

Principal component analysis: theory and concepts

Introduction to Statistical Modelling

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Goal of dimensionality reduction

- Pre-processing
 - Remove collinear predictors (multicollinearity)
- Computational efficiency
 - Retain important features to speed up computational processing
- Visualization

Learning outcomes

At the end of this lecture, you should be able to:

- 1 Explain the ideas behind PCA
- 2 Do a PCA by hand given a covariance matrix
- 3 Do a PCA with R
- 4 Interpret and explain the PCA results
- 5 Build and explain a PCR model

References

- *Introduction to statistical modeling*. Chapter available on Ufora.
- *An Introduction to Statistical Learning*. Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. Available for free online at <https://www.statlearning.com/>.
 - PCA: section 6.3

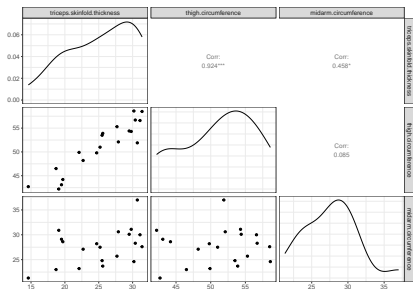
Reminder: multicollinearity

Bodyfat dataset: 20 observations, predict amount of body fat from three body measurements.

- Linear regression model:

$$\begin{aligned}\text{bodyfat} = & 117.085 \\ & + 4.334 \cdot \text{triceps} \\ & - 2.857 \cdot \text{thigh} \\ & - 2.186 \cdot \text{midarm}\end{aligned}$$

- Do you see anything wrong with this?**



Call:

```
lm(formula = bodyfat ~ ., data = bodyfat)
```

Residuals:

Min	1Q	Median	3Q	Max
-3.7263	-1.6111	0.3923	1.4656	4.1277

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	117.085	99.782	1.173	0.258
triceps.skinfold.thickness	4.334	3.016	1.437	0.170
thigh.circumference	-2.857	2.582	-1.106	0.285
midarm.circumference	-2.186	1.595	-1.370	0.190

Residual standard error: 2.48 on 16 degrees of freedom

Multiple R-squared: 0.8014, Adjusted R-squared: 0.7641

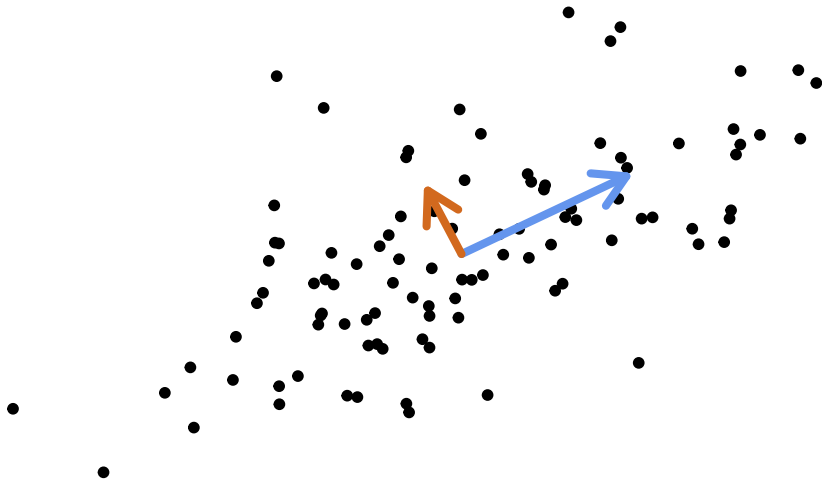
F-statistic: 21.52 on 3 and 16 DF, p-value: 7.343e-06

Principal component analysis

Directions of maximal variability

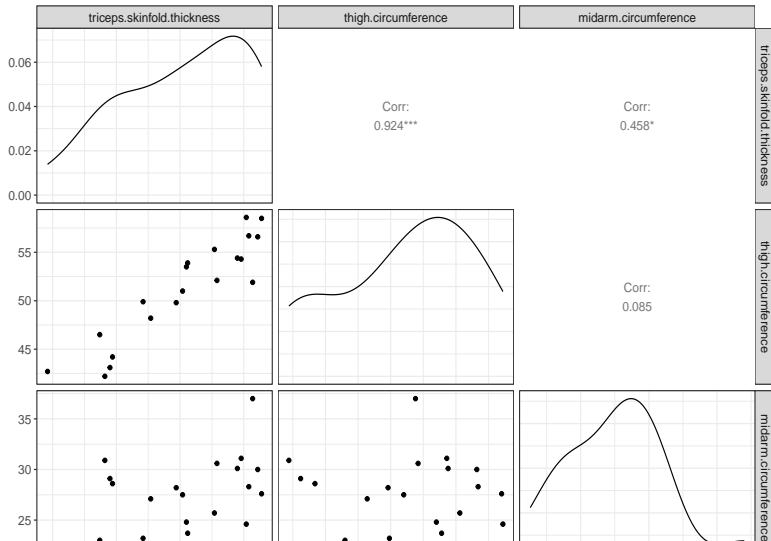
Intuitively:

- Find directions of maximal variability in the dataset
- Discard directions in which there is negligible variability



Directions of less variability

Since triceps and thigh are highly correlated, specifying both is superfluous. What do we lose if we throw away one of these variables?



Notation

Dataset:

- N observations \mathbf{x}_k , $k = 1, \dots, N$
- Each observation is a (column) vector in \mathbb{R}^D

Data matrix:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix} \in \mathbb{R}^{N \times D}$$

Columns of the data matrix:

- Referred to as features, predictors, independent variables
- Denoted by \mathbf{X}_i , $i = 1, \dots, D$

Notation: example (body fat dataset)

- 20 observations with 3 features each
- Data matrix is 20×3 matrix
- Features:
 - X_1 : `triceps.skinfold.thickness`
 - X_2 : `thigh.circumference`
 - X_3 : `midarm.circumference`

The covariance matrix

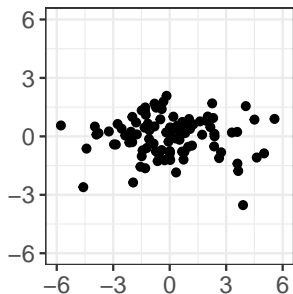
Given observations $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$, the variance-covariance matrix \mathbf{S} is defined as:

$$\mathbf{S} = \frac{1}{N} \sum_{k=1}^N (\mathbf{x}_k \mathbf{x}_k^T - \bar{\mathbf{x}} \bar{\mathbf{x}}^T).$$

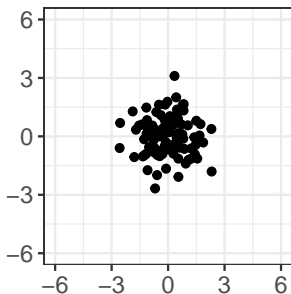
Structure: variances and covariances between components of the data.

$$\mathbf{S} = \begin{bmatrix} \text{Var}(x_1) & \text{Cov}(x_1, x_2) & \cdots & \text{Cov}(x_1, x_D) \\ \text{Cov}(x_2, x_1) & \text{Var}(x_2) & \cdots & \text{Cov}(x_2, x_D) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(x_D, x_1) & \text{Cov}(x_D, x_2) & \cdots & \text{Var}(x_D) \end{bmatrix}$$

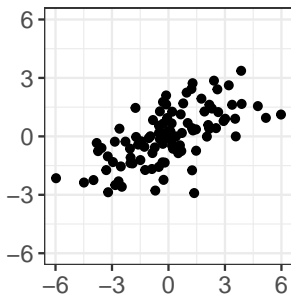
The covariance matrix: examples



$$\mathbf{S} = \begin{bmatrix} 6 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mathbf{S} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mathbf{S} = \begin{bmatrix} 5 & 2 \\ 2 & 2 \end{bmatrix}$$

Clearly the covariance matrix will help us find directions of maximum variability, but how?

Linear combination of features

- The **first principal component** \mathbf{Z}_1 is a linear combination of the columns of \mathbf{X} :

$$\mathbf{Z}_1 = v_1 \mathbf{X}_1 + \cdots + v_D \mathbf{X}_D,$$

where we will choose the coefficients v_i so that the variances is maximal, in some sense.

- The coefficients v_i are referred to as the **loadings** and the vector

$$\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_D \end{bmatrix}$$

is the **loadings vector**.

- Variance of \mathbf{Z}_1 :

$$\text{Var}(\mathbf{Z}_1) = \mathbf{v}^T \mathbf{S} \mathbf{v}.$$

Maximizing the variance

- Idea: choose loadings \mathbf{v} so that $\text{Var}(\mathbf{Z}_1)$ is **maximal**.
- Problem: just by increasing the norm of \mathbf{v} , variance can become as large as we want. Solution: impose that $\|\mathbf{v}\| = 1$.

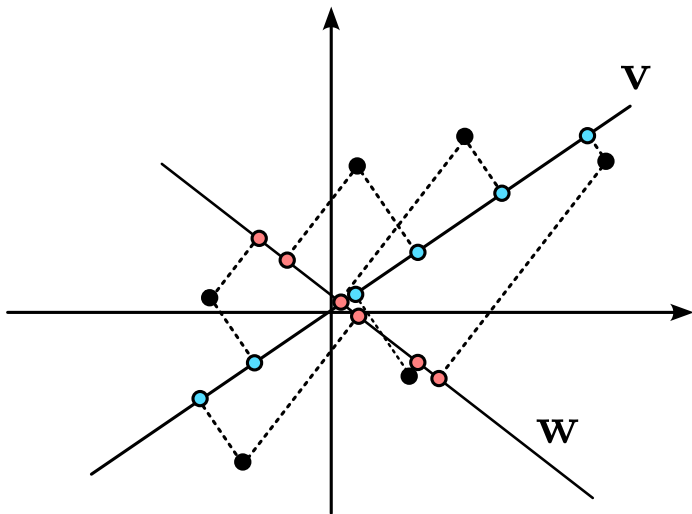
💡 PC1: maximization of variance

The loadings vector \mathbf{v} for the first principal component is found by solving the following maximization problem:

$$\text{maximize } \mathbf{v}^T \mathbf{S} \mathbf{v} \text{ so that } \mathbf{v}^T \mathbf{v} = 1.$$

Geometric interpretation

- Z_1 : projection of data on the line in the direction of \mathbf{v} .
- Find direction \mathbf{v} so that variance is maximal (blue)



Eigenvalue problem

Through Lagrange multipliers, can show that maximizing variance is equivalent to finding eigenvalues and eigenvectors of \mathbf{S} .

💡 PC1: eigenvalues

The loadings vector \mathbf{v} for the first principal component is the eigenvector of \mathbf{S} with the largest eigenvalue:

$$\mathbf{S}\mathbf{v} = \lambda\mathbf{v}$$

Eigenvectors are typically quite efficient to compute.

Amount of variance explained

Take the eigenvalue equation

$$\mathbf{S}\mathbf{v} = \lambda\mathbf{v},$$

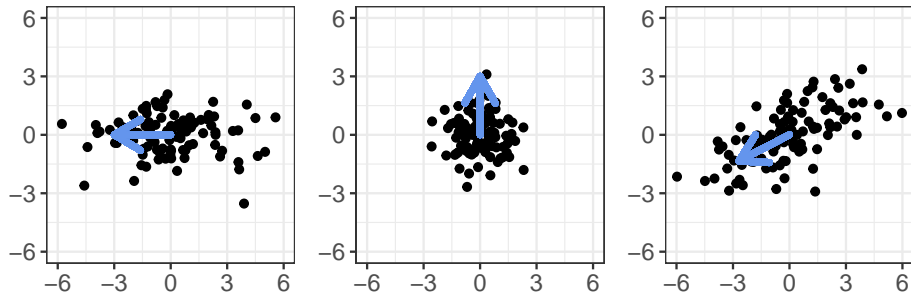
and left-multiply by \mathbf{v}^T to get

$$\lambda = \lambda\mathbf{v}^T\mathbf{v} = \mathbf{v}^T\mathbf{S}\mathbf{v} = \text{Var}(\mathbf{Z}_1).$$

i Eigenvalues and eigenvectors

- The largest eigenvalue of \mathbf{S} is equal to the variance contained in (“explained by”) the first principal component \mathbf{Z}_1 .
- The corresponding eigenvector gives the loadings vector \mathbf{v} .

Example



The loadings vectors may point in the opposite direction of what you expected... Why is this not a problem?

The remaining principal components

Next principal components $\mathbf{Z}_2, \mathbf{Z}_3, \dots$ involve variation in the data after \mathbf{Z}_1 has been taken into account.

- For \mathbf{Z}_2 :

maximize $\text{Var}(\mathbf{Z}_2)$ so that $\text{Cov}(\mathbf{Z}_1, \mathbf{Z}_2) = 0$

- Equivalent to: find second largest eigenvalue λ_2 and eigenvector \mathbf{v}_2 .

Same story for remaining principal components.

Note

The principal components are *uncorrelated* linear combinations of features that *maximize variance*.

How many principal components are there?

Recall:

- \mathbf{S} is a symmetric $D \times D$ matrix
- Such a matrix always has D eigenvalues and eigenvectors

When $D \leq N$ (more data points than features)

- In general, D non-zero principal components

When $D > N$:

- \mathbf{S} has rank at most N : N non-zero principal components
- Can happen in high-dimensional datasets (e.g. gene assays)

Percentage of variance explained

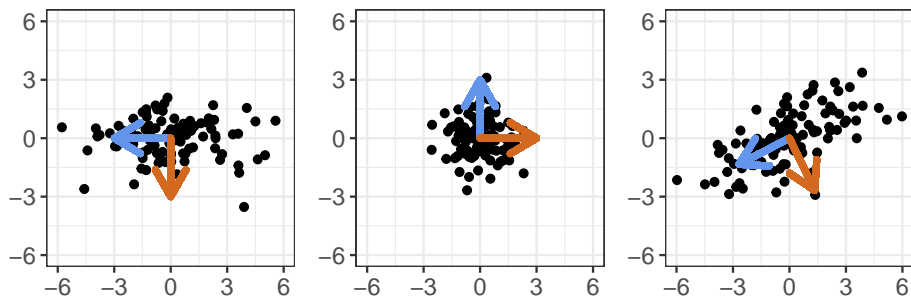
- Eigenvalue λ_i is amount of variance explained by PC i .
- Total amount of variance: $\lambda_1 + \lambda_2 + \dots + \lambda_D$
- Percentage of variance explained by PC i :

$$\frac{\lambda_i}{\lambda_1 + \dots + \lambda_D}$$

In many cases, the first few PCs will explain the majority of variance (80% to 90%).

Dimensionality reduction: we can omit the remaining principal components with only a small loss of information

Example



Blue: first PC, red: second PC.

Worked out example (by hand)

Dataset is chosen so that

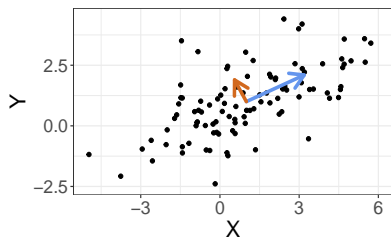
$$\mathbf{S} = \begin{bmatrix} 5 & 2 \\ 2 & 2 \end{bmatrix}.$$

Eigenvalues:

$$\lambda_1 = 6, \quad \lambda_2 = 1.$$

Eigenvectors:

$$\mathbf{v}_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} -1 \\ 2 \end{bmatrix}.$$



Worked out example (with R)

```
prcomp(df)
```

Standard deviations (1, ..., p=2):

```
[1] 2.44949 1.00000
```

Rotation (n x k) = (2 x 2):

	PC1	PC2
X	0.8944272	-0.4472136
Y	0.4472136	0.8944272

Note:

- Standard deviations are **square roots** of eigenvalues
- Columns of rotation matrix give loadings vectors

Example: body fat dataset

```
pca <- prcomp(bodyfat_predictors)
pca
```

Standard deviations (1, .., p=3):
[1] 7.2046011 3.7432587 0.1330841

Rotation (n x k) = (3 x 3):

	PC1	PC2	PC3
triceps.skinfold.thickness	0.6926671	0.1511979	0.7052315
thigh.circumference	0.6985058	-0.3842734	-0.6036751
midarm.circumference	0.1797272	0.9107542	-0.3717862

Percentage of variance explained

```
summary(pca)
```

Importance of components:

	PC1	PC2	PC3
Standard deviation	7.2046	3.7433	0.13308
Proportion of Variance	0.7872	0.2125	0.00027
Cumulative Proportion	0.7872	0.9997	1.00000

- First 2 PCs explain over 99% of variance in data
- Interpretation:

$$PC_1 = 0.693 \cdot \text{triceps} + 0.699 \cdot \text{thigh} + 0.179 \cdot \text{midarm}$$

$$PC_2 = 0.151 \cdot \text{triceps} - 0.384 \cdot \text{thigh} - 0.910 \cdot \text{midarm}$$

Standardizing the features

Often, data are standardized before running PCA:

$$\mathbf{Y}_i = \frac{\mathbf{X}_i - \bar{\mathbf{X}}_i}{\text{SD}(\mathbf{X}_i)}$$

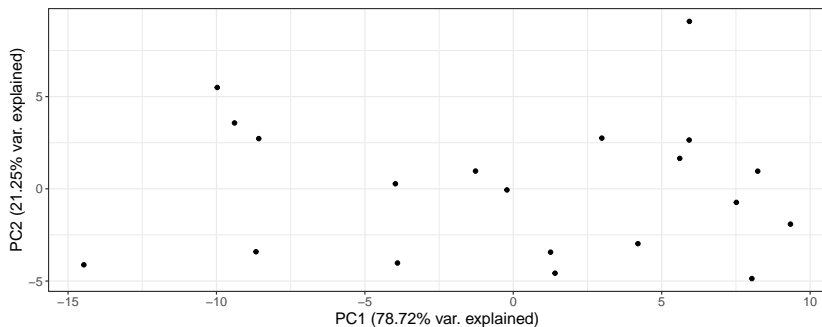
- Standardization puts all features on the same scale and affects the outcome of your PCA.
- Often a good idea when features have different units (e.g. mm, Watt, sec).
- **Not** a good idea when features have the same units (e.g. pixel intensities in an image).

In R: `prcomp(df, center = TRUE, scale = TRUE)`.

Interpretation of PCA results

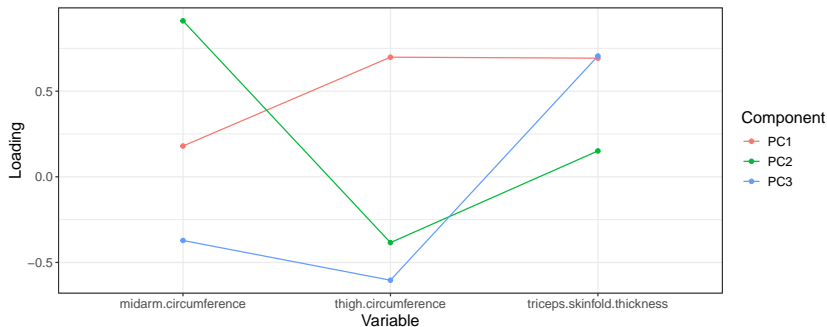
Score plot

- Scatter plot of two PC (usually PC1 and PC2)
- Can be used to spot patterns in data (see later)



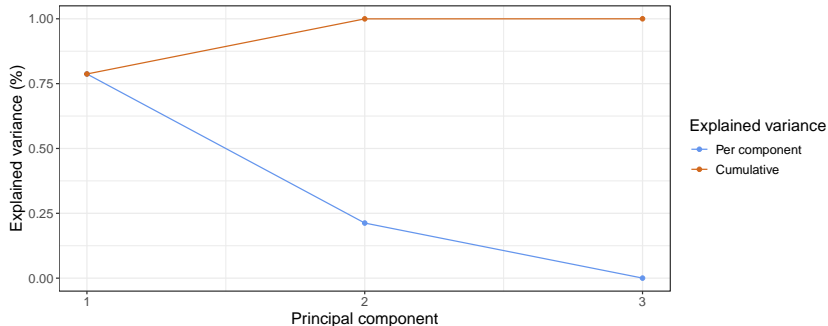
Loadings plot

- Shows how much each variable contributes to each PC
- Useful to discern patterns in PCs



Scree plot

- Shows percentage of variance explained per PC
- Useful to determine the PCs that contribute most to variance
- Can be made with R's `screeplot` command, but better to make your own (it's just a line plot)



Selecting the number of principal components to retain

Many heuristics exist for selecting “optimal” number of PCs:

- Explain fixed percentage (e.g. 80%) of variance
- “Elbow” in scree plot
- ...

Can also determine number of PCs dynamically (e.g. if doing regression on PCs, look at R^2)



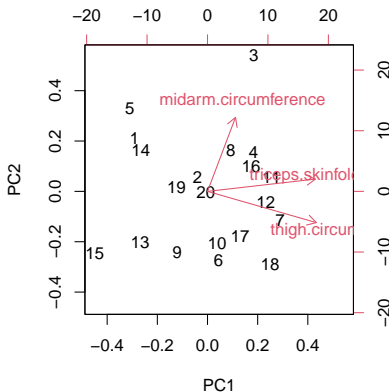
Image credit:

<https://en.wikipedia.org/wiki/Scree> (Kevin Lenz, CC BY-SA 2.5)

Biplot

- Biplot = loadings plot + score plot
- Numbers: data for first two PC
- Arrows: contribution of variables to first two PC

```
biplot(pc)
```



Principal component regression

Principal component regression (PCR)

Idea:

- Do a PCA (usually with standardized features)
- Build a linear model on reduced number of PCs

Why do we do this?

- PCs are uncorrelated, so takes care of multicollinearity
- Results in a simpler model where only important features play a role

Not always the right thing to do, alternatives exist (e.g. ridge regression, see later)

PCR by hand: starting with PC 1

```
pc1 <- pc$x[, "PC1"]  
model_1 <- lm(bodyfat$bodyfat ~ pc1)  
summary(model_1)
```

Call:

```
lm(formula = bodyfat$bodyfat ~ pc1)
```

Residuals:

Min	1Q	Median	3Q	Max
-5.1357	-1.8821	0.2682	1.7107	3.4992

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	20.19500	0.58688	34.411	< 2e-16 ***
pc1	0.61366	0.08358	7.343	8.13e-07 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.625 on 18 degrees of freedom

Multiple R-squared: 0.7497, Adjusted R-squared: 0.7358

F-statistic: 53.91 on 1 and 18 DF, p-value: 8.128e-07

PCR by hand: adding PC 2

Call:

```
lm(formula = bodyfat$bodyfat ~ pc1 + pc2)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-3.9876	-1.8822	0.2562	1.3209	4.0285

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	20.19500	0.56604	35.678	< 2e-16 ***
pc1	0.61366	0.08061	7.613	7.12e-07 ***
pc2	-0.23785	0.15514	-1.533	0.144

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

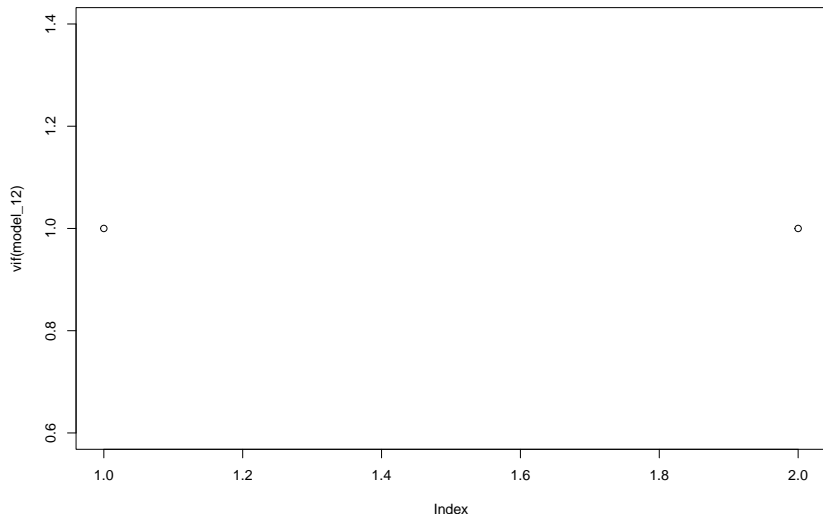
Residual standard error: 2.531 on 17 degrees of freedom

Multiple R-squared: 0.7801, Adjusted R-squared: 0.7542

F-statistic: 30.15 on 2 and 17 DF, p-value: 2.564e-06

Aside: variance inflation factors

Reminder: principal components are uncorrelated by definition, so all the VIFs will be equal to 1.



PCR by hand: putting together the final model

- We would probably select `model_1`:

$$\text{bodyfat} = 20.195 + 0.614 \cdot \text{PC}_1$$

- This model uses the principal components as predictors, but we typically want the original predictors. Recall

$$\text{PC}_1 = 0.693 \cdot \text{triceps} + 0.699 \cdot \text{thigh} + 0.179 \cdot \text{midarm}$$

- Putting these two together gives the final PCR model:

$$\begin{aligned} \text{bodyfat} = & 20.195 + \\ & 0.426 \cdot \text{triceps} + 0.429 \cdot \text{thigh} + 0.110 \cdot \text{midarm} \end{aligned}$$

Stepwise building a model and rewriting it back in terms of the original predictors is a lot of work. Is there a better way?

PCR via the pls package

```
library(pls)

pcr_model <- pcr(bodyfat ~ ., data = bodyfat, validation = "CV")
summary(pcr_model)
```

Data: X dimension: 20 3

Y dimension: 20 1

Fit method: svdpc

Number of components considered: 3

VALIDATION: RMSEP

Cross-validated using 10 random segments.

	(Intercept)	1 comps	2 comps	3 comps
CV	5.239	2.711	2.735	2.867
adjCV	5.239	2.695	2.713	2.832

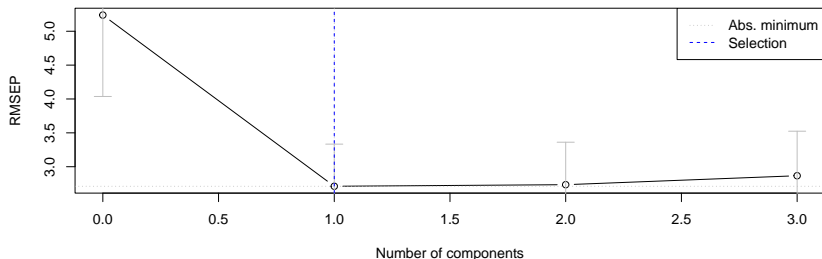
TRAINING: % variance explained

	1 comps	2 comps	3 comps
X	78.72	99.97	100.00
bodyfat	74.97	78.01	80.14

Selecting the optimal number of components

- “1-sigma rule”: select model with least number of components whose cross-validation error is at most 1 standard deviation away from optimal model
- In human language: 2 PCs gives lowest RMSEP, but we can go down to 1 PC without losing too much

```
selectNcomp(pcr_model, method = "onesigma", plot = TRUE)
```



```
[1] 1
```

Ridge regression (optional)

- PCR is not the only way to “regularize” a regression model
- Ridge regression: like ordinary regression, but punish model for coefficients that become too large.
- Objective function:

$$J_{\text{ridge}}(\alpha, \beta) = J(\alpha, \beta) + \lambda(\alpha^2 + \beta^2).$$

- Parameter λ set to a fixed value or determined via cross-validation.
 - $\lambda = 0$: ridge regression = ordinary regression
 - $\lambda \rightarrow \infty$: all coefficients become zero
- Can be done with the `glmnet` package (not very userfriendly)

Example session

```
library(glmnet)
predictors <- data.matrix(bodyfat_predictors)
outcome <- bodyfat$bodyfat

lambdas <- 10^seq(2, -2, by = -.1)
ridge_cv <- cv.glmnet(predictors, outcome, alpha = 0, lambda = lambdas)

best <- ridge_cv$lambda.min
best
```

```
[1] 0.06309573
```

```
best_ridge <- glmnet(predictors, outcome, alpha = 0, lambda = best)
coef(best_ridge)
```

4 x 1 sparse Matrix of class "dgCMatrix"

	s0
(Intercept)	-4.6532088
triceps.skinfold.thickness	0.6433295
thigh.circumference	0.2965686
midarm.circumference	-0.2391984