Saarland University

The Elements of Stastical Learning

Assignement 5

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Problem 1

Principal Components Analysis The first principal component is the direction of maximum variance in the data. Show that this first principal component also minimizes the residual sum of squares, which is here the squared distance between the projected data point and the original data point.

The RSS is given by:

$$RSS = \sum_{i=1}^{n}(y_i - f(x_i))^2$$

The least squares regression model is given by the equation 6.16 and 6.17 of ISRL:

$$Z_m = \sum_{j=1}^{p} \phi_{jm} X_j \qquad \text{(6.16, ISLR)}$$

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \varepsilon_i, \quad i = 1, ..., n \qquad \text{(6.17, ISLR)}$$

In the RSS equation, $f(x)$ correspond to the value projected on the first component line and is given by: $f(x) = \phi(x_i - \bar{x})$ (6.19, ISLR). So we have RSS:

$$RSS = \sum_{i=1}^{n}(\theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \varepsilon_i - \phi(x_i - \bar{x}))^2$$

The first component has the highest variance so $Var(f(x))$ is a maximum and so the RSS is minimized.

Problem 2

Show that regression splines of degree d with K knots form a vector space of dimension d + K + 1 by providing a balance of the degrees of freedom in every region of the input data range and the lost degrees of freedom due to the smoothness constraints at the knots. Do not use bases of the spline vector space for your argument.

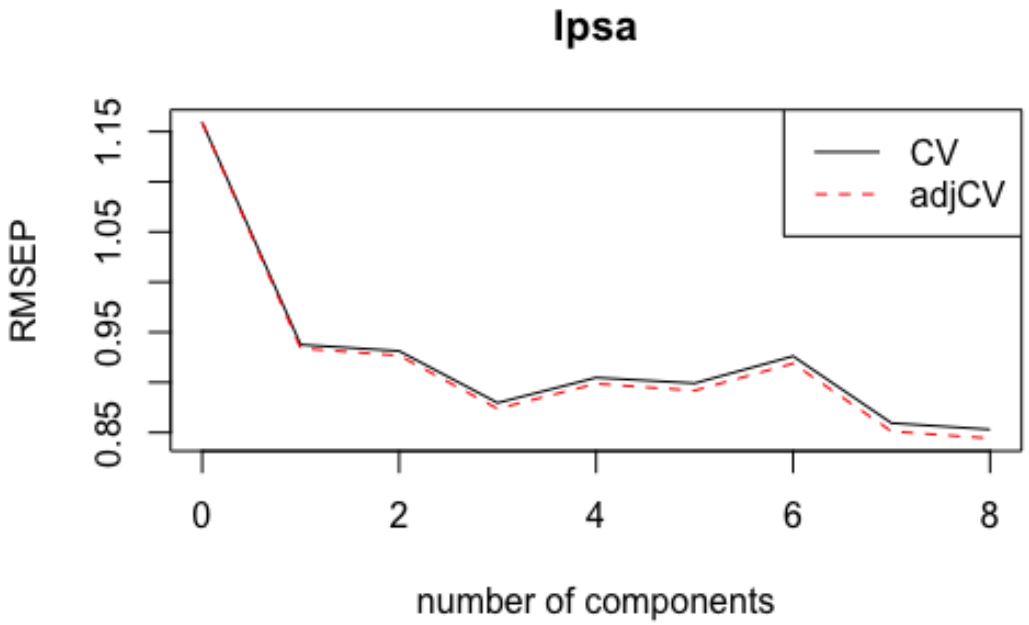
Problem 3

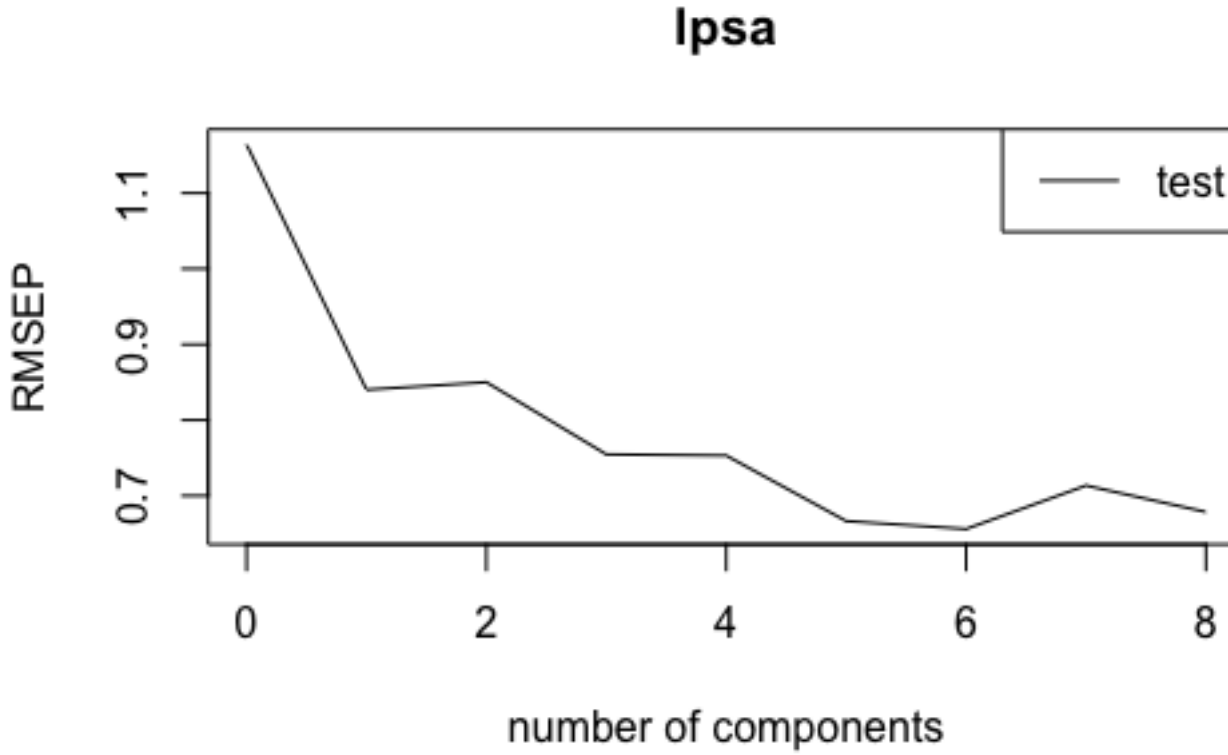
Consider the truncated power series representation for cubic splines with K interior knots. Let

$$f(x) = \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3$$

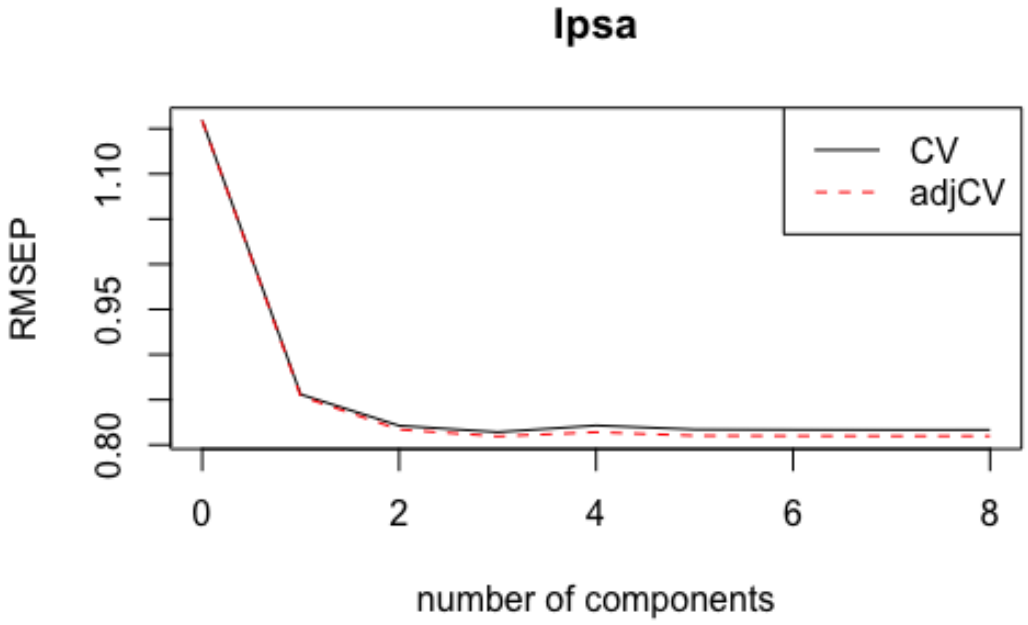
Problem 4

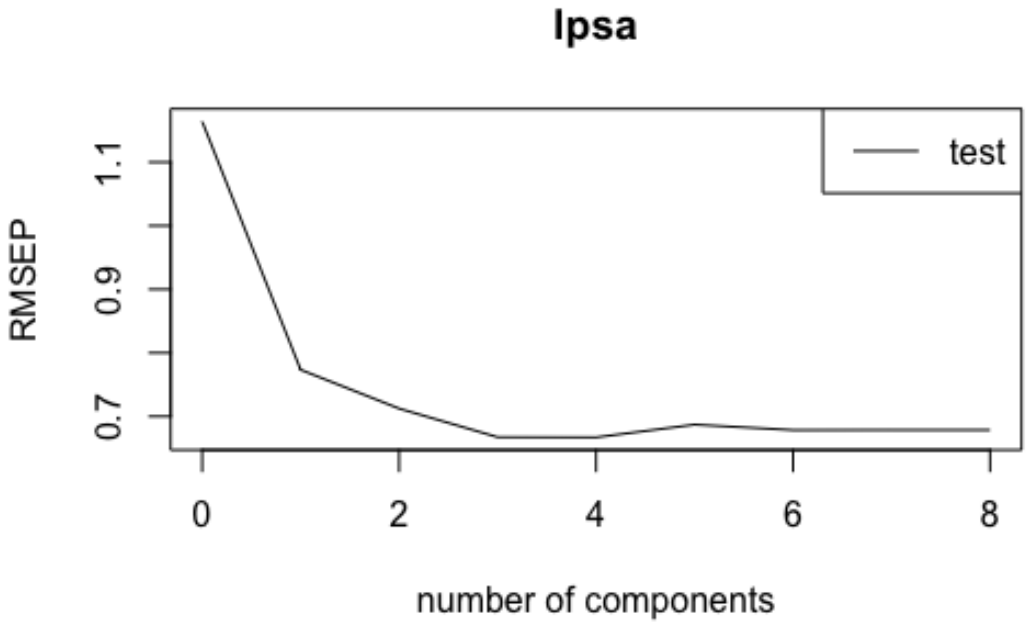
1. For the principal component regression models the plots of training error v.s. number of components and test error v.s. number of principal components are below, respectively. Based on the training data, 8 components would be best, while 7 or possibly 3 components could produce comparable results. The test data suggests that 5 or 6 components would be best, and 8 components could produce comparable results.





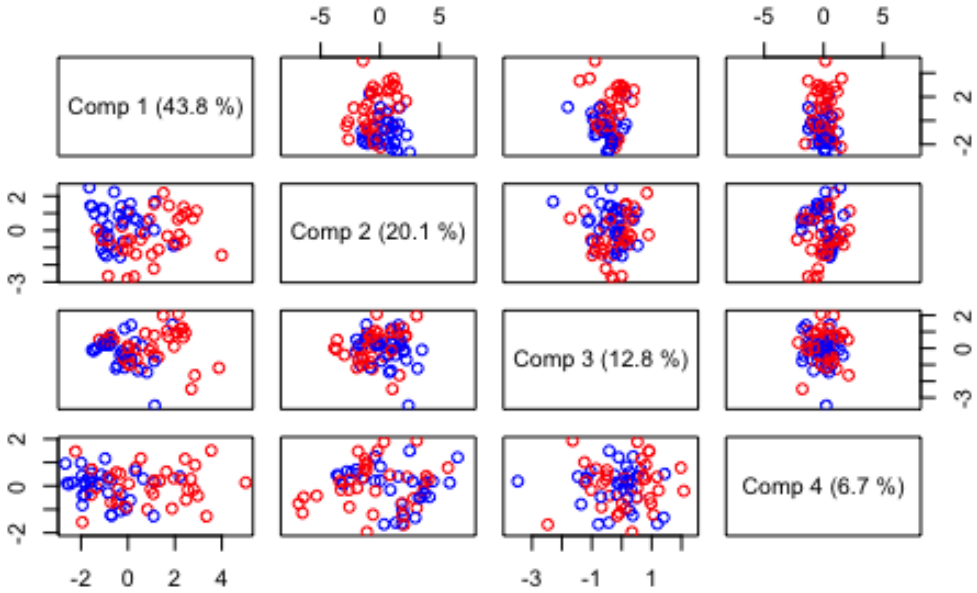
2. For the partial least squares model, the training error v.s. number of principal components and test error v.s number of principal components are shown below. Here, the training data suggests 3 principal components would be best, with 2 and 4-8 components being about as good. The test data also suggests that 3 components would be best.

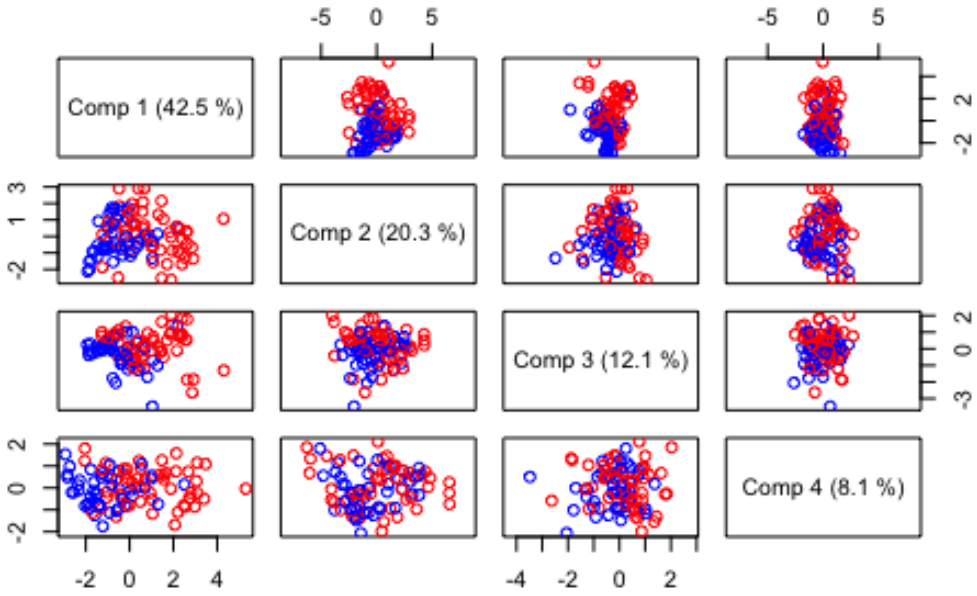




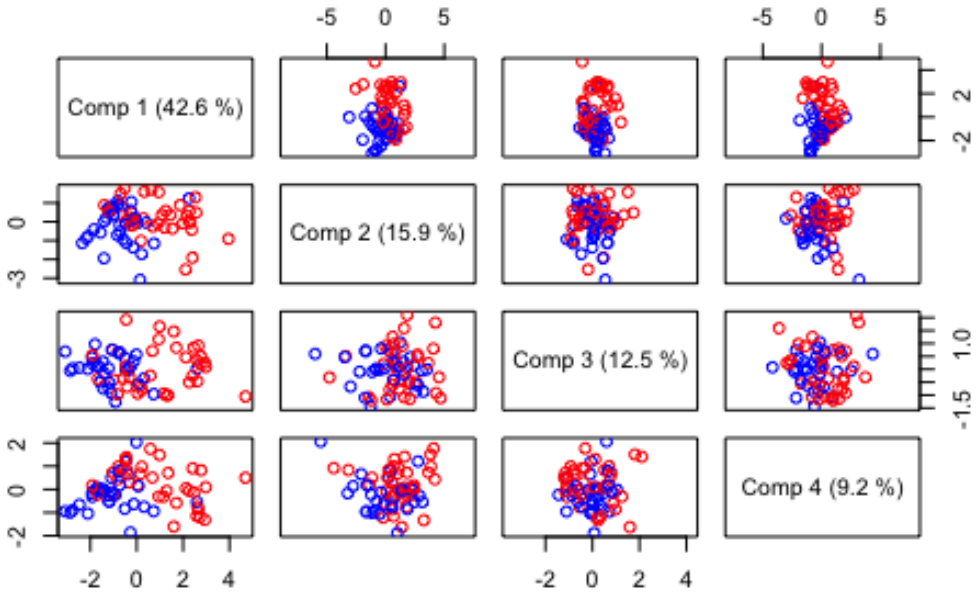
3. The visualizations of just the training set then the whole data set for the first for principal components are below. With the addition of the test data the first com-

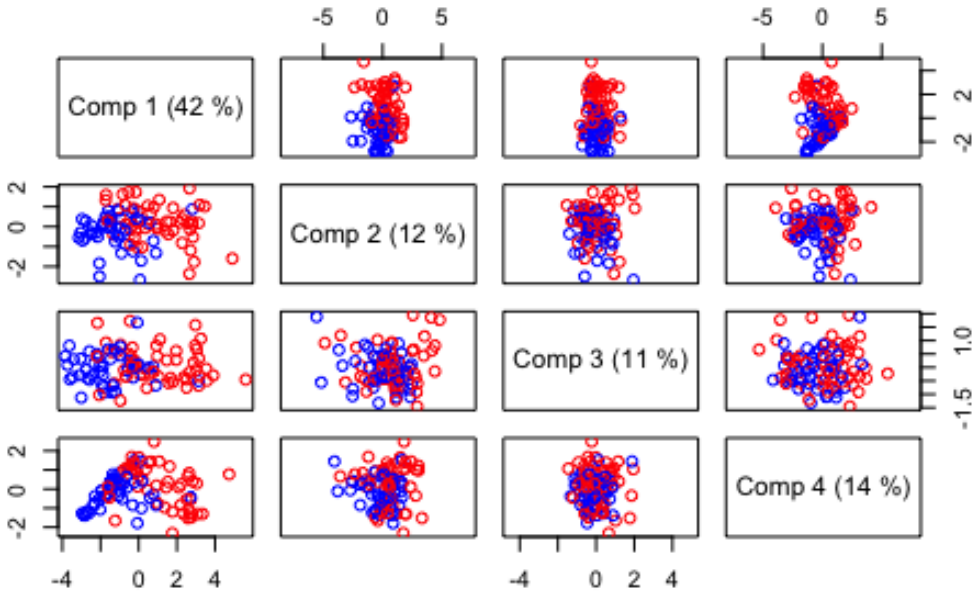
ponent clearly appears to capture the separability of the data much better than with just training data alone.





4. The visualizations of just the training set then the whole data set for the first four PLS directions are below. Here both graphs seem to be much more similar to one another, than for PCR. I both cases the first PLS direction seems to accurately capture separability in the data.





5. For PCR, the training and test data suggest very different M values, with little overlap. Here I would chose 8 components. For PLS, the training and test data suggest more similar values for M. This makes sense since PLS is a supervised alternative to PCR that takes into account the response.