLS} \\ &= \mathbf{Z}\mathbf{V}^{\mathsf{T}}\hat{\boldsymbol{\beta}}_{OLS} \\ &= \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR}\end{aligned}$$

$$\begin{aligned}\hat{\mathbf{y}} &= \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR} \\ &= \mathbf{X}\mathbf{V}\hat{\boldsymbol{\beta}}_{PCR} \\ &= \mathbf{X}\hat{\boldsymbol{\beta}}_{OLS}\end{aligned}$$

Notice when using all PCs, $\mathbf{X} = \mathbf{Z}\mathbf{V}^{\mathsf{T}}$, OLS $\hat{\mathbf{y}}$ is the same as PCR $\hat{\mathbf{y}}$

PCR Coefficients transition formula

In general, you can always reexpress the PCR coefficients in terms of the original variables:

$$
\begin{aligned}
\hat{\mathbf{y}} &= \mathbf{Z}\hat{\boldsymbol{\beta}}_{PCR} \\
&= \mathbf{X}\mathbf{V}\hat{\boldsymbol{\beta}}_{PCR}
\end{aligned}
$$

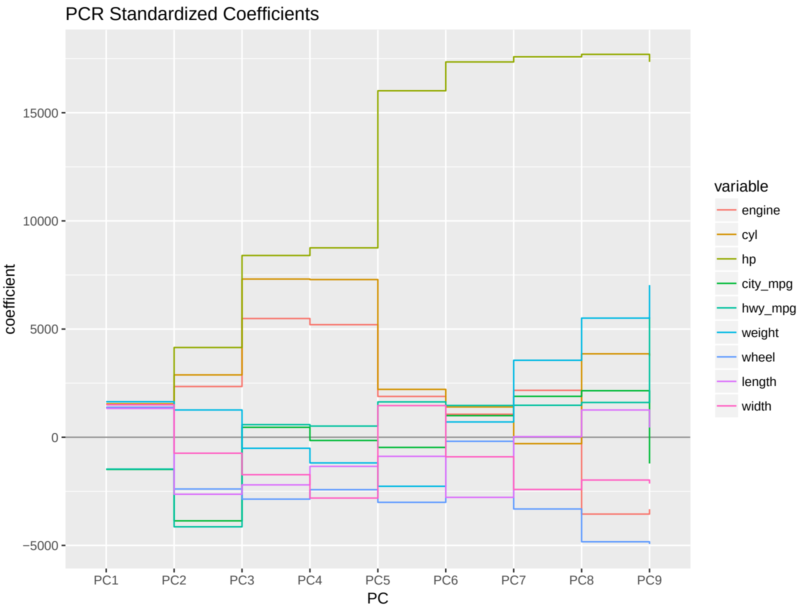
by premultiplying $\hat{\boldsymbol{\beta}}_{PCR}$ by the loadings $\mathbf{V}$

PC Regression Coefficients

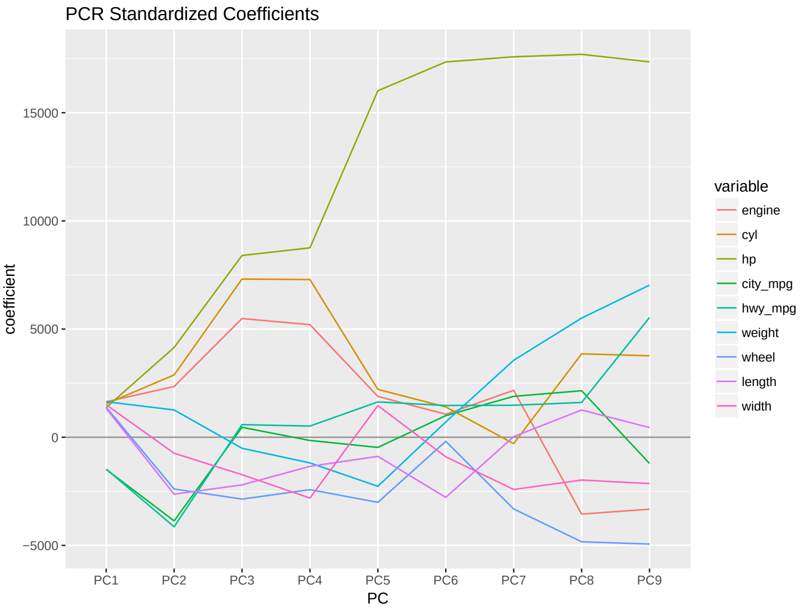
Regression coefficients in terms of the original variables, for each of the 9 PC regressions:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
engine	1641	2345	5487	5203	1887	1064	2168.5	-3551	-3327
cyl	1544	2881	7312	7289	2213	1401	-295.5	3856	3766
hp	1377	4148	8402	8755	16016	17348	17585.7	17700	17352
city_mpg	-1487	-3864	459	-149	-470	999	1891.3	2151	-1213
hwy_mpg	-1472	-4140	583	516	1633	1468	1477.9	1607	5536
weight	1642	1261	-510	-1187	-2266	707	3557.7	5507	7033
wheel	1385	-2392	-2860	-2422	-3009	-187	-3315.7	-4832	-4938
length	1332	-2634	-2202	-1346	-883	-2778	28.2	1260	447
width	1501	-738	-1731	-2811	1464	-904	-2413.8	-1978	-2142

The solution with 9 PCs matches the OLS solution.



PCR Standardized Coefficients
coefficient
15000
10000
5000
0
−5000
PC1
PC2
PC3
PC4
PC5
PC6
PC7
PC8
PC9
PC
variable
engine
cyl
hp
city_mpg
hwy_mpg
weight
wheel
length
width


PCR Standardized Coefficients
coefficient
15000
10000
5000
0
−5000
PC1
PC2
PC3
PC4
PC5
PC6
PC7
PC8
PC9
PC
variable
engine
cyl
hp
city_mpg
hwy_mpg
weight
wheel
length
width

How to choose an "optimal" number of PCs?

Number of PCs

- The main challenge in PCR is the choice for k, the number of PCs
- k is also known as the tuning parameter
- k is usually chosen via cross-validation

Regression with PC1

$$\hat{\mathbf{y}} = \hat{\beta}_1 \mathbf{z_1} = \mathbf{X}(\hat{\beta}_1 \mathbf{v_1})$$

	correlation	coefficient
engine	0.5997873	1640.623
cyl	0.6544123	1543.678
hp	0.8360930	1376.699
city_mpg	-0.4854130	-1487.103
hwy_mpg	-0.4694315	-1471.922
weight	0.4760867	1641.840
wheel	0.2035464	1385.197
length	0.2096682	1331.796
width	0.3135383	1500.565

Regression with PC1 and PC2

$$\hat{\mathbf{y}} = \hat{\beta}_1 \mathbf{z_1} + \hat{\beta}_2 \mathbf{z_2} = \mathbf{X}\mathbf{V}_{1:2}\hat{\boldsymbol{\beta}}_{1:2}$$

	correlation	coefficient
engine	0.5997873	2345.1254
cyl	0.6544123	2881.3726
hp	0.8360930	4148.0459
city_mpg	-0.4854130	-3864.4992
hwy_mpg	-0.4694315	-4139.9870
weight	0.4760867	1260.7474
wheel	0.2035464	-2391.5824
length	0.2096682	-2634.3174
width	0.3135383	-738.1835

Number of PCs via Cross-Validation

- Optionally: divide the data into training and test sets.
- If you don't have a test set, then all your data is the training set.
- Divide the training set into m parts (of similar size).
- For each possible number k of PCs do:
  - For each part, use the rest of the data to fit the PC regression, and use the part to compute the MSE.
  - Repeat for each part, and average the MSE's.
- Select the number of PCs with smallest MSE.

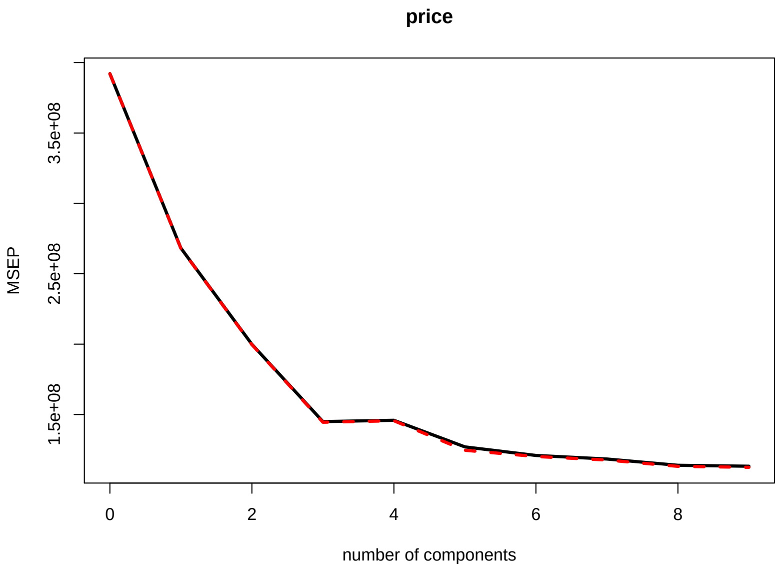
PCR Coefficients

```r
library(pls)
set.seed(2)

pcr_fit <- pcr(price ~ ., data = cars2004, scale = TRUE, validation = "CV")

summary(pcr_fit)

validationplot(pcr_fit, val.type = "MSEP")
```

`pcr()` standardizes the predictors, but not the response

PCR Coefficients

```
Data:  X dimension: 385 9
Y dimension: 385 1
Fit method: svdpc
Number of components considered: 9

VALIDATION: RMSEP
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 com
CV           19802    16377    14138    12041    12079    11270    10996    108
adjCV        19802    16370    14129    12021    12066    11162    10962    108
       8 comps  9 comps
CV       10674    10643
adjCV    10639    10607

TRAINING: % variance explained
       1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X        70.04    83.47    90.23    93.30    95.67    97.79    98.79    99.58
price    32.22    50.11    64.60    64.82    70.87    72.40    73.15    74.21
```

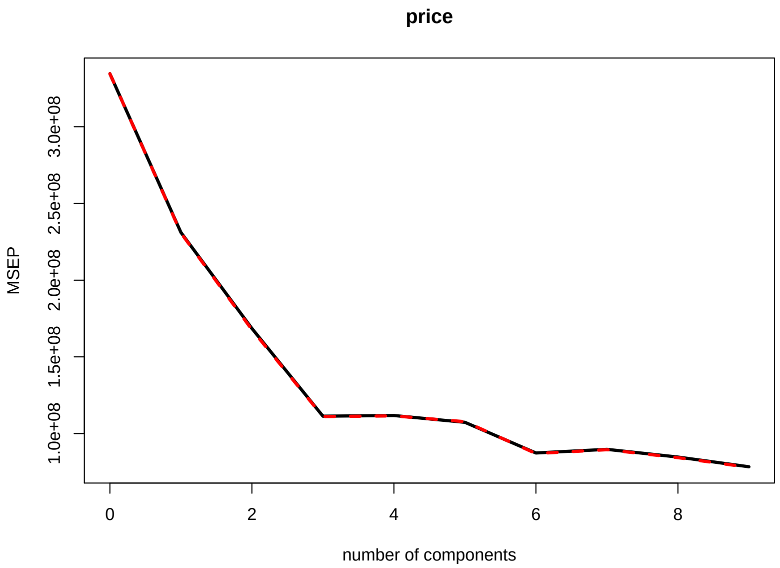

price
MSEP
3.5e+08
2.5e+08
1.5e+08
0
2
4
6
8
number of components

PCR Coefficients

```r
# train set
set.seed(1)
train <- sample(c(TRUE, FALSE), nrow(cars2004), replace = TRUE)
test <- (!train)

pcr_fit <- pcr(price ~ ., data = cars2004, subset = train,
               scale = TRUE, validation = "CV")

summary(pcr_fit)

validationplot(pcr_fit, val.type = "MSEP")
```

PCR Coefficients

```
Data:  X dimension: 208 9
Y dimension: 208 1
Fit method: svdpc
Number of components considered: 9

VALIDATION: RMSEP
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 com
CV           18291    15203    12983    10552    10572    10361     9346     94
adjCV        18291    15190    12952    10540    10560    10381     9327     94
       8 comps  9 comps
CV        9203     8852
adjCV     9182     8832

TRAINING: % variance explained
       1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X        68.61    82.49    90.05    93.57    95.98    97.91    98.80    99.58
price    32.49    53.06    67.70    67.80    68.57    75.55    75.66    76.96
```



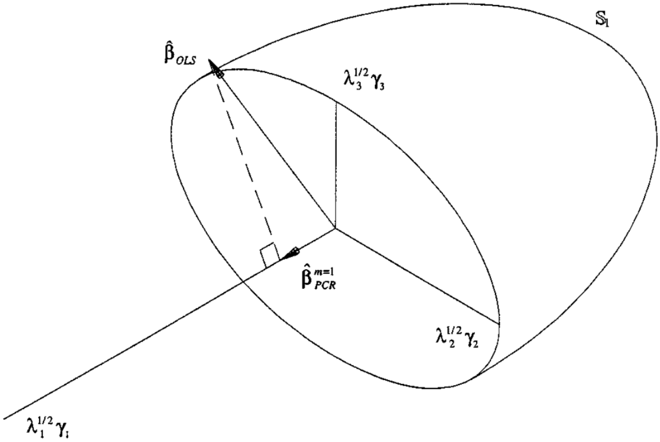
price
MSEP
1.0e+08
1.5e+08
2.0e+08
2.5e+08
3.0e+08
0
2
4
6
8
number of components

Number of PCs via Cross-Validation

- PCR with CV suggests using all $k = 9$ PCs.
- The PCR solution coincides with the OLS.
- There is not really an advantage of PCR in this particular example.
- As this example shows: the PCs with large variation may not necessarily be good predictors.
- However, a regression on PC1 may still be an interesting case.

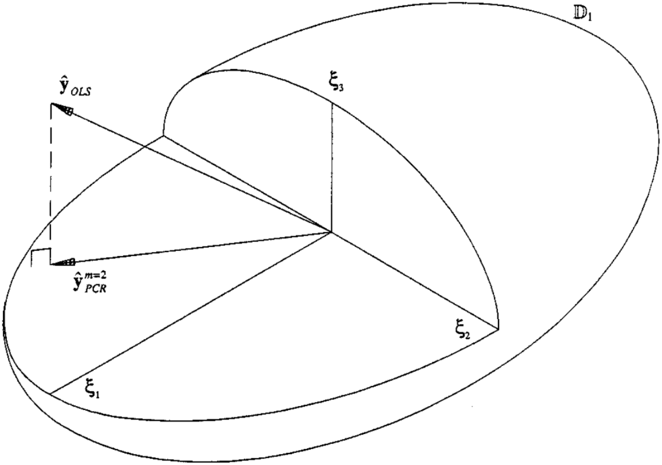
Geometry of PCR

PCR Geometry



PCR fitted vector with first PC (Phatak & de Jong, 1997)

PCR Geometry



PCR fitted vector with two first PCs (Phatak & de Jong, 1997)

PCR Geometry

"The geometric interpretation of principal component regression is quite straightforward. $\hat{\beta}^{m}_{PCR}$ is simply the orthogonal projection of $\hat{\beta}_{OLS}$ onto the subspace spanned by the eigenvectors corresponding to the PCs retained in the regression."

(Phatak & de Jong, 1997)

PC Regression rationale

- The main advantage of PC regression occurs when multicollinearities are present.
- Finding regression coefficients is more straightforward with $\mathbf{Z}$ because its columns are orthogonal.
- Calculation of OLS estimates via PC regression may be numerically more estable.
- PCR assumes that the new predictors (i.e. the PCs), explain the reponse, especially those PCs with larger variance.

PC Regression Issues

- The first PCs may not be necessarily related to the response.
- PCR is not a feature selection method.
- Each of the PCs used in the regression is a linear combination of all p predictor variables.
- PCR is not scaling-invariant.

References

- **Principal Component Analysis** by Ian Jolliffe (2004). *Chapter 8: Principal Components in Regression Analysis*.
- **Linear Models with R** by Julian Faraway (2015). *Chapter 11: Shrinkage Methods*.
- **Modern Regression Methods** by Thomas Ryan (1997). *Chapter 12, sec 9: Other Biased Estimators*.
- **The Geometry of Partial Least Squares** by Aloke Phatak and Sijmen de Jong (1997). *Journal of Chemometrics, Vol. 11, 311-338*.