PCA -- In practice

- The basic goal of PCA is to reduce the dimensionality of the data. Thus, one usually chooses:

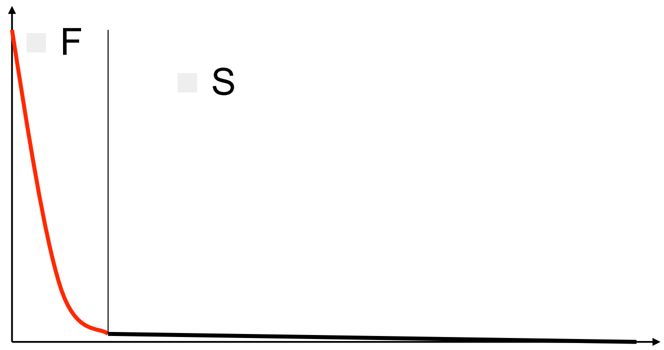
$$n << q$$

- But how do we select the number of components *n* ?

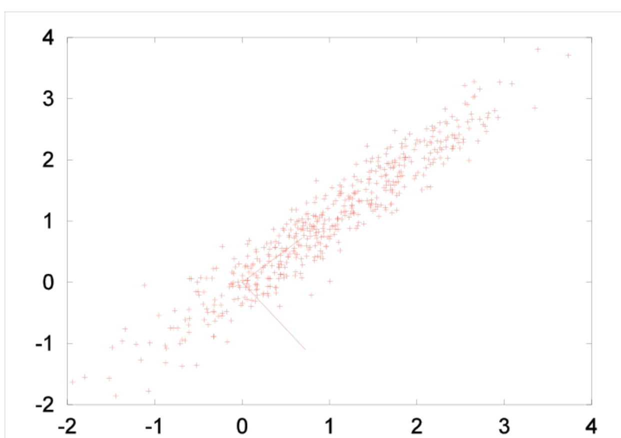
Determining the number of components

- Plot the eigenvalues – each eigenvalue is related to the amount of variation explained by the corresponding axis (eigenvector);
- If the points on the graph tend to level out (show an “elbow” shape), these eigenvalues are usually close enough to zero that they can be ignored.
- In general: Limit the variance accounted for.

Critical information lies in low dimensional subspaces



- A typical eigenvalue spectrum and its division into two orthogonal subspaces



$\lambda_1 = 1.98, \quad \lambda_2 = 0.05$

Determining the number of components

$x_i \in \Re^q, \quad i = 1, \cdots, N$

$w_1, w_2, \cdots, w_q$: q eigenvectors (principal component directions)

$\|w_i\| = 1$ (the w_is are orthonormal vectors)

Representation of x_i in eigenvector space :

$$y_i = (w_1^T x_i) w_1 + (w_2^T x_i) w_2 + \cdots + (w_q^T x_i) w_q$$

Suppose we retain the first k principal components :

$$y_i^k = (w_1^T x_i) w_1 + (w_2^T x_i) w_2 + \cdots + (w_k^T x_i) w_k$$

Then :

$$y_i - y_i^k = (w_{k+1}^T x_i) w_{k+1} + \cdots + (w_q^T x_i) w_q$$

Determining the number of components

$$(y_i - y_i^k)^T (y_i - y_i^k) =$$

$$\left[(w_{k+1}^T x_i) w_{k+1} + \cdots + (w_q^T x_i) w_q\right]^T \left[(w_{k+1}^T x_i) w_{k+1} + \cdots + (w_q^T x_i) w_q\right] =$$

$$w_{k+1}^T (w_{k+1}^T x_i)^2 w_{k+1} + \cdots + w_q^T (w_q^T x_i)^2 w_q =$$

(note $w_i^T w_j = 0 \; \forall i \neq j$ since w_i and w_j are orthogonal vectors)

$$(w_{k+1}^T x_i)^2 w_{k+1}^T w_{k+1} + \cdots + (w_q^T x_i)^2 w_q^T w_q =$$

$$(w_{k+1}^T x_i)^2 + \cdots + (w_q^T x_i)^2 =$$

$$(w_{k+1}^T x_i)(x_i^T w_{k+1}) + \cdots + (w_q^T x_i)(x_i^T w_q) =$$

$$w_{k+1}^T (x_i x_i^T) w_{k+1} + \cdots + w_q^T (x_i x_i^T) w_q$$

Determining the number of components

$$\frac{1}{N}\sum_{i=1}^{N}\left(y_i - y_i^k\right)^T\left(y_i - y_i^k\right) =$$

Mean square error

$$\frac{1}{N}\sum_{i=1}^{N}\left[\boldsymbol{w}_{k+1}^T\left(\boldsymbol{x}_i\boldsymbol{x}_i^T\right)\boldsymbol{w}_{k+1} + \cdots + \boldsymbol{w}_q^T\left(\boldsymbol{x}_i\boldsymbol{x}_i^T\right)\boldsymbol{w}_q\right] =$$

$$\boldsymbol{w}_{k+1}^T\left[\frac{1}{N}\sum_{i=1}^{N}\left(\boldsymbol{x}_i\boldsymbol{x}_i^T\right)\right]\boldsymbol{w}_{k+1} + \cdots + \boldsymbol{w}_q^T\left[\frac{1}{N}\sum_{i=1}^{N}\left(\boldsymbol{x}_i\boldsymbol{x}_i^T\right)\right]\boldsymbol{w}_q =$$

$$\boldsymbol{w}_{k+1}^T\Sigma\boldsymbol{w}_{k+1} + \cdots + \boldsymbol{w}_q^T\Sigma\boldsymbol{w}_q$$

We have: $\Sigma\boldsymbol{w}_{k+1} = \lambda_{k+1}\boldsymbol{w}_{k+1}, \cdots, \Sigma\boldsymbol{w}_q = \lambda_q\boldsymbol{w}_q$

Thus:

$$\boldsymbol{w}_{k+1}^T\Sigma\boldsymbol{w}_{k+1} + \cdots + \boldsymbol{w}_q^T\Sigma\boldsymbol{w}_q =$$

$$\boldsymbol{w}_{k+1}^T\lambda_{k+1}\boldsymbol{w}_{k+1} + \cdots + \boldsymbol{w}_q^T\lambda_q\boldsymbol{w}_q =$$

$$\lambda_{k+1} + \cdots + \lambda_q$$

Determining the number of components

$$\frac{1}{N}\sum_{i=1}^{N}\left(y_i - y_i^k\right)^T\left(y_i - y_i^k\right) = \lambda_{k+1} + \cdots \lambda_q$$

⟹ The mean square error of the truncated representation is equal to the sum of the remaining eigenvalues.

In general: choose *k* so that 90-95% of the variance of the data is captured.