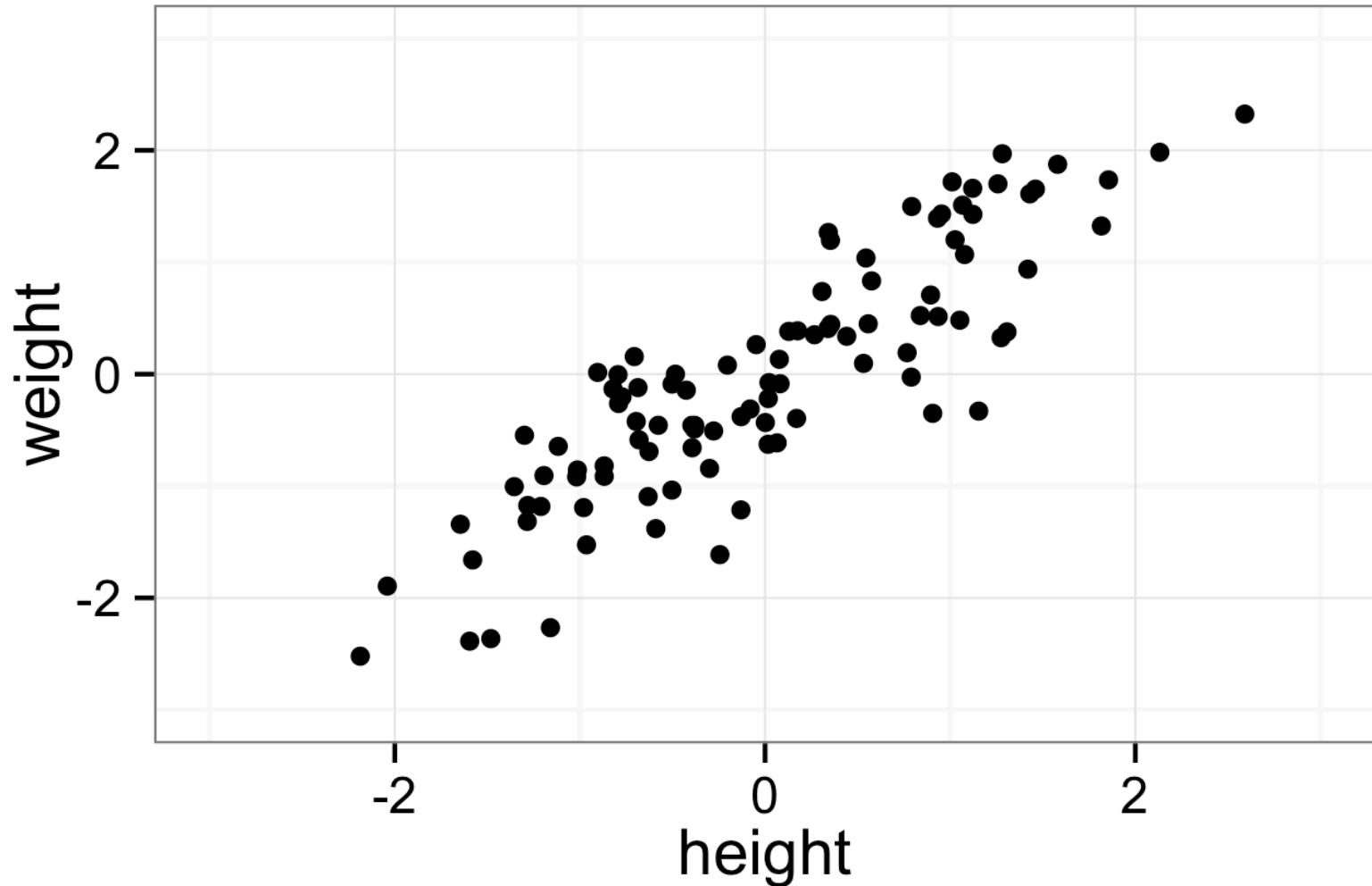


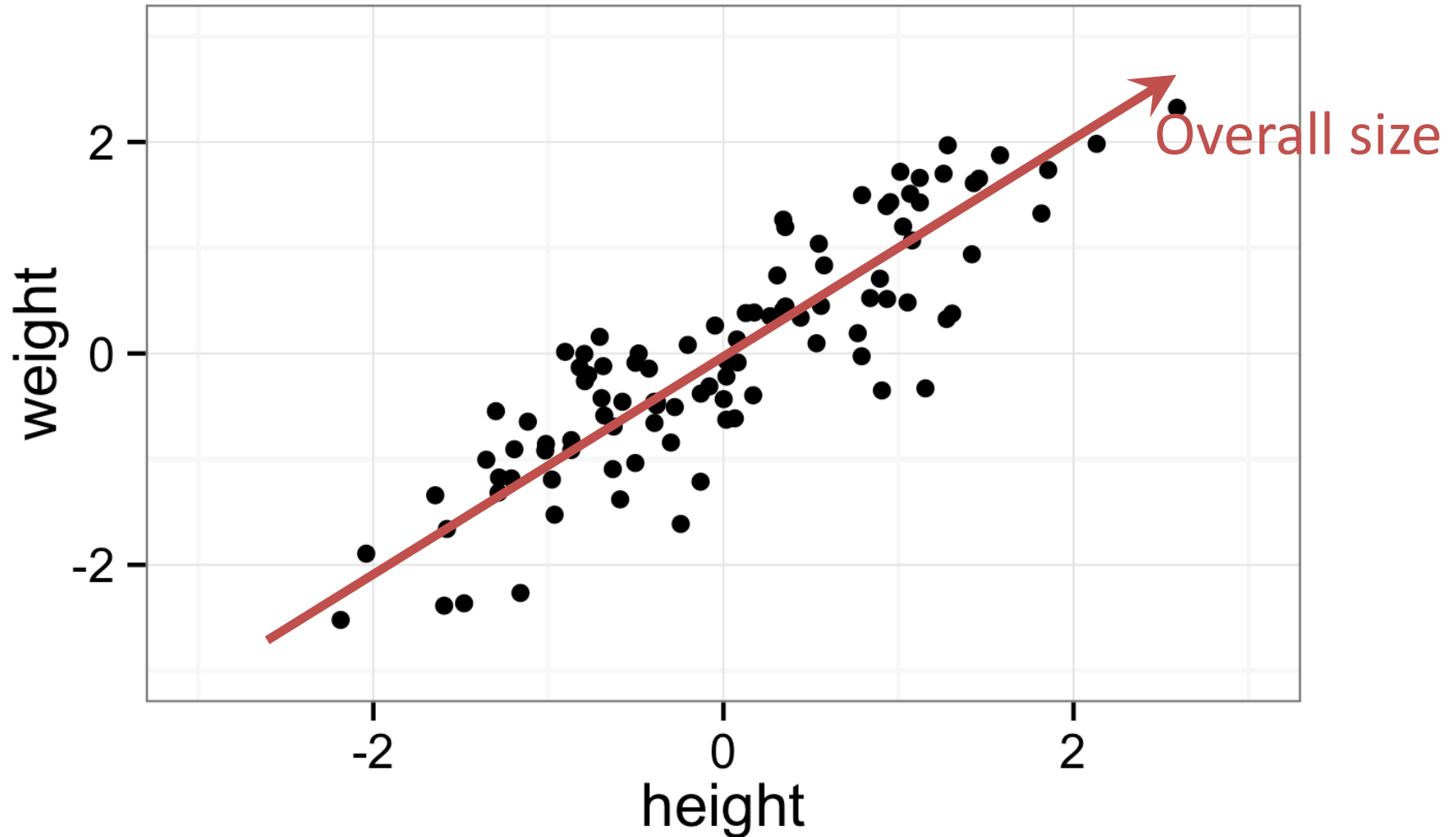
Principal Components Analysis (PCA)

Exploratory data analysis of high-dimensional data sets.

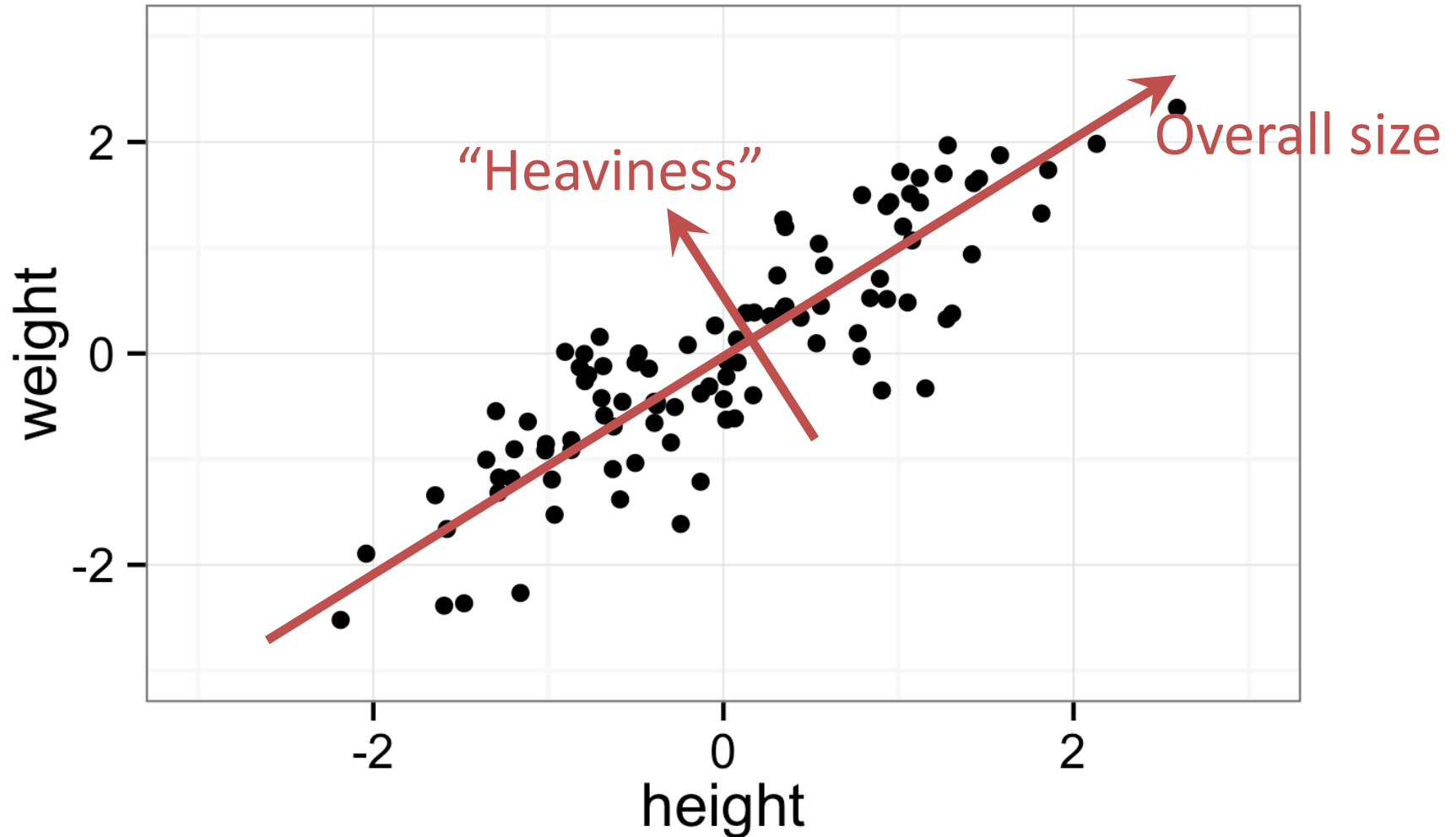
Example: Consider a data set of heights and weights of people



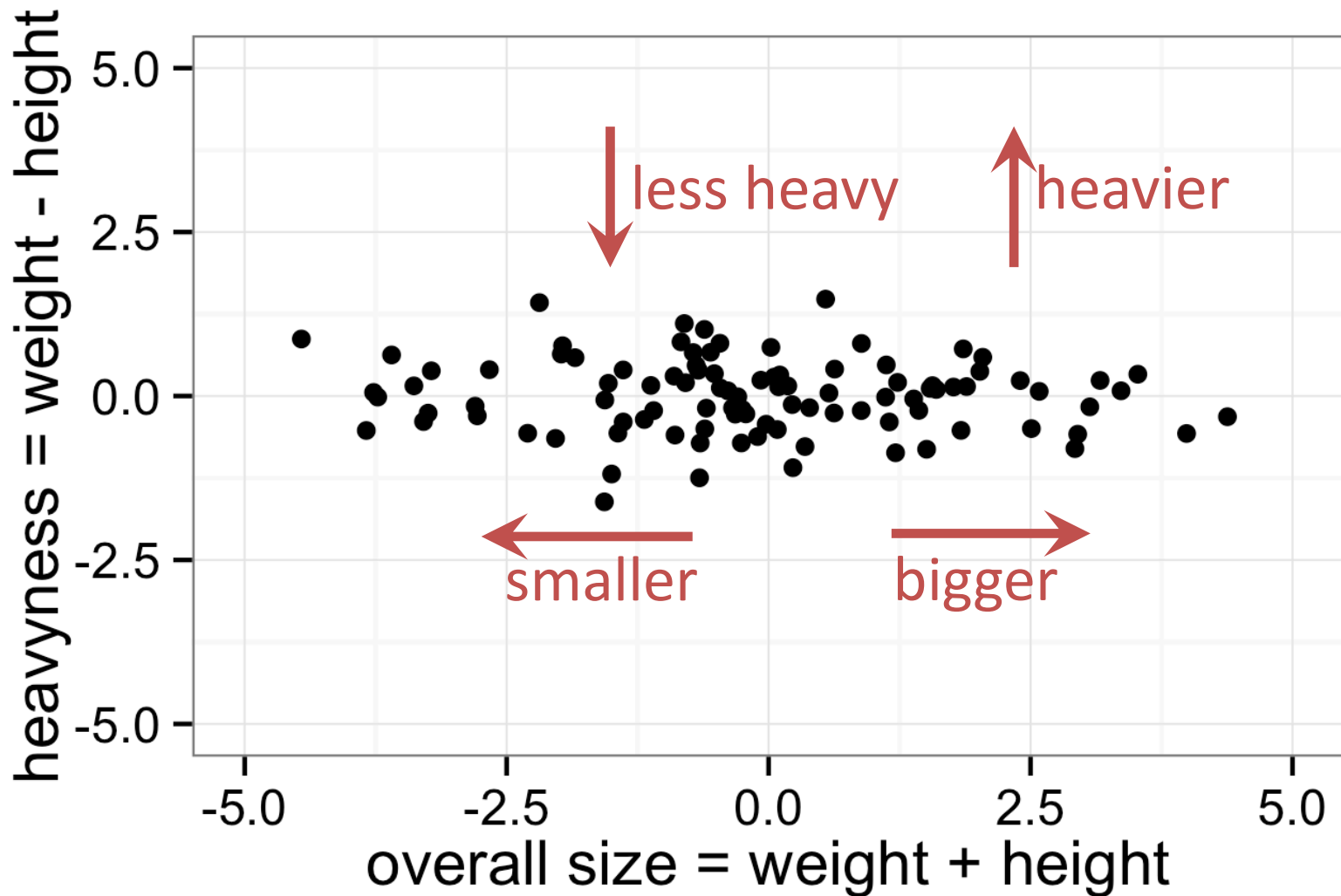
Example: Consider a data set of heights and weights of people



Example: Consider a data set of heights and weights of people



PCA on this data set reframes data in terms of overall size and heavyness



The math behind PCA

Variance of one variable:

$$\text{Var}(X) = \frac{1}{n} \sum_j (\bar{x} - x_j)^2 = \sigma_X^2$$

Covariance of two variables:

$$\text{Cov}(X, Y) = \frac{1}{n} \sum_j (\bar{x} - x_j)(\bar{y} - y_j) = \sigma_{XY}^2$$

The math behind PCA

Covariance matrix of n variables $X_1 \dots X_n$:

$$\mathbf{C} = \begin{pmatrix} \sigma_{11}^2 & \sigma_{12}^2 & \cdots & \sigma_{1n}^2 \\ \sigma_{21}^2 & \sigma_{22}^2 & \cdots & \sigma_{2n}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1}^2 & \sigma_{n2}^2 & \cdots & \sigma_{nn}^2 \end{pmatrix}$$

The math behind PCA


PCA diagonalizes the covariance matrix \mathbf{C} :

$$\mathbf{C} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$
$$= \mathbf{U} \begin{pmatrix} \lambda_1^2 & 0 & \cdots & 0 \\ 0 & \lambda_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^2 \end{pmatrix} \mathbf{U}^T$$

The math behind PCA

PCA diagonalizes the covariance matrix \mathbf{C} :

$$\mathbf{C} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$


rotation matrix 

$$= \mathbf{U} \begin{pmatrix} \lambda_1^2 & 0 & \cdots & 0 \\ 0 & \lambda_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^2 \end{pmatrix} \mathbf{U}^T$$

The math behind PCA

PCA diagonalizes the covariance matrix \mathbf{C} :

$$\mathbf{C} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$

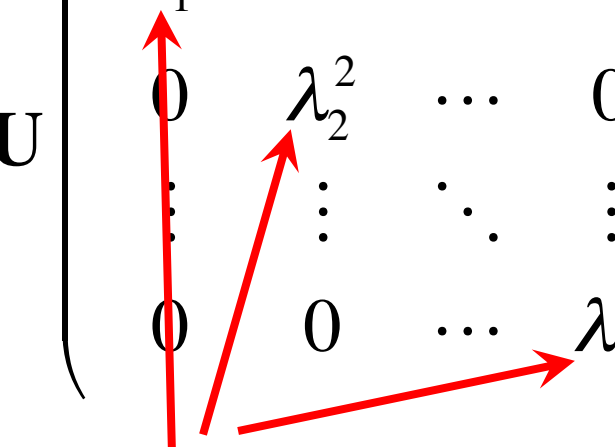
diagonal matrix 

$$= \mathbf{U} \begin{pmatrix} \lambda_1^2 & 0 & \cdots & 0 \\ 0 & \lambda_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^2 \end{pmatrix} \mathbf{U}^T$$

The math behind PCA

PCA diagonalizes the covariance matrix \mathbf{C} :

$$\mathbf{C} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$

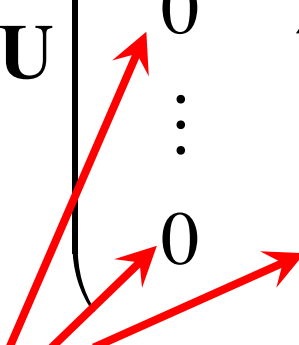
$$= \mathbf{U} \begin{pmatrix} \lambda_1^2 & 0 & \dots & 0 \\ 0 & \lambda_2^2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n^2 \end{pmatrix} \mathbf{U}^T$$


eigenvalues (= variance explained
by each component)

The math behind PCA

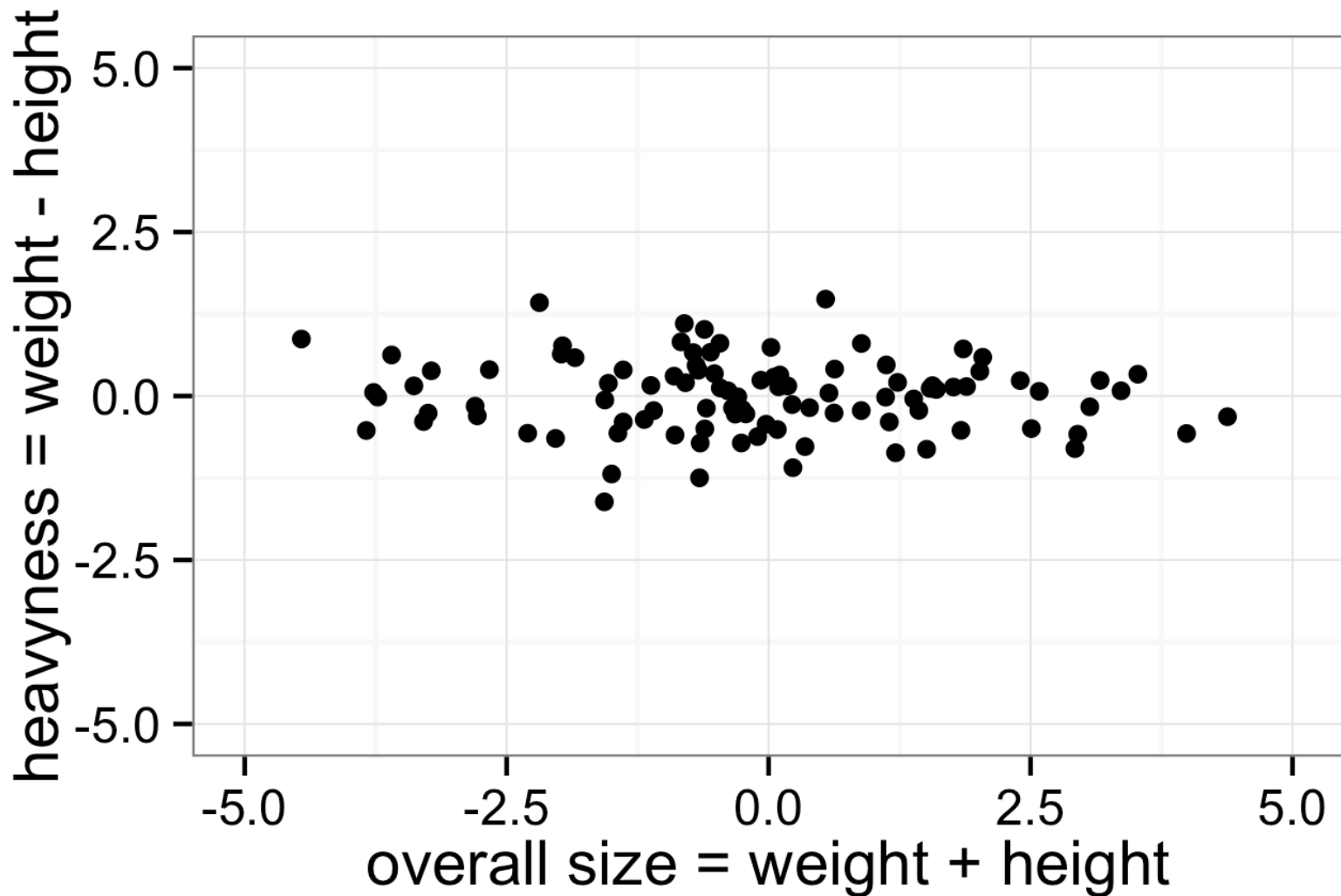
PCA diagonalizes the covariance matrix \mathbf{C} :

$$\mathbf{C} = \mathbf{U}\mathbf{D}\mathbf{U}^T$$

$$= \mathbf{U} \begin{pmatrix} \lambda_1^2 & 0 & \cdots & 0 \\ 0 & \lambda_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^2 \end{pmatrix} \mathbf{U}^T$$


covariance between components
is zero (they are uncorrelated)

In our earlier example, overall size and heaviness are uncorrelated



Doing a PCA in R

```
iris %>%  
  select(-Species) %>% # remove Species column  
  scale() %>% # scale to zero mean  
  # and unit variance  
  prcomp() -> # do PCA  
  pca # store result  
  # in variable "pca"
```

Doing a PCA in R

```
> pca
```

```
Standard deviations:
```

```
[1] 1.7083611 0.9560494 0.3830886 0.1439265
```

```
Rotation:
```

	PC1	PC2	PC3	PC4
Sepal.Length	0.5210659	-0.37741762	0.7195664	0.2612863
Sepal.Width	-0.2693474	-0.92329566	-0.2443818	-0.1235096
Petal.Length	0.5804131	-0.02449161	-0.1421264	-0.8014492
Petal.Width	0.5648565	-0.06694199	-0.6342727	0.5235971

Doing a PCA in R

```
> pca
```

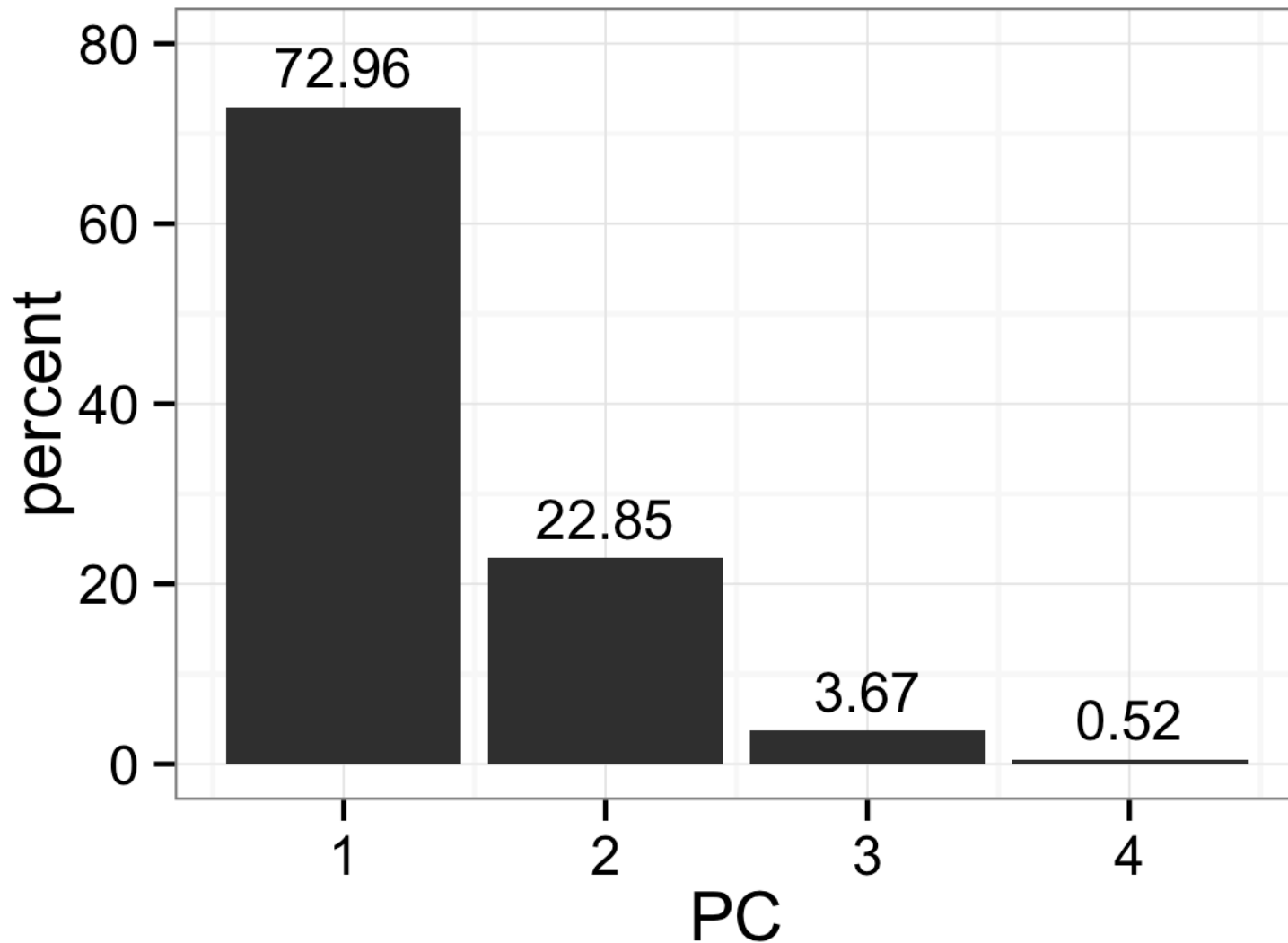
```
Standard deviations:
```

```
[1] 1.7083611 0.9560494 0.3830886 0.1439265
```

```
Rotation:
```

	PC1	PC2	PC3	PC4
Sepal.Length	0.5210659	-0.37741762	0.7195664	0.2612863
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Petal.Width	0.5648565	-0.06694199	-0.6342727	0.5235971

Squares of the std. devs represent the % variance explained by each PC



Doing a PCA in R

```
> pca
```

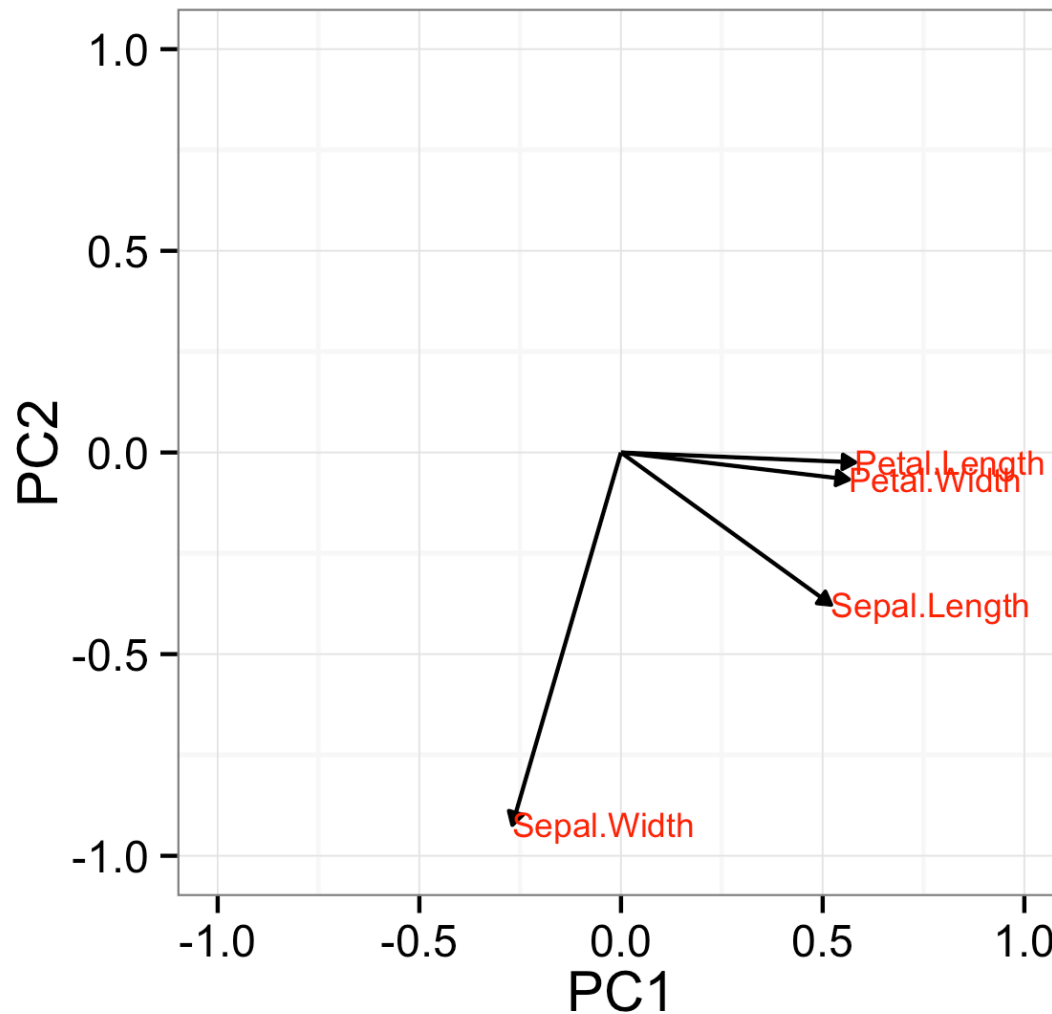
```
Standard deviations:
```

```
[1] 1.7083611 0.9560494 0.3830886 0.1439265
```

```
Rotation:
```

	PC1	PC2	PC3	PC4
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Petal.Width	0.5648565	-0.06694199	-0.6342727	0.5235971

The rotation matrix tells us which variables contribute to which PCs



We can also recover each original observation expressed in PC coordinates

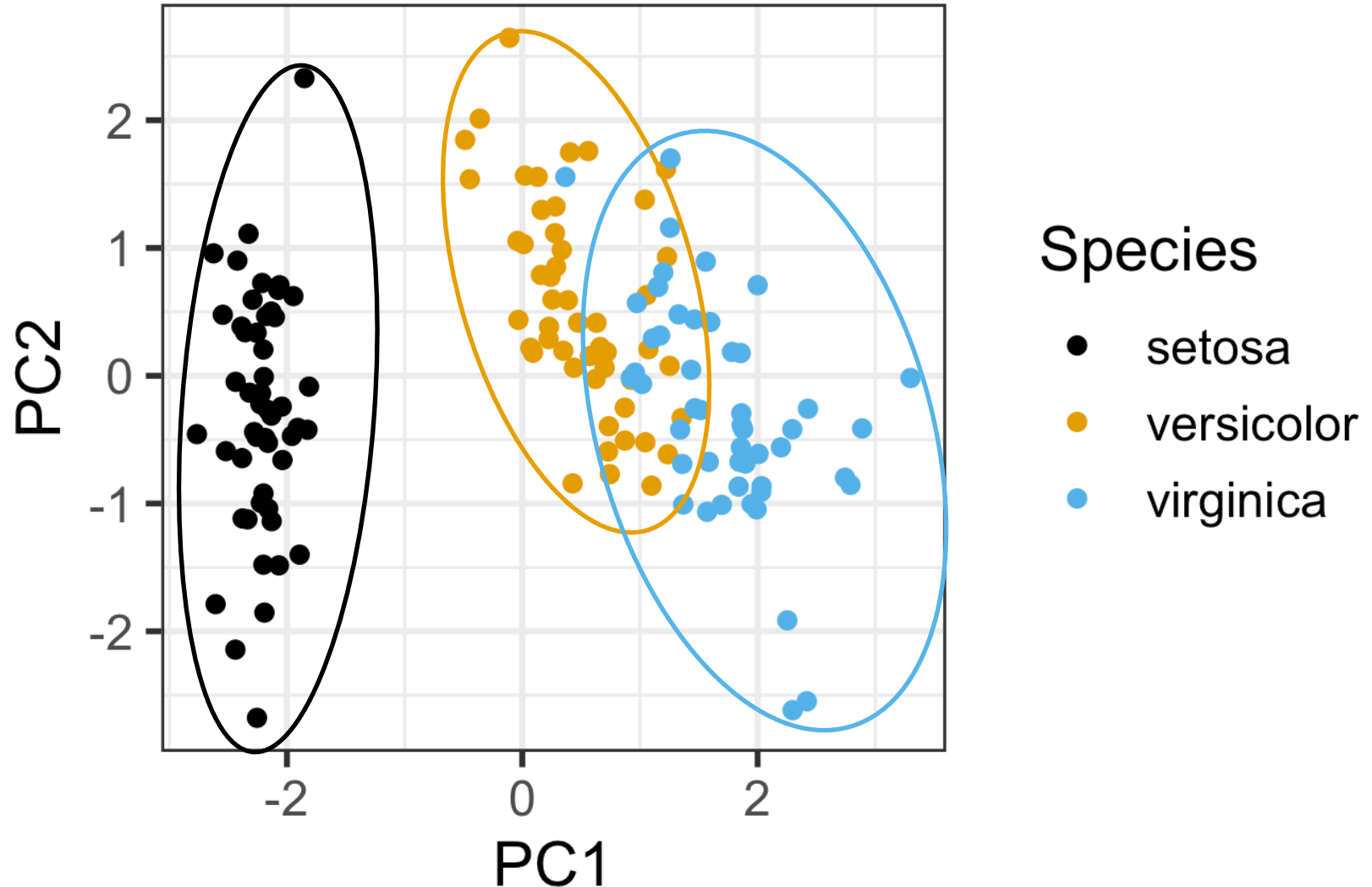
```
> pca$x
```

We can also recover each original observation expressed in PC coordinates

```
> pca$x
```

	PC1	PC2	PC3	PC4
[1,]	-2.25714118	-0.478423832	0.127279624	0.024087508
[2,]	-2.07401302	0.671882687	0.233825517	0.102662845
[3,]	-2.35633511	0.340766425	-0.044053900	0.028282305
[4,]	-2.29170679	0.595399863	-0.090985297	-0.065735340
[5,]	-2.38186270	-0.644675659	-0.015685647	-0.035802870
[6,]	-2.06870061	-1.484205297	-0.026878250	0.006586116
[7,]	-2.43586845	-0.047485118	-0.334350297	-0.036652767
[8,]	-2.22539189	-0.222403002	0.088399352	-0.024529919
[9,]	-2.32684533	1.111603700	-0.144592465	-0.026769540
[10,]	-2.17703491	0.467447569	0.252918268	-0.039766068
[11,]	-2.15907699	-1.040205867	0.267784001	0.016675503
[12,]	-2.31836413	-0.132633999	-0.093446191	-0.133037725
[13,]	-2.21104370	0.726243183	0.230140246	0.002416941

Plot of iris plants in PC coordinates reveals differences among species



These differences are much harder to see in the original variables

