

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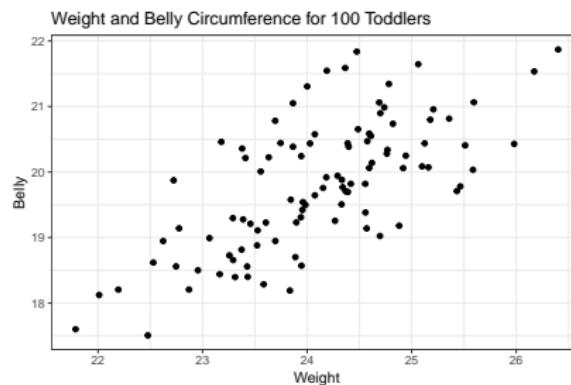
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One solution is to perform variable selection and drop some less useful predictors.

- 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.

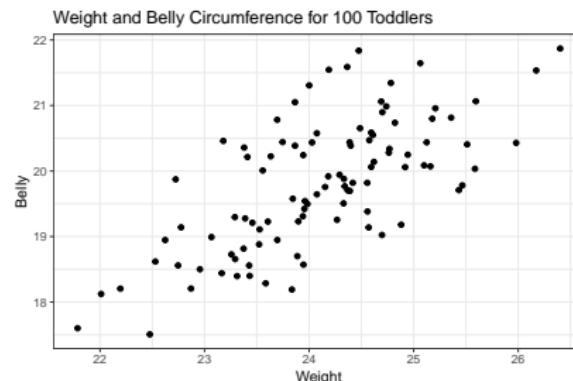
PCA Overview

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



PCA Overview

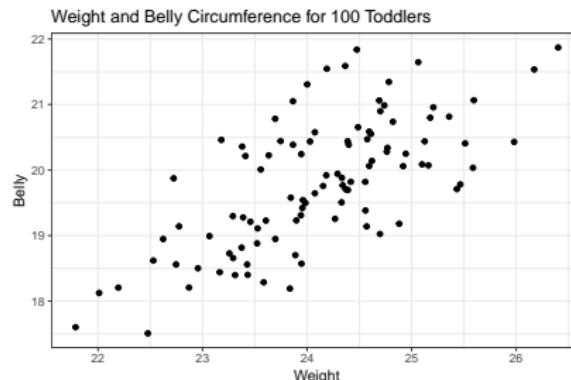
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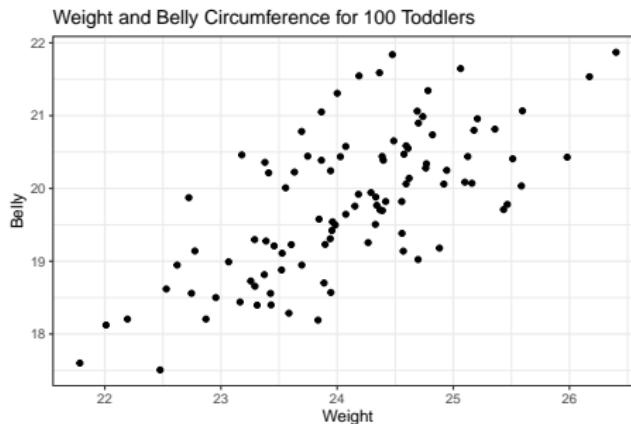


What are the approximate standard deviations of Weight and Belly?

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

PCA Overview

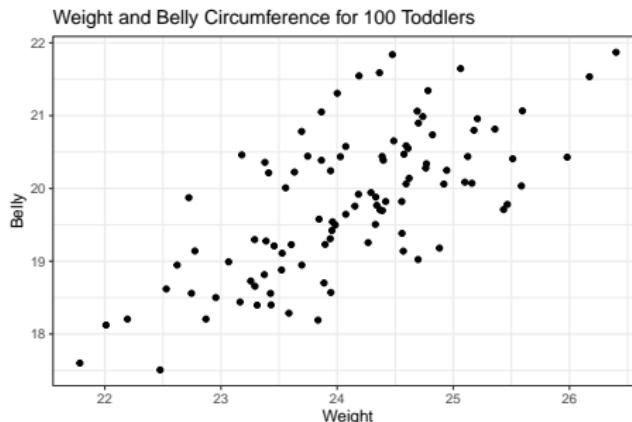
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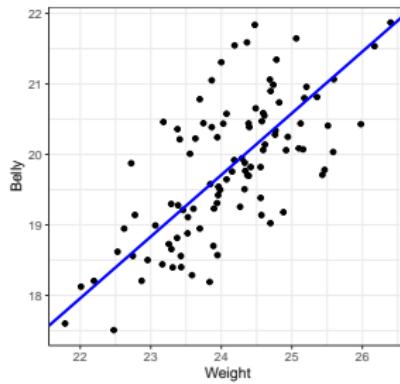
```
##          R_sq
## 1 0.4673515
```

PCA Overview

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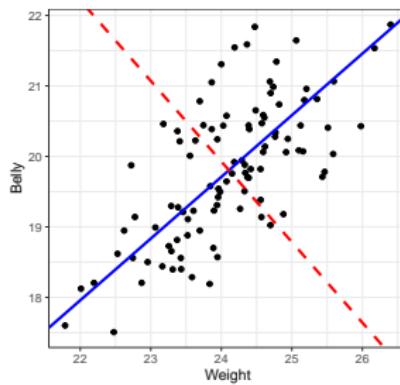
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PCA Overview

How much variation occurs perpendicular to this line?



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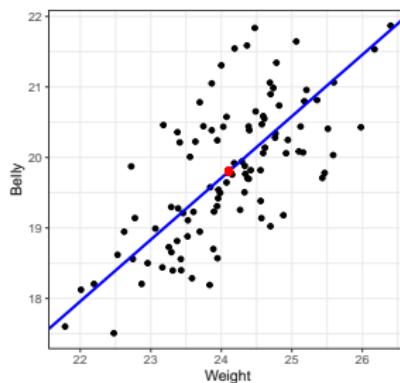
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- Alternatively, we could express Z_1 as an affine linear combination of the predictors themselves (affine meaning including a constant term)

PCA Example

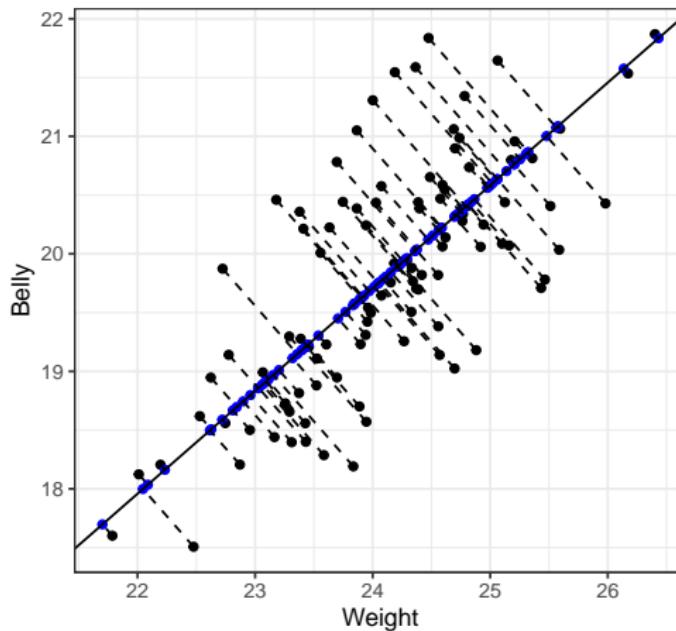
The first principal component



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

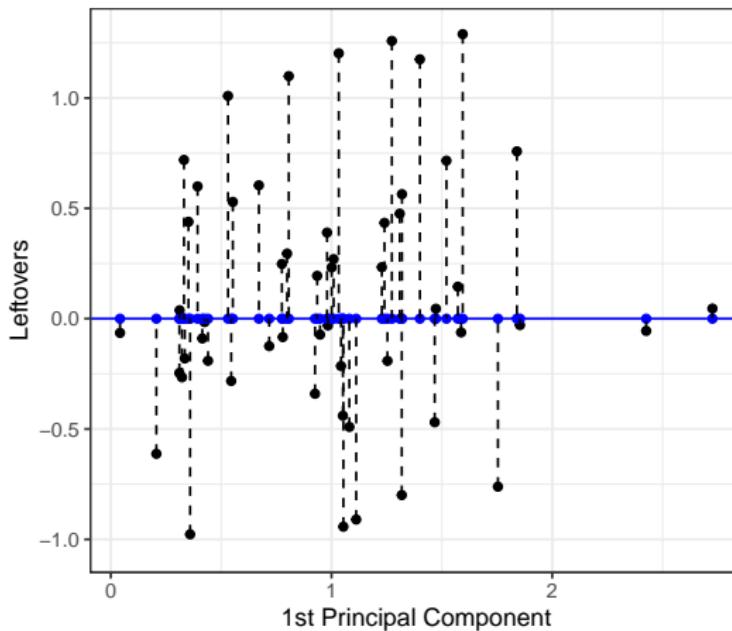
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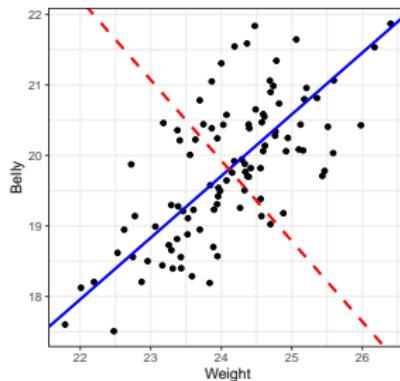
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For the case when $p = 2$, the 2nd principal component corresponds to the line perpendicular to the line for the 1st principal component.

Generally, the k th 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



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

Principal Comoponent Regression

The PCR approach to linear regression constructs the first M principal components Z_1, \dots, Z_M of a data set with p predictors (so $M \leq p$), and then uses these as predictors in a linear regression model.

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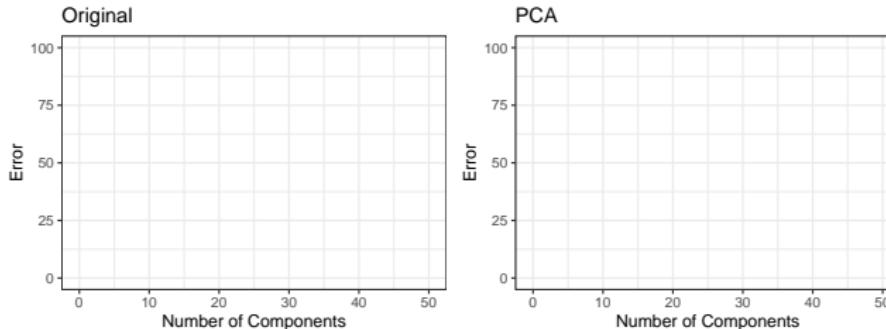
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- Goal: Use a small number of predictors which explain most of the variability in the data set, as well as their relationship to the response.

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



Principal Component Regression in R

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
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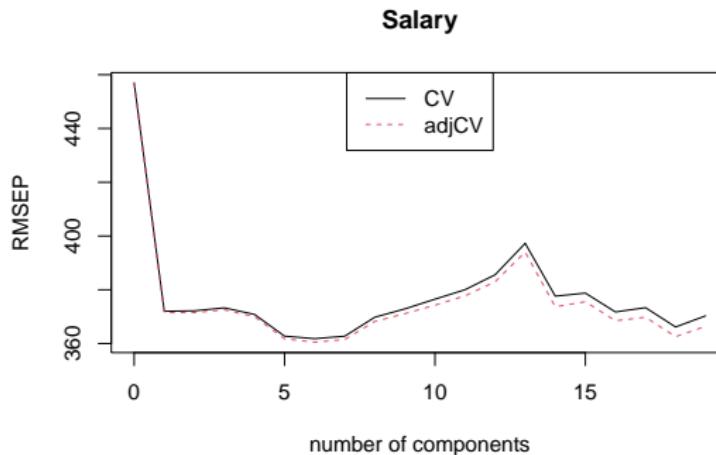
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- Note: pcr reports RSE, so values need to be squared to get MSE.

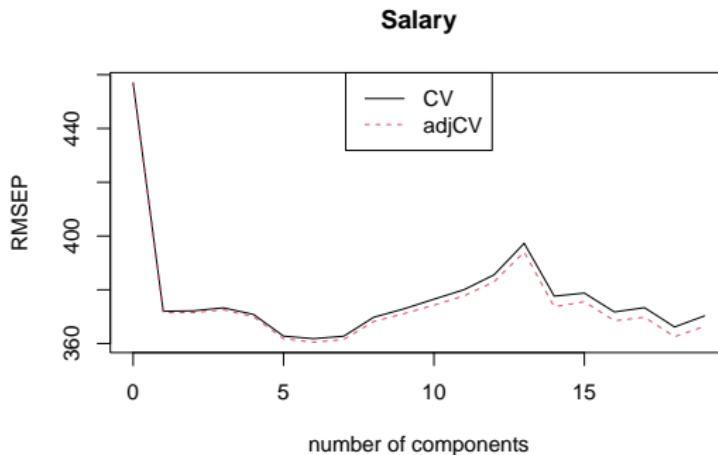
Validation Plot

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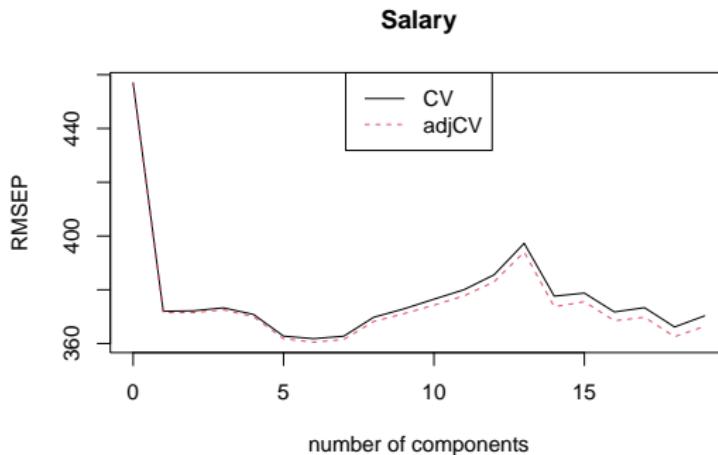
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- Note: The smallest CV error occurs at $M = 17$ (which is close to the maximum number of predictors $p = 19$.)
- However, a relatively low CV error is also obtained at $M = 5$, suggesting fewer components are sufficient

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.
```