Principal Component Regression

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Math 243: Stat Learning

December 3rd, 2021

Outline

In today's class, we will...

- Discuss Principal Component Analysis as a means of dimensionality reduction for regression
- Implement PCR in R

Section 1

Principal Component Regression

Dimensionality Reduction

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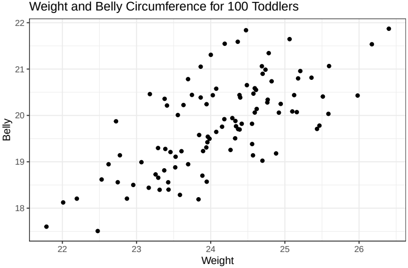
One solution is to perform variable selection and drop some less useful predictors.

- But dropping variables completely loses possible valuable information.
- Instead, we can combine variables into new ones that adequately describe the variance in the data, and drop those that have limited utility in explaining that variance.

PCA Overview

Consider the weight and belly circumference for a random sample of 100 toddlers.



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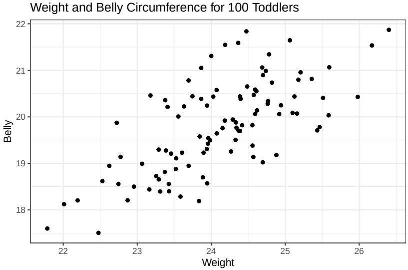

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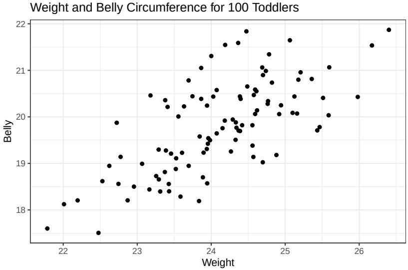

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```
##   sd_Weight  sd_Belly
## 1 0.8981994 0.9843542
```

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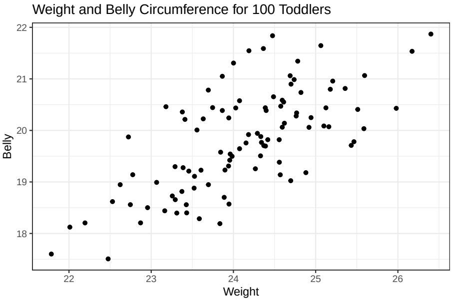

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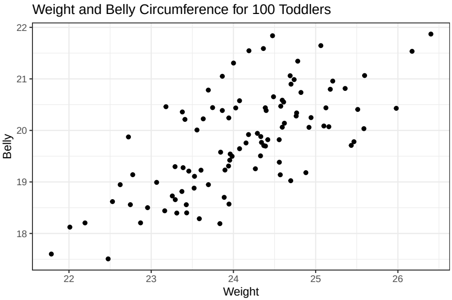

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```
##         R_sq
## 1 0.4673515
```

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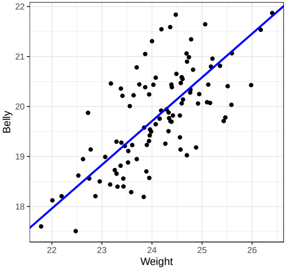
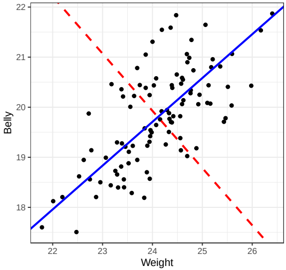


PCA Overview

How much variation occurs perpendicular to this line?



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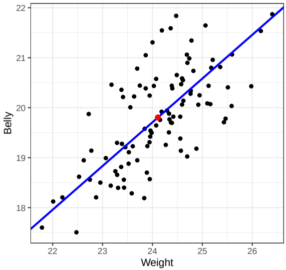
- Alternatively, we could express Z_1 as an affine linear combination of the predictors themselves (affine meaning including a constant term)

PCA Example

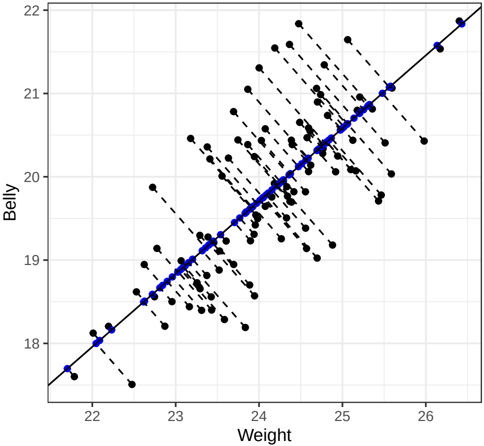
The first principal component



$$Z_1 = 0.66 \cdot (\text{Weight} - 24.1) + 0.75 \cdot (\text{Belly} - 19.8)$$

PCA Example

What is leftover?



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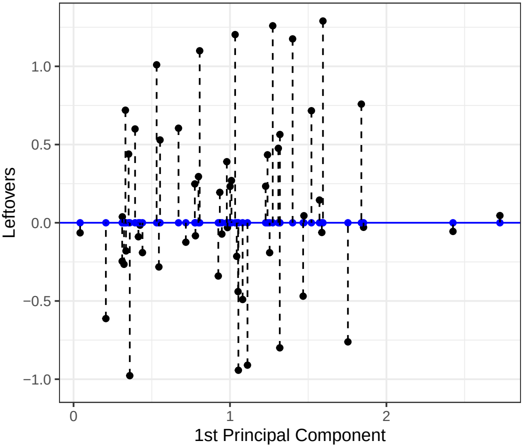

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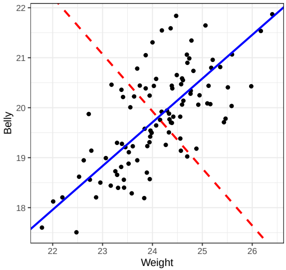
Generally, the kth principal component is obtained by finding a linear combination of centered variables that is uncorrelated with all previous principal components, and has the largest variance subject to this constraint.

PCA Example

The second principal component



$$Z_2 = 0.75 \cdot (\text{Weight} - 24.1) - 658(\text{Belly} - 19.8)$$

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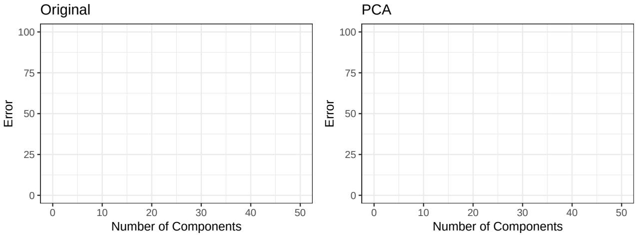
In general, PCR tends to produce linear models with higher accuracy than models fit with the original predictors.



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We can use the `pcr` function in the `pls` library to quickly perform PCR in R.

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The `Hitters` data set from the `ISLR` package contains `Salary` and 18 other predictors for 263 baseball players

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set.seed(1)
library(pls)
my_pcr <- pcr( Salary ~ ., data = Hitters_train, scale = T, validation = "CV")
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- Setting `scale = T` standardizes each predictor
- Setting `validation = "CV"` causes pcr to compute the 10-fold CV error for each value of M (number of principal components used)

PCR Results

```
summary(my_pcr)
```

```
## Data:    X dimension: 197 19
##  Y dimension: 197 1
## Fit method: svdpc
## Number of components considered: 19
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV           456.9    372.0    372.2    373.3    370.8    362.7    361.8
## adjCV        456.9    371.5    371.5    372.5    370.0    361.8    360.5
##        7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
## CV       362.7    369.8    372.9     376.5     380.0     385.6     397.3
## adjCV    361.5    368.2    371.1     374.3     377.7     383.0     394.0
##        14 comps  15 comps  16 comps  17 comps  18 comps  19 comps
## CV        377.6     378.8     371.7     373.3     366.2     370.3
## adjCV     373.7     375.6     368.5     369.8     362.6     366.4
##
## TRAINING: % variance explained
##         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
## X         37.56    60.41    71.20    78.91    84.05    88.33    92.15    94.81
## Salary    36.31    37.53    37.83    39.43    42.56    43.89    44.30    44.39
##         9 comps  10 comps  11 comps  12 comps  13 comps  14 comps  15 comps
## X         96.13     97.12     97.90     98.61     99.12     99.45     99.74
## Salary    44.62     45.59     45.82     45.87     46.18     50.77     50.88
##         16 comps  17 comps  18 comps  19 comps
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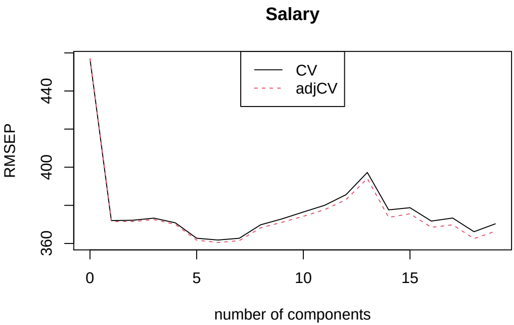
- Note: `pcr` reports RSE, so values need to be squared to get MSE.

Validation Plot

```
validationplot(my_pcr, val.type = "RMSEP", legendpos = "top")
```



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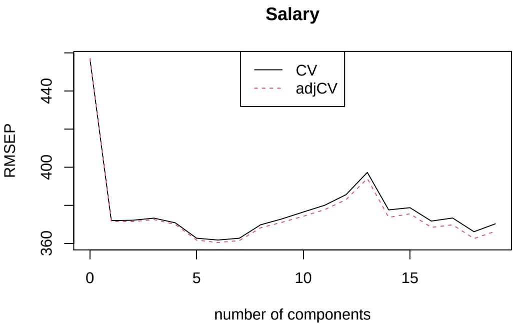

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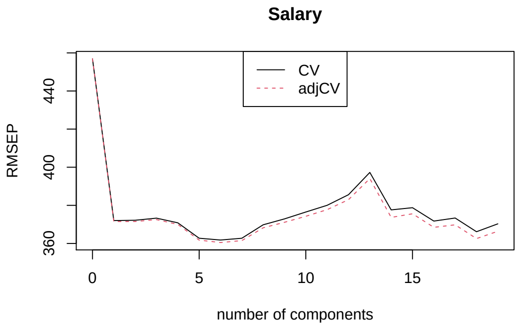

- Note: The smallest CV error occurs at $M = 17$ (which is close to the maximum number of predictors $p = 19$.)
- However, a relatively low CV error is also obtained at $M = 5$, suggesting fewer components are sufficient

Make Predictions

Finally, to actually implement the PCR model on training data, we use the `predict` function

```
pcr_preds5 <- predict(my_pcr, Hitters_test, ncomp = 5)
pcr_preds17 <- predict(my_pcr, Hitters_test, ncomp = 17)
pcr_preds19 <- predict(my_pcr, Hitters_test, ncomp = 19)

results <- data.frame(obs = Hitters_test$Salary, pcr_preds5, pcr_preds17,pcr_preds19) %>%
  pivot_longer(!obs, names_to = "model", values_to = "preds")

library(yardstick)
results %>% group_by(model) %>% rmse(truth = obs, estimate = preds ) %>% arrange(.estimate)
```

```
## # A tibble: 3 x 4
##   model           .metric .estimator .estimate
##   <chr>           <chr>   <chr>          <dbl>
## 1 Salary.5.comps  rmse    standard        299.
## 2 Salary.17.comps rmse    standard        312.
## 3 Salary.19.comps rmse    standard        329.
```