## Partial least squares regression

A possible drawback of PCR is that we have no guarantee that the selected principal components are associated with the outcome. Here, the selection of the principal components to incorporate in the model is not supervised by the outcome variable.

An alternative to PCR is the **Partial Least Squares** (PLS) regression, which identifies new principal components that not only summarizes the original predictors, but also that are related to the outcome. These components are then used to fit the regression model. So, compared to PCR, PLS uses a dimension reduction strategy that is supervised by the outcome.
Like PCR, PLS is convenient for data with highly-correlated predictors. The number of PCs used in PLS is generally chosen by cross-validation. Predictors and the outcome variables should be generally standardized, to make the variables comparable.

## Loading required R packages

- `tidyverse` for easy data manipulation and visualization
- `caret` for easy machine learning workflow
- `pls`, for computing PCR and PLS

```
library(tidyverse)
library(caret)
library(pls)
```

## Preparing the data

We'll use the `Boston` data set [in `MASS` package], introduced in Chapter @ref(regression-analysis), for predicting the median house value (`mdev`), in Boston Suburbs, based on multiple predictor variables.
We'll randomly split the data into training set (80% for building a predictive model) and test set (20% for evaluating the model). Make sure to set seed for reproducibility.

```
# Load the data
data("Boston", package = "MASS")
# Split the data into training and test set
set.seed(123)
training.samples <- Boston$medv %>%
  createDataPartition(p = 0.8, list = FALSE)
train.data  <- Boston[training.samples, ]
test.data <- Boston[-training.samples, ]
```

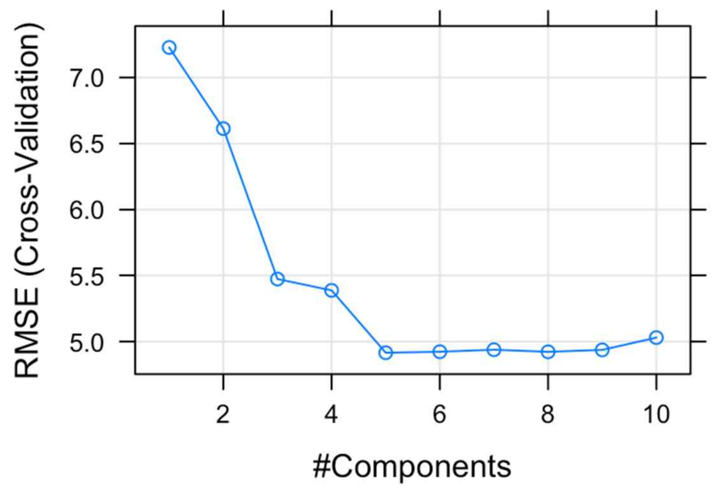
## Computation

The R function `train()` [`caret` package] provides an easy workflow to compute PCR and PLS by invoking the `pls` package. It has an option named `method`, which can take the value `pcr` or `pls`.
An additional argument is `scale = TRUE` for standardizing the variables to make them comparable.
`caret` uses cross-validation to automatically identify the optimal number of principal components (`ncomp`) to be incorporated in the model.

Here, we'll test 10 different values of the tuning parameter ncomp. This is specified using the option tuneLength. The optimal number of principal components is selected so that the cross-validation error (RMSE) is minimized.

## Computing principal component regression

```
# Build the model on training set
set.seed(123)
model <- train(
  medv~., data = train.data, method = "pcr",
  scale = TRUE,
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
  )
# Plot model RMSE vs different values of components
plot(model)
# Print the best tuning parameter ncomp that
# minimize the cross-validation error, RMSE
model$bestTune
##   ncomp
## 5     5
# Summarize the final model
summary(model$finalModel)
## Data:    X dimension: 407 13
##  Y dimension: 407 1
## Fit method: svdpc
## Number of components considered: 5
## TRAINING: % variance explained
##           1 comps  2 comps  3 comps  4 comps  5 comps
## X           47.48    58.40    68.00    74.75    80.94
## .outcome    38.10    51.02    64.43    65.24    71.17
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance metrics
data.frame(
  RMSE = caret::RMSE(predictions, test.data$medv),
  Rsquare = caret::R2(predictions, test.data$medv)
)
##   RMSE Rsquare
## 1 5.18   0.645
```



The plot shows the prediction error (RMSE, Chapter @ref(regression-model-accuracy-metrics)) made by the model according to the number of principal components incorporated in the model.

Our analysis shows that, choosing five principal components (ncomp = 5) gives the smallest prediction error RMSE.

The `summary()` function also provides the percentage of variance explained in the predictors (x) and in the outcome (`medv`) using different numbers of components.
For example, 80.94% of the variation (or information) contained in the predictors are captured by 5 principal components (`ncomp = 5`). Additionally, setting ncomp = 5, captures 71% of the information in the outcome variable (`medv`), which is good.
Taken together, cross-validation identifies ncomp = 5 as the optimal number of PCs that minimize the prediction error (RMSE) and explains enough variation in the predictors and in the outcome.

## Computing partial least squares

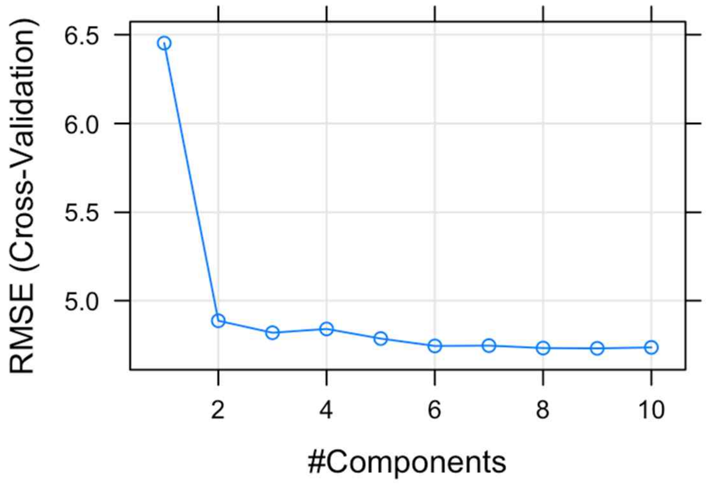
The R code is just like that of the PCR method.

```
# Build the model on training set
set.seed(123)
model <- train(
  medv~., data = train.data, method = "pls",
  scale = TRUE,
  trControl = trainControl("cv", number = 10),
  tuneLength = 10
  )
# Plot model RMSE vs different values of components
plot(model)
# Print the best tuning parameter ncomp that
# minimize the cross-validation error, RMSE
model$bestTune
```

```
##   ncomp
## 9     9
```

```
# Summarize the final model
```

```
summary(model$finalModel)
## Data:    X dimension: 407 13
##  Y dimension: 407 1
## Fit method: oscorespls
## Number of components considered: 9
## TRAINING: % variance explained
##           1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X           46.19    57.32    64.15    69.76    75.63    78.66    82.85
## .outcome    50.90    71.84    73.71    74.71    75.18    75.35    75.42
##           8 comps  9 comps
## X           85.92    90.36
## .outcome    75.48    75.49
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance metrics
data.frame(
  RMSE = caret::RMSE(predictions, test.data$medv),
  Rsquare = caret::R2(predictions, test.data$medv)
)
##   RMSE Rsquare
## 1 4.99   0.671
```



The optimal number of principal components included in the PLS model is 9. This captures 90% of the variation in the predictors and 75% of the variation in the outcome variable (medv).
In our example, the cross-validation error RMSE obtained with the PLS model is lower than the RMSE obtained using the PCR method. So, the PLS model is the best model, for explaining our data, compared to the PCR model.

## Discussion

This chapter describes principal component based regression methods, including principal component regression (PCR) and partial least squares regression (PLS). These methods are very useful for multivariate data containing correlated predictors.

The presence of correlation in the data allows to summarize the data into few non-redundant components that can be used in the regression model.

Compared to ridge regression and lasso (Chapter @ref(penalized-regression)), the final PCR and PLS models are more difficult to interpret, because they do not perform any kind of variable selection or even directly produce regression coefficient estimates.