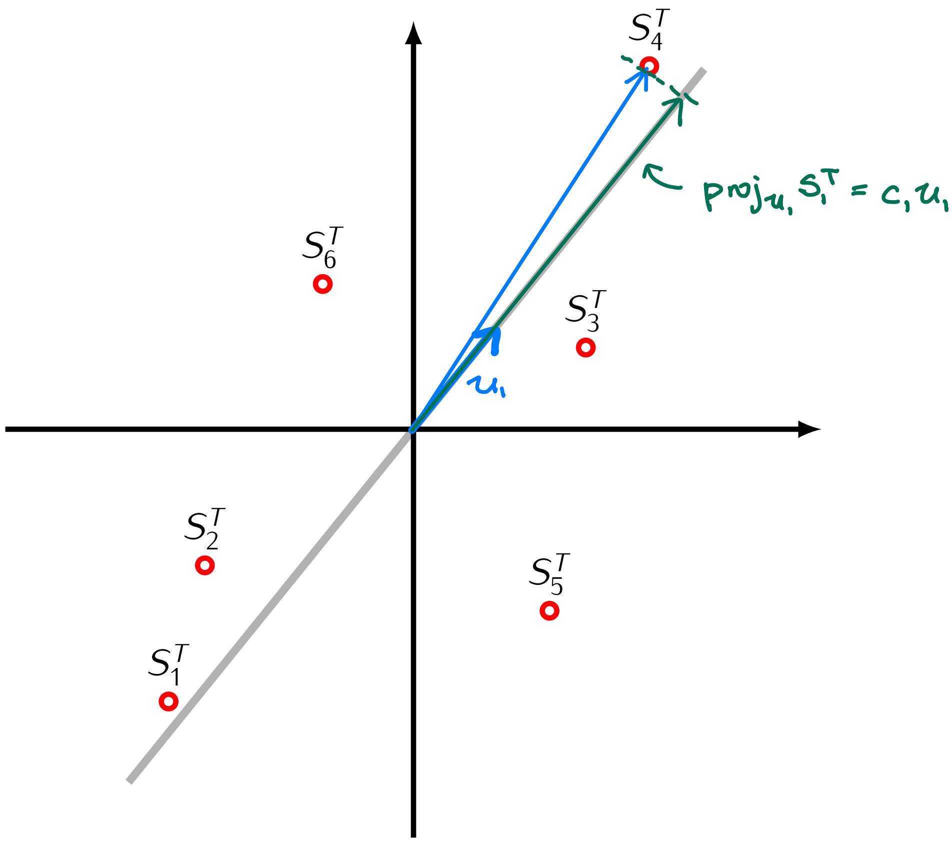
Example.

Demeaned data matrix:

$$A = \begin{array}{r} \\ \text{Aly} \\ \text{Bob} \\ \text{Chen} \\ \text{Deb} \\ \text{Emma} \\ \text{Finn} \end{array} \begin{array}{c} \begin{array}{cc} \text{Ex 1} & \text{Ex 2} \end{array} \\ \begin{bmatrix} -27 & -30 \\ -23 & -15 \\ 19 & 6 \\ 26 & 40 \\ 15 & -20 \\ -10 & 16 \end{bmatrix} \end{array} = \begin{bmatrix} \boxed{X_1} & \boxed{X_2} \end{bmatrix} = \begin{bmatrix} \boxed{S_1} \\ \boxed{S_2} \\ \boxed{S_3} \\ \boxed{S_4} \\ \boxed{S_5} \\ \boxed{S_6} \end{bmatrix}$$

Let $\mathbf{u}_1$ be the 1^{st} principal axis of A, and let Y_1 be the 1^{st} principal component of A:

$$Y_1 = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} = \begin{bmatrix} S_1\mathbf{u}_1 \\ S_2\mathbf{u}_1 \\ \vdots \\ S_N\mathbf{u}_1 \end{bmatrix}$$



The projection matrix

The projection matrix:

$$P = \begin{bmatrix} (\mathrm{proj}_{u_1} S_1^T)^T \\ (\mathrm{proj}_{u_1} S_2^T)^T \\ \vdots \\ (\mathrm{proj}_{u_1} S_N^T)^T \end{bmatrix} = \underbrace{\begin{bmatrix} c_1 u_1^T \\ c_2 u_1^T \\ \vdots \\ c_N u_1^T \end{bmatrix}}_{y_1 u_1^T} = \begin{bmatrix} s_1 u_1 u_1^T \\ s_2 u_1 u_1^T \\ \vdots \\ s_N u_1 u_1^T \end{bmatrix} = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{bmatrix} u_1 u_1^T$$

$$= A u_1 u_1^T$$

The difference matrix

$$\underbrace{D = A - P}$$

the information that is not captured by the 1st principal component of A

To understand this information better we can use the 1st principal component of D:

Definition

Let A an $N \times M$ demeaned data matrix

$$A = \begin{bmatrix} \boxed{S_1} \\ \boxed{S_1} \\ \vdots \\ \boxed{S_N} \end{bmatrix}$$

Let $\mathbf{u}_1$ be the 1st principal axis of A, and let Y_1 be the 1st principal component of A.

The *2nd principal axis* of A is the 1st principal axis of the difference matrix

$$D_1 = A - Y_1 \mathbf{u}_1^T$$

The *2nd principal component* Y_2 of A is the 1st principal component of the matrix D_1.

Computation of the 2^{nd} principal ~~component~~ axis of A

The 2^{nd} princ. axis of A = the 1^{st} pric. axis of $D = A - P$

= the eigenvector of $C_D = \frac{1}{N}D^TD$ corresponding to the largest eigenvalue of C_D.

Consider the orthogonal diagonalization of $C_A = \frac{1}{N}A^TA$:

$$C_A = \frac{1}{N}A^TA = \underbrace{\begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix}}_{\substack{\text{orthonormal} \\ \text{eigenvectors of } C_A}} \underbrace{\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{bmatrix}}_{\substack{\text{eigenvalues} \\ \text{of } C_A,\ \lambda_1 \geq \lambda_2 \geq \ldots \lambda_N \geq 0}} \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_N^T \end{bmatrix}$$

We have:

$$C_D = \frac{1}{N}D^TD = \frac{1}{N}(A-P)^T(A-P) = \frac{1}{N}(A^TA - A^TP - P^TA + P^TP) = C_A - \frac{1}{N}A^TP - \frac{1}{N}P^TA + \frac{1}{N}P^TP$$

$$\frac{1}{N}A^TP = \underbrace{\frac{1}{N}A^TA}_{C_A}u_1u_1^T \underset{C_Au_1 = \lambda_1u_1}{=} \lambda_1u_1u_1^T$$

$$\frac{1}{N}P^TA = \left(\frac{1}{N}A^TP\right)^T = (\lambda_1u_1u_1^T)^T = \lambda_1u_1u_1^T$$

$$\frac{1}{N}P^TP = \frac{1}{N}(Au_1u_1^T)^T(Au_1u_1^T) = \frac{1}{N}u_1u_1^TA^TAu_1u_1^T = u_1u_1^TC_Au_1u_1^T \overset{C_Au_1 = \lambda_1u_1}{=} u_1u_1^T(\lambda_1u_1)u_1^T$$

$$= \lambda_1u_1(u_1^Tu_1)u_1^T \underset{u_1^Tu_1 = 1}{=} \lambda_1u_1u_1^T$$

This gives:

$$C_D = C_A - \lambda_1u_1u_1^T - \cancel{\lambda_1u_1u_1^T} + \cancel{\lambda_1u_1u_1^T} = C_A - \lambda_1u_1u_1^T =$$

$$= \begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{bmatrix} \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_N^T \end{bmatrix} - \begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_N^T \end{bmatrix}$$

$$= \begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix} \left(\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{bmatrix} - \begin{bmatrix} \lambda_1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} \right) \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_N^T \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} u_1 & u_2 & \cdots & u_N \end{bmatrix}}_{\substack{\text{orthonormal} \\ \text{eigenvectors of } C_D}} \underbrace{\begin{bmatrix} 0 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{bmatrix}}_{\substack{\text{eigenvalues of} \\ C_D}} \begin{bmatrix} u_1^T \\ u_2^T \\ \vdots \\ u_N^T \end{bmatrix}$$

Upshot

1) The 2^{nd} principal axis of A = the 1^{st} pricipal axis of D
= the eigenvector u_2 of C_A corresponding to the second largest eigenvalue λ_2 of C_A.

2) The 2^{nd} principal component of A = the 1^{st} princ. comp. of D

$$Y_2 = D u_2 = (A-P)u_2 = Au_2 - Au_1\underbrace{u_1^T u_2}_{0} = Au_2$$

$\leftarrow$ since u_1 is orthogonal to u_2

3) $$\mathrm{Var}(Y_2) = \frac{1}{N} Y_2^T Y_2 = \frac{1}{N}(Au_2)^T(Au_2) = \frac{1}{N} u_2^T A^T A u_2 =$$
$$= u_2^T C_A u_2 \underset{C_A u_2 = \lambda_2 u_2}{=} \lambda_2 u_2^T u_2 \underset{u_2^T u_2 = 1}{=} \lambda_2$$

4) $$\mathrm{Cov}(Y_1, Y_2) = \frac{1}{N} Y_1^T Y_2 = \frac{1}{N}(Au_1)^T(Au_2) = \frac{1}{N} u_1^T A^T A u_2$$
$$= u_1^T C_A u_2 \underset{C_A u_2 = \lambda_2 u_2}{=} u_1^T \lambda_2 u_2 = \lambda_2 u_1^T u_2 = 0$$

since u_1, u_2 are orthogonal

Proposition

Given a demeaned data matrix A, let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$$

be eigenvalues of the covariance matrix C_A and let $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N$ be orthonormal vectors such that $\mathbf{u}_i$ is an eigenvector of C_A corresponding to the eigenvalue λ_i.

- The 2^{nd} *principal axis* of A is the vector $\mathbf{u}_2$.
- The 2^{nd} *principal component* of A is the vector $Y_2 = A\mathbf{u}_2$.
- We have $\mathrm{Var}(Y_2) = \lambda_2$.
- In addition, $\mathrm{Cov}(Y_1, Y_2) = 0$.

The i^{th} principal component

Let u_1, u_2 – the 1^{st} and 2^{nd} principal axes of A

$$D_2 = \underbrace{A - \underbrace{\begin{bmatrix} (\mathrm{proj}_{u_1} s_1^T)^T \\ (\mathrm{proj}_{u_1} s_2^T)^T \\ \vdots \\ (\mathrm{proj}_{u_2} s_N^T)^T \end{bmatrix}}_{\text{from the } 1^{st} \text{ principal component}} - \underbrace{\begin{bmatrix} (\mathrm{proj}_{u_2} s_1^T)^T \\ (\mathrm{proj}_{u_2} s_2^T)^T \\ \vdots \\ (\mathrm{proj}_{u_2} s_N^T)^T \end{bmatrix}}_{\text{from the } 2^{nd} \text{ principal component}}}_{\text{the information not captured by the } 1^{st} \text{ and } 2^{nd} \text{ principal component of } A}$$

<u>Define:</u>

The 3^{rd} principal axis / component of A

$\parallel$

The 1^{st} principal axis / component of D_2

$\vdots$

Proposition/Definition

Given a demeaned data matrix A, let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$$

be eigenvalues of the covariance matrix C_A and let $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N$ be orthonormal vectors such that $\mathbf{u}_i$ is an eigenvector of C_A corresponding to the eigenvalue λ_i.

- The i^{th} *principal axis* of A is the vector $\mathbf{u}_i$.
- The i^{th} *principal component* of A is the vector $Y_i = A\mathbf{u}_i$.
- We have $\mathrm{Var}(Y_i) = \lambda_i$.
- In addition, $\mathrm{Cov}(Y_i, Y_j) = 0$ if $i \neq j$.