19) Principal Components Regression, and Partial Least Squares

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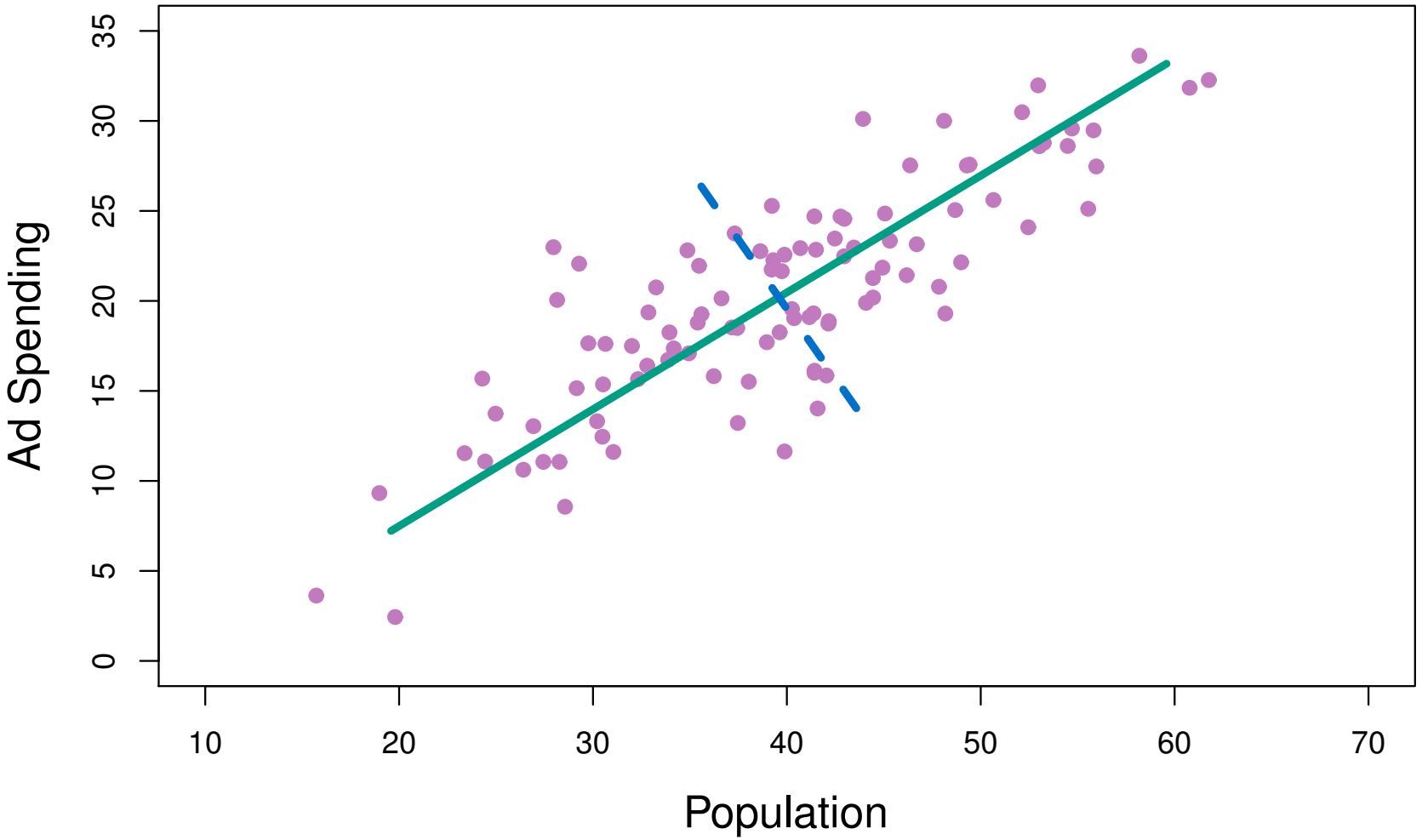
Reference

Tables, Graphics, and Figures from

James et al. (2017): Chapters: 6.3, and 6.7

Hastie et al. (2017): Chapter: 3.5

Advertising Data



Principal Components Analysis (PCA)

$$Z_1 = \phi_{11}(pop - \bar{pop}) + \phi_{21}(ad - \bar{ad})$$

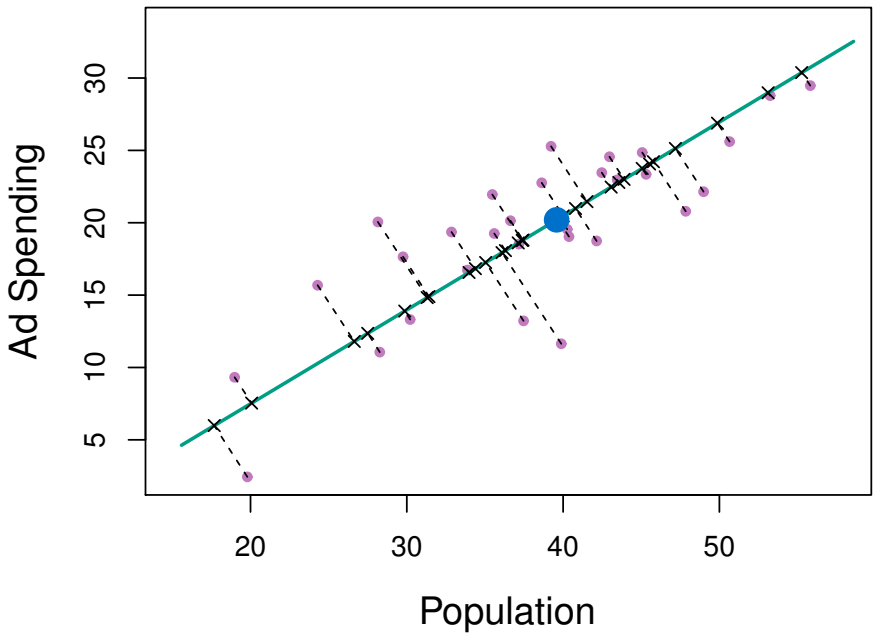
$$Z_1 = 0.839(pop - \bar{pop}) + 0.544(ad - \bar{ad})$$

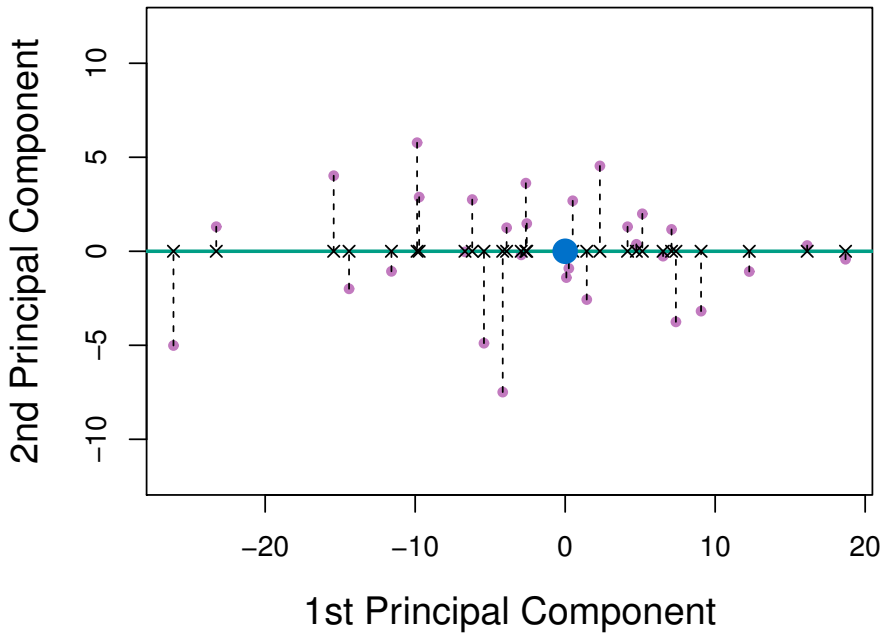
$$Var[\phi_{11}(pop - \bar{pop}) + \phi_{21}(ad - \bar{ad})]$$

$$\phi_{11}^2 + \phi_{21}^2 = 1$$

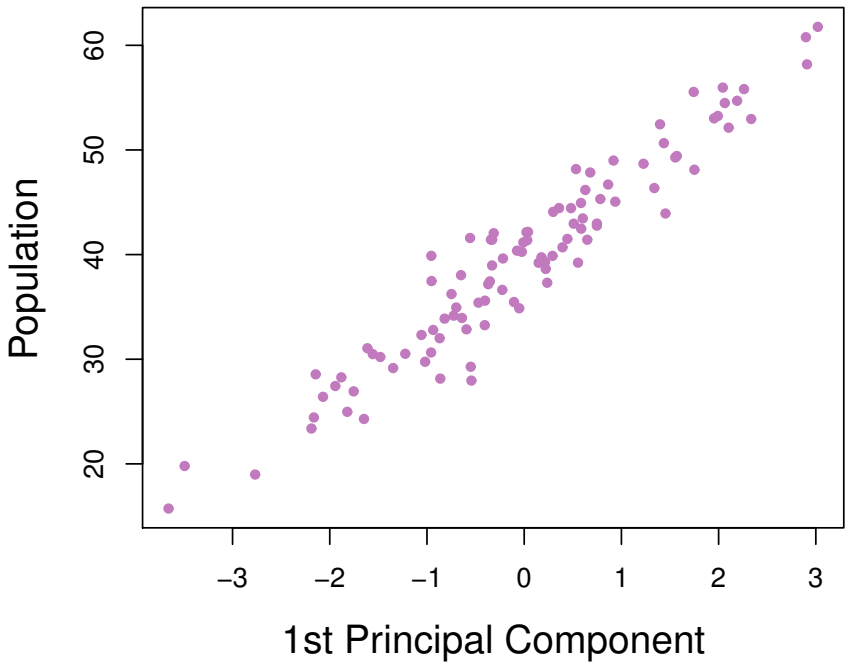
$$z_{i1} = 0.839(pop_i - \bar{pop}) + 0.544(ad_i - \bar{ad})$$

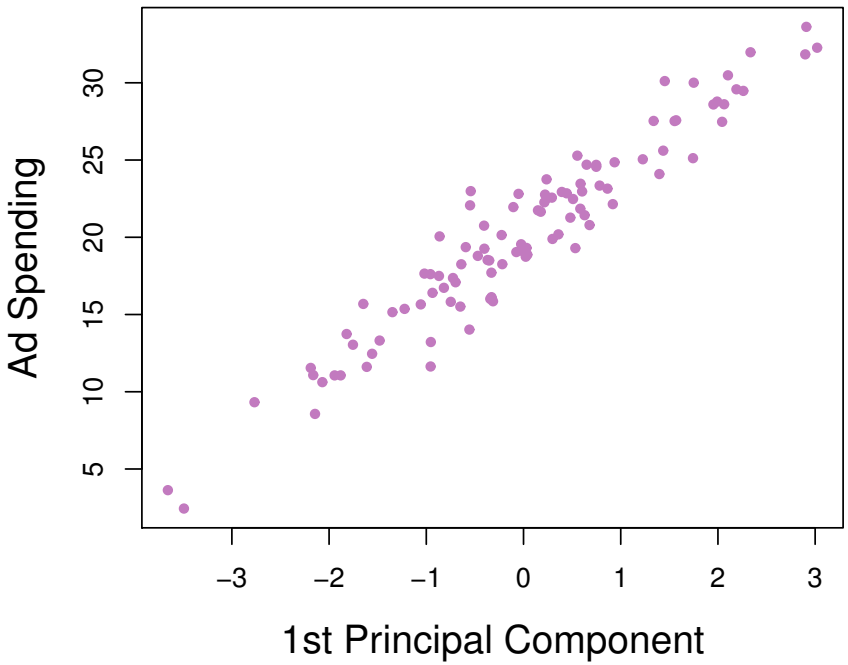
First and Second Principal Component



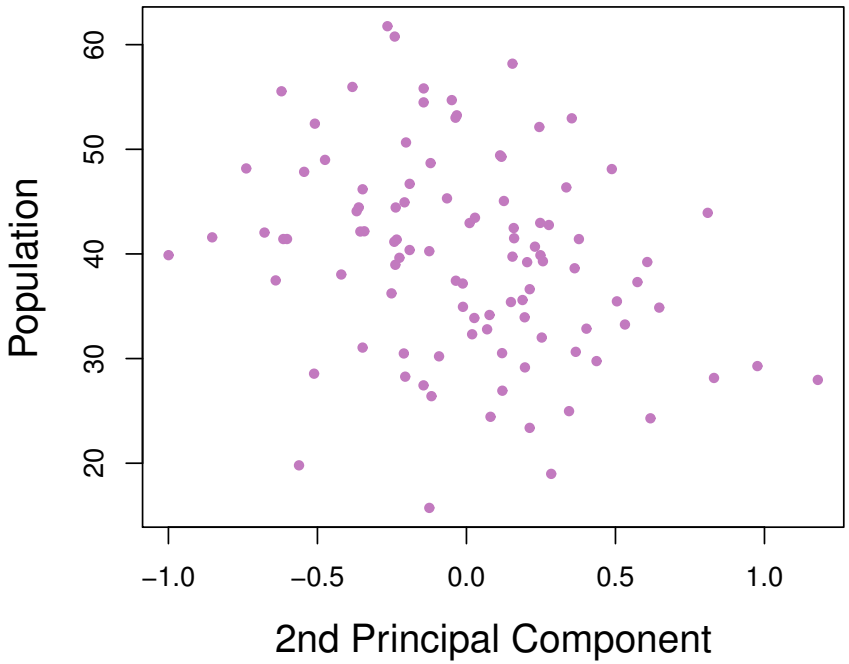


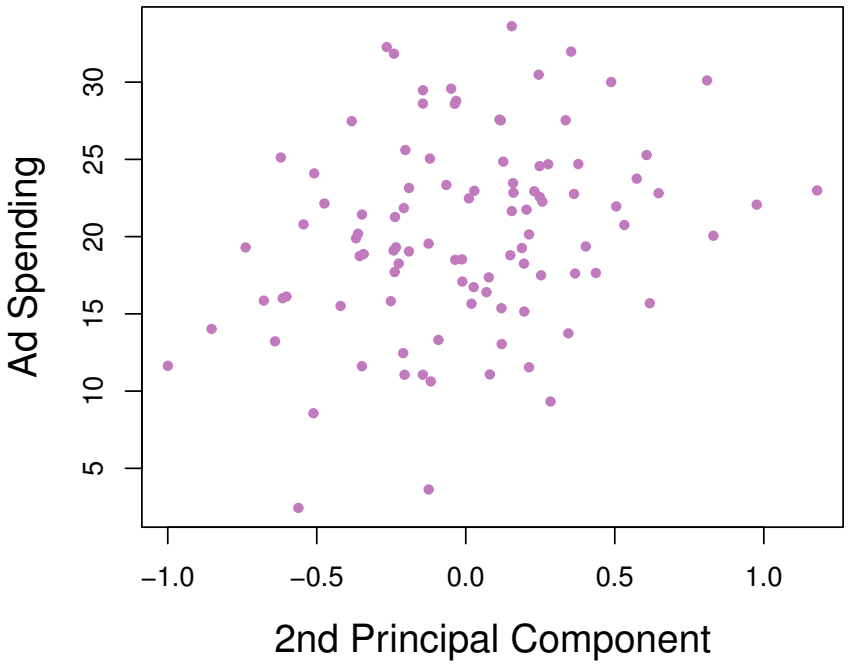
First Principal Component Scores z_{i1} vs pop and ad





Second Principal Component Scores z_{i2} vs pop and ad





Dimension Reduction

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

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

$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{jm} x_{ij}$$

$$= \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{jm} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij}$$

Principal Components Regression (PCR)

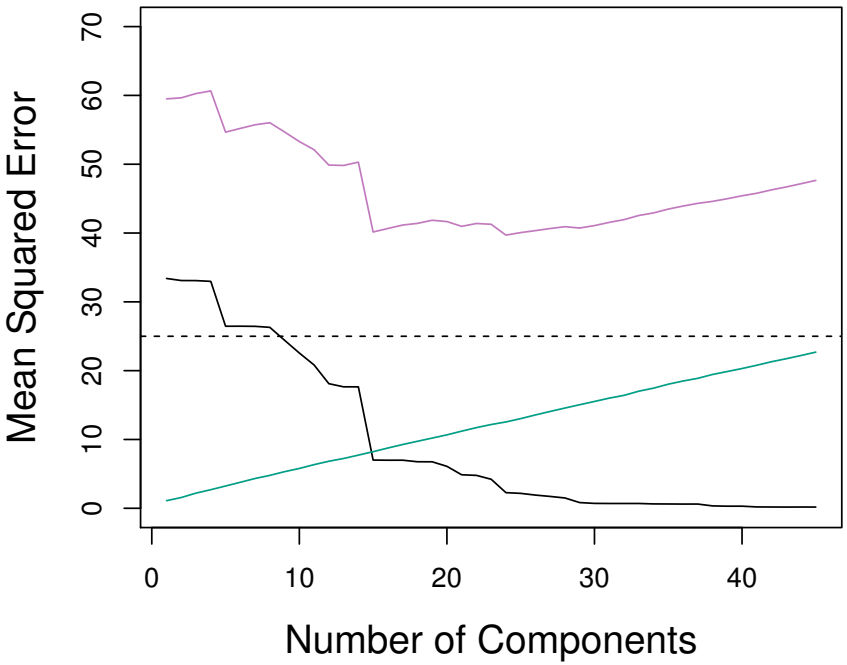
$$\hat{y}^{pcr}_{(M)} = \bar{y}1 + \sum_{m=1}^{M} \hat{\theta}_m z_m$$

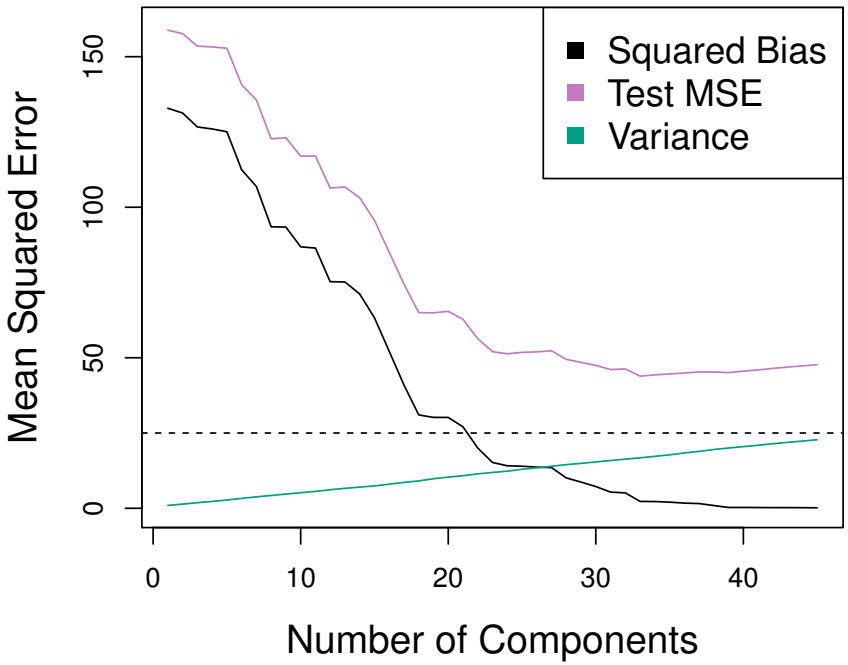
$$\hat{\beta}^{pcr}_{(M)} = \sum_{m=1}^{M} \hat{\theta}_m v_m$$

$$\hat{\theta}_m = \frac{\langle z_m, y \rangle}{\langle z_m, z_m \rangle}$$

Principal Components Regression (PCR) for Simulated Data

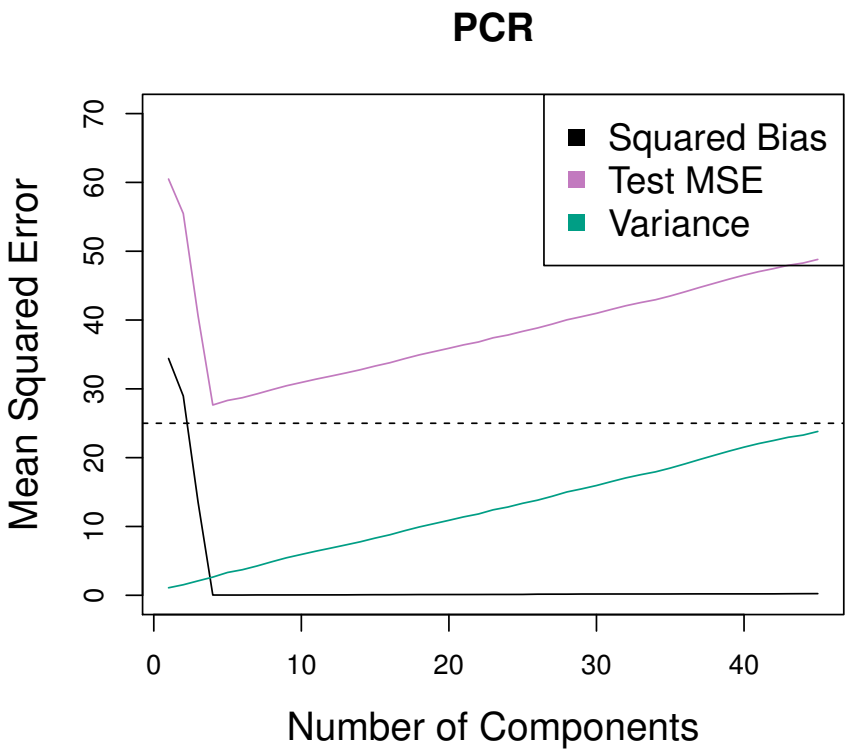
Horizontal Dashed Line: $Var(\epsilon)$

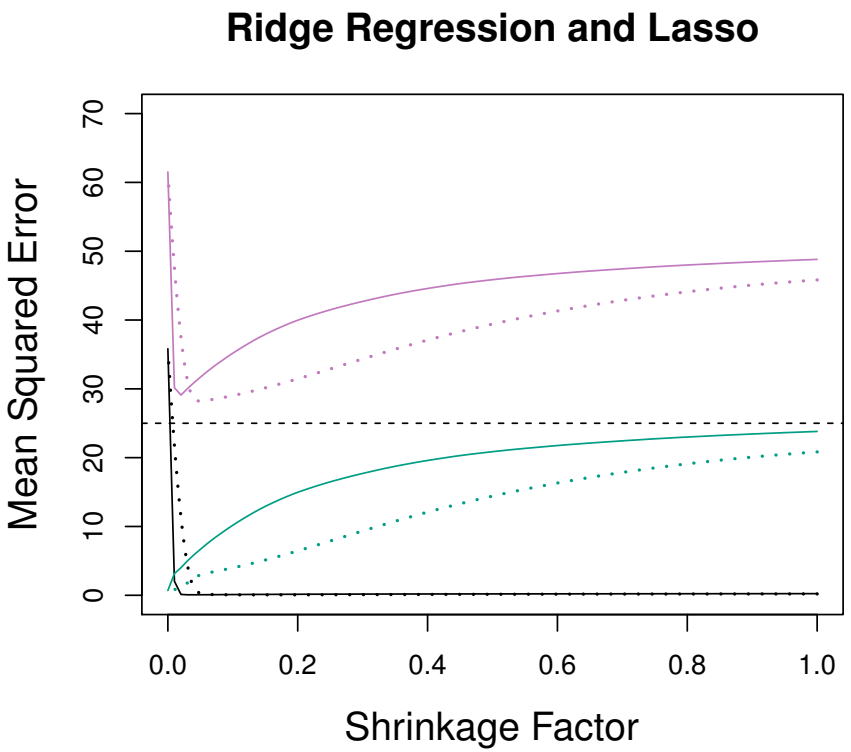




Simulated Data in which the first 5 PC of X contain all the information about Y

Solid (lasso), Dotted(ridge)





PCR Optimization

$$\max_{\alpha} Var(X\alpha)$$

Subject to $||\alpha|| = 1$ and $\alpha^T S v_l = 0$

S is the sample covariance matrix of the X

$z_m = X\alpha$ is uncorrelated with all the previous linear combinations $z_l = Xv_l$

Partial Least Squares (PLS)

$$\max_{\alpha} Corr^2(y, X\alpha) Var(X\alpha)$$

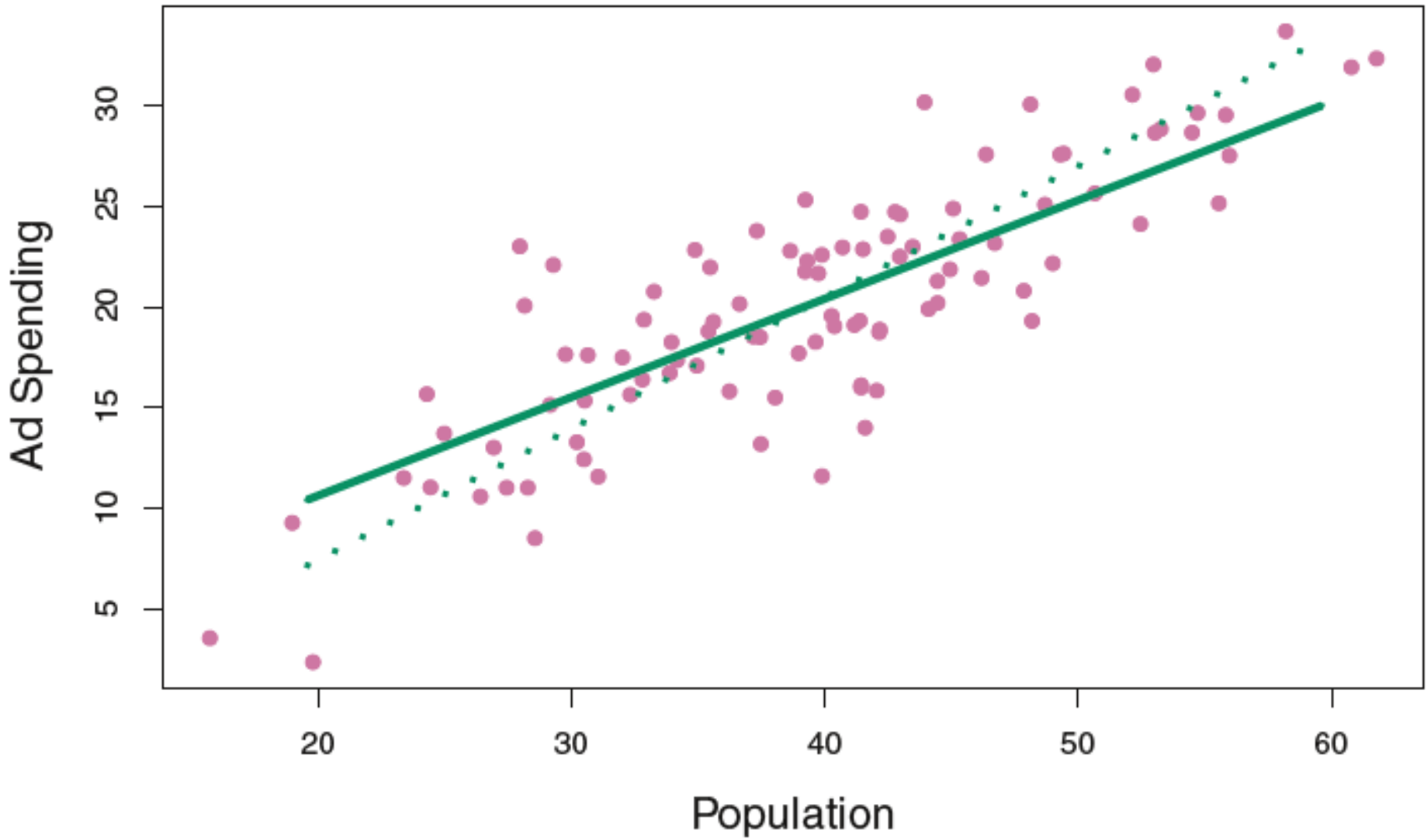
Subject to $||\alpha|| = 1$ and $\alpha^T S \hat{\varphi}_l = 0$

$$l = 1, ..., m - 1$$

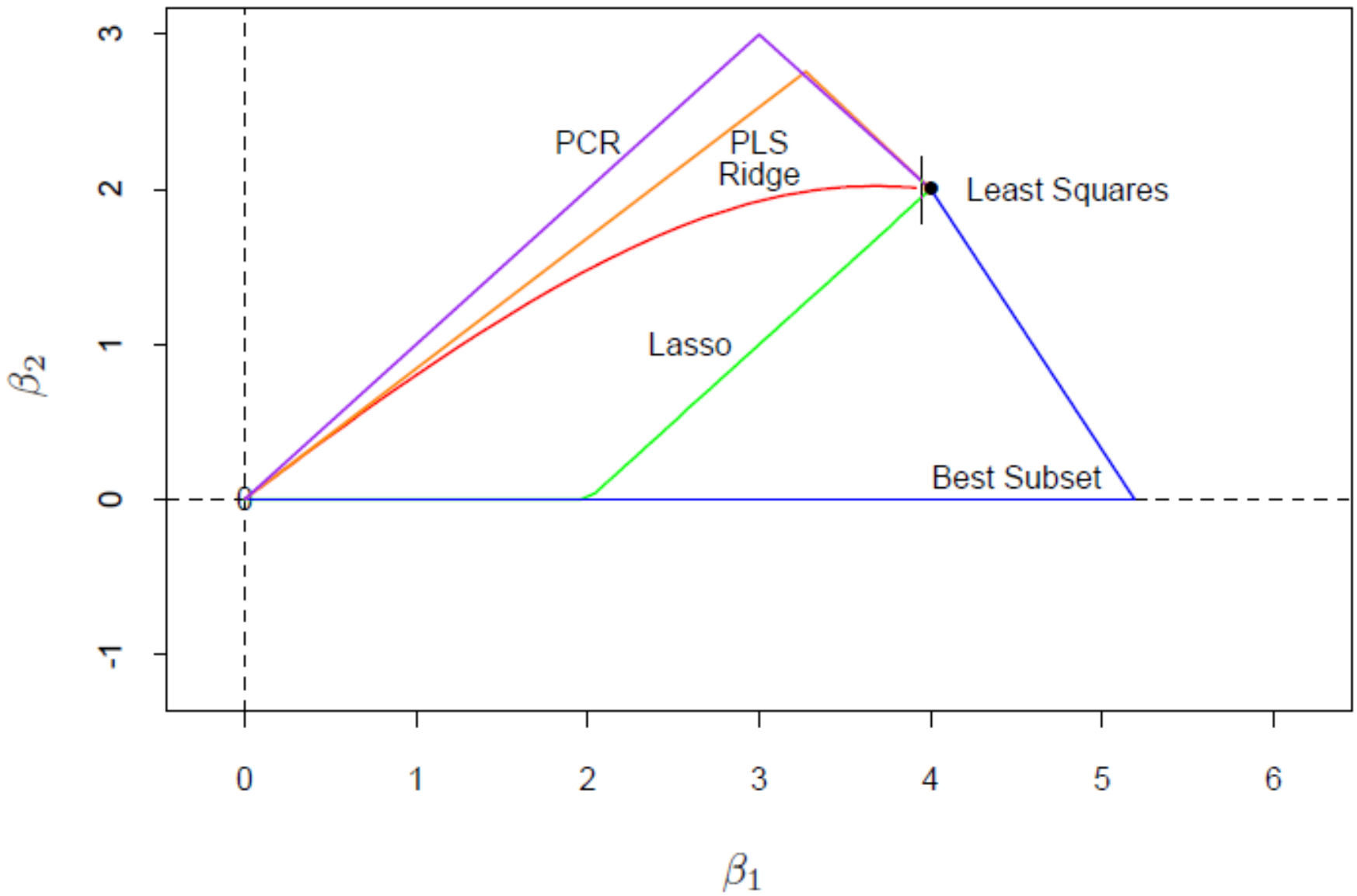
$$\hat{\varphi}_{1j} = \langle x_j, y \rangle$$

First PLS Direction (solid line) and First PCR Direction (dotted line)

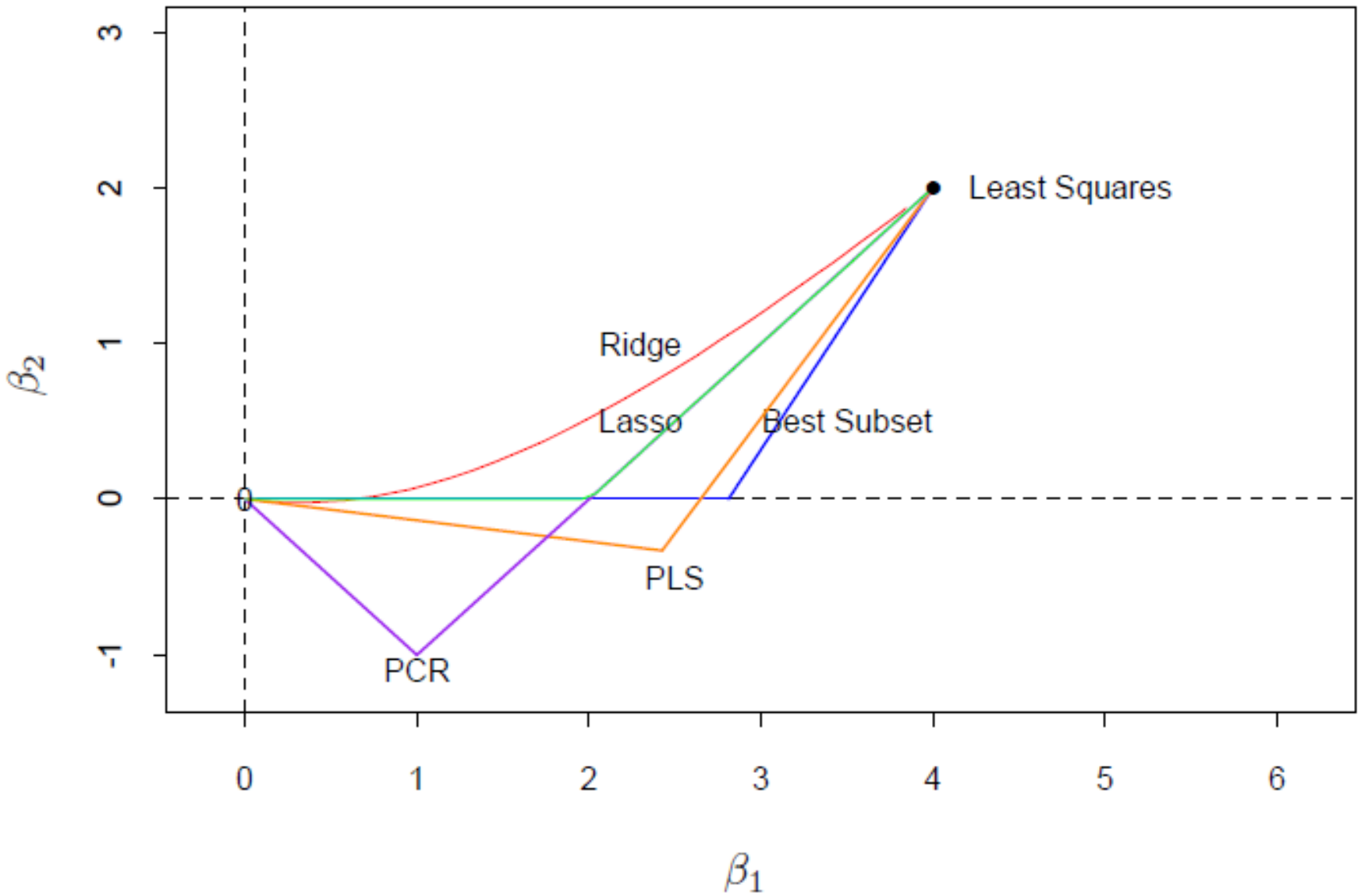
$Y = \text{Sales}$



$\rho = 0.5$


PCR
PLS
Ridge
Least Squares
Lasso
Best Subset
β_2
β_1
3
2
1
0
-1
0
1
2
3
4
5
6

$\rho = -0.5$


Least Squares
Ridge
Lasso
Best Subset
PLS
PCR
β_1
β_2
0
1
2
3
4
5
6
-1
0
1
2
3

Prostate Cancer Data

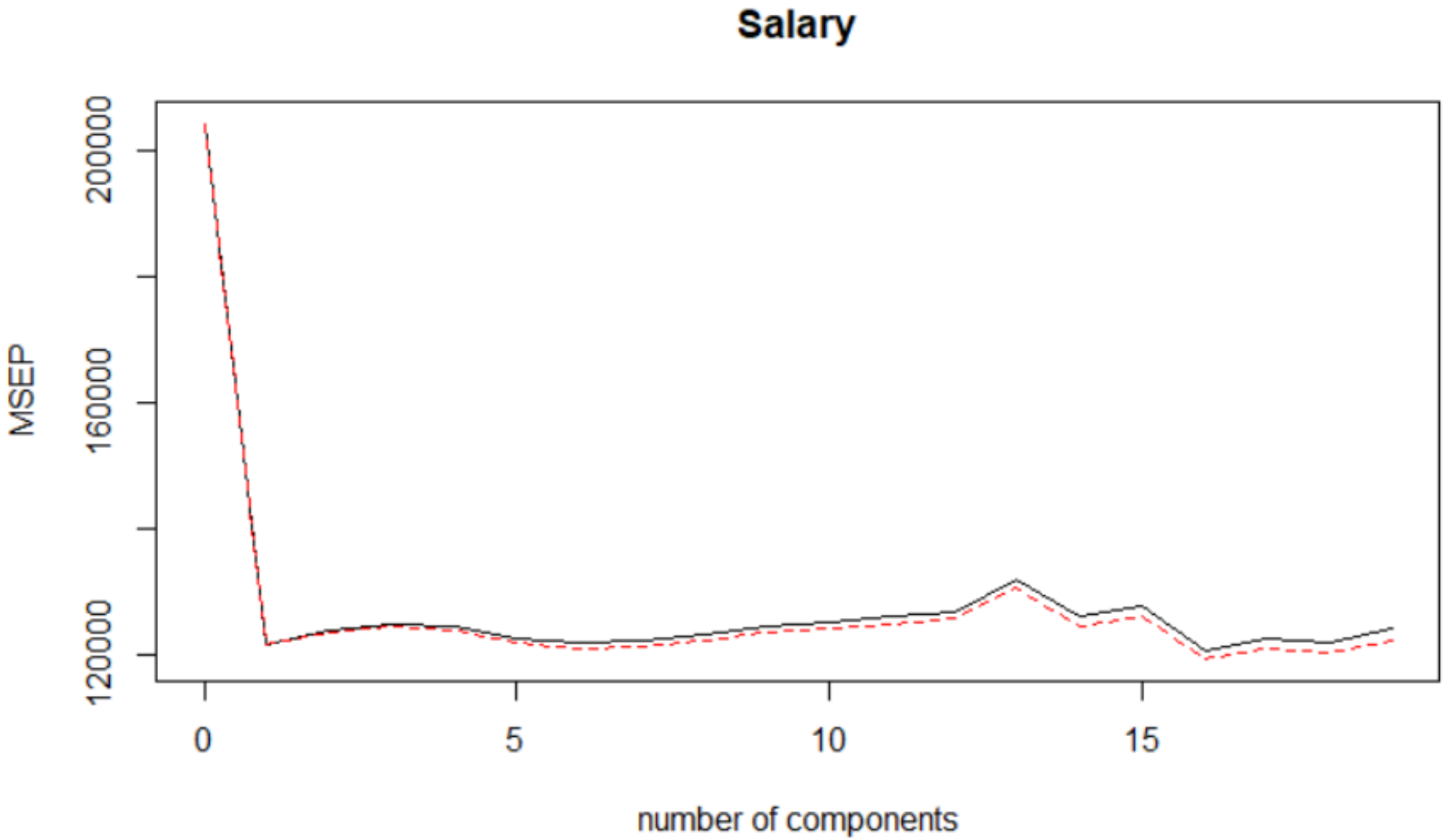
Term	LS	Best Subset	Ridge	Lasso	PCR	PLS
Intercept	2.465	2.477	2.452	2.468	2.497	2.452
lcavol	0.680	0.740	0.420	0.533	0.543	0.419
lweight	0.263	0.316	0.238	0.169	0.289	0.344
age	−0.141		−0.046		−0.152	−0.026
lbph	0.210		0.162	0.002	0.214	0.220
svi	0.305		0.227	0.094	0.315	0.243
lcp	−0.288		0.000		−0.051	0.079
gleason	−0.021		0.040		0.232	0.011
pgg45	0.267		0.133		−0.056	0.084
Test Error	0.521	0.492	0.492	0.479	0.449	0.528
Std Error	0.179	0.143	0.165	0.164	0.105	0.152

library (pls); set.seed (2)

pcr.fit=pcr(Salary~., data=Hitters, scale=TRUE,validation="CV"); summary(pcr.fit)

```
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
CV             452    348.9    352.2    353.5    352.8    350.1    349.1
adjCV          452    348.7    351.8    352.9    352.1    349.3    348.0
       7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
CV       349.6    350.9    352.9     353.8     355.0     356.2     363.5
adjCV    348.5    349.8    351.6     352.3     353.4     354.5     361.6
       14 comps  15 comps  16 comps  17 comps  18 comps  19 comps
CV        355.2     357.4     347.6     350.1     349.2     352.6
adjCV     352.8     355.2     345.5     347.6     346.7     349.8

TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X         38.31    60.16    70.84    79.03    84.29    88.63    92.26    94.96
Salary    40.63    41.58    42.17    43.22    44.90    46.48    46.69    46.75
        9 comps  10 comps  11 comps  12 comps  13 comps  14 comps  15 comps
X         96.28     97.26     97.98     98.65     99.15     99.47     99.75
Salary    46.86     47.76     47.82     47.85     48.10     50.40     50.55
```

validationplot(pcr.fit,val.type="MSEP")



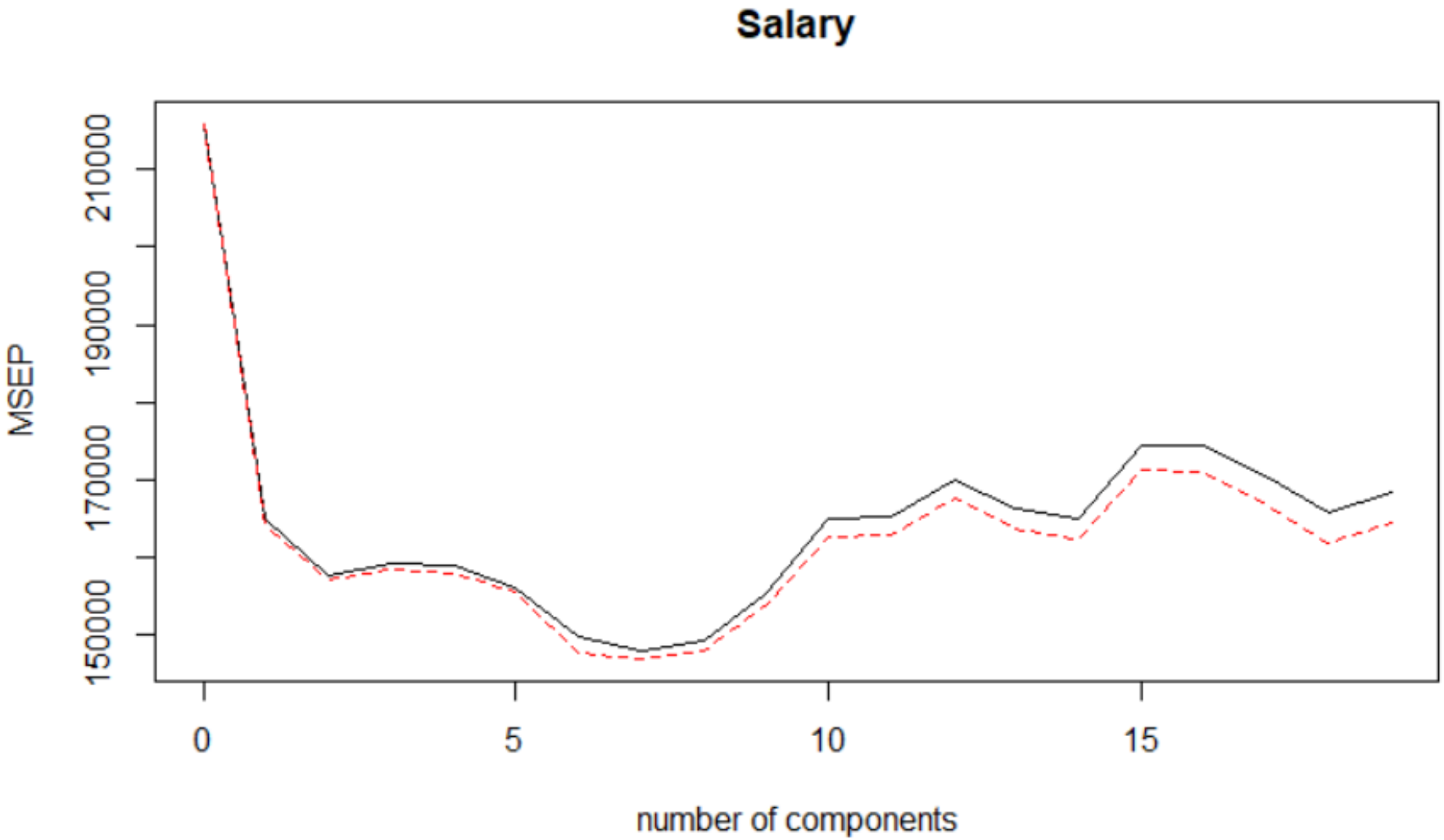
Training and Test Data Set

```
x=model.matrix(Salary~.,Hitters)[,-1]
y=Hitters$Salary; set.seed(1)
train=sample(1:nrow(x), nrow(x)/2)
test=(-train); y.test=y[test]

set.seed(1)
pcr.fit=pcr(Salary~., data=Hitters,
subset=train,scale=TRUE, validation="CV")
```

summary(pcr.fit)

```
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
CV           464.6    406.1    397.1    399.1    398.6    395.2    386.9
adjCV        464.6    405.2    396.3    398.1    397.4    394.5    384.5
       7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
CV       384.8    386.5    394.1     406.1     406.5     412.3     407.7
adjCV    383.3    384.8    392.0     403.4     403.7     409.3     404.6
       14 comps  15 comps  16 comps  17 comps  18 comps  19 comps
CV        406.2     417.8     417.6     413.0     407.0     410.2
adjCV     402.8     413.9     413.5     408.3     402.4     405.5

TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X         38.89    60.25    70.85    79.06    84.01    88.51    92.61    95.20
Salary    28.44    31.33    32.53    33.69    36.64    40.28    40.41    41.07
        9 comps  10 comps  11 comps  12 comps  13 comps  14 comps  15 comps
X         96.78     97.63     98.27     98.89     99.27     99.56     99.78
Salary    41.25     41.27     41.41     41.44     43.20     44.24     44.30
```

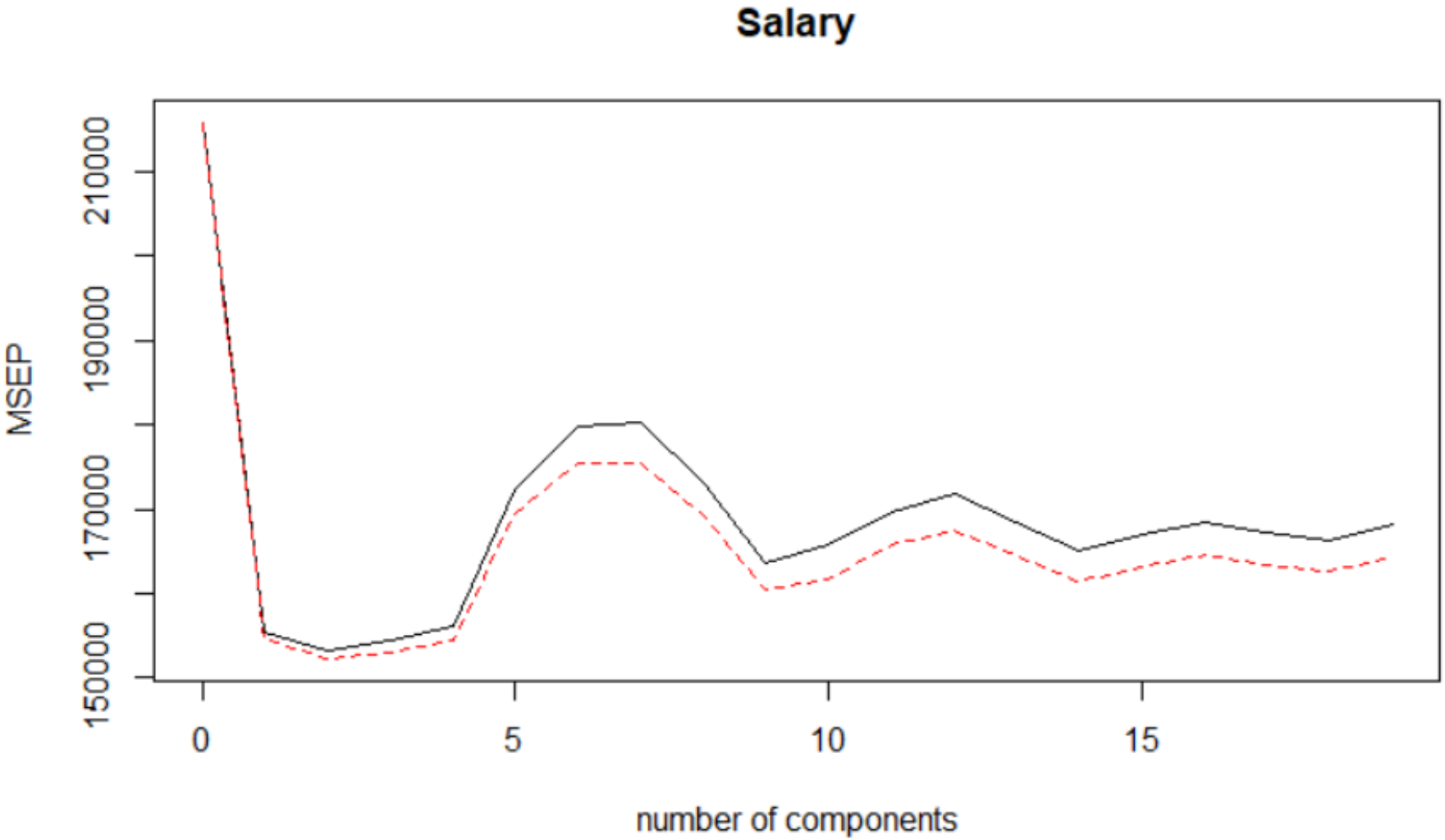
validationplot(pcr.fit,val.type="MSEP")



Partial Least Squares (PLS)

set.seed(1)

pls.fit=plsr(Salary~., data=Hitters, subset=train, scale=TRUE, validation="CV"); summary(pls.fit)

```
Cross-validated using 10 random segments.
       (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
CV           464.6    394.2    391.5    393.1    395.0    415.0    424.0
adjCV        464.6    393.4    390.2    391.1    392.9    411.5    418.8
       7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
CV       424.5    415.8    404.6     407.1     412.0     414.4     410.3
adjCV    418.9    411.4    400.7     402.2     407.2     409.3     405.6
       14 comps  15 comps  16 comps  17 comps  18 comps  19 comps
CV        406.2     408.6     410.5     408.8     407.8     410.2
adjCV     401.8     403.9     405.6     404.1     403.2     405.5

TRAINING: % variance explained
         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
X          38.12    53.46    66.05    74.49    79.33    84.56    87.09    90.74
Salary     33.58    38.96    41.57    42.43    44.04    45.59    47.05    47.53
         9 comps  10 comps  11 comps  12 comps  13 comps  14 comps  15 comps
X          92.55     93.94     97.23     97.88     98.35     98.85     99.11
Salary     48.42     49.68     50.04     50.54     50.78     50.92     51.04
```

validationplot(pls.fit,val.type="MSEP")