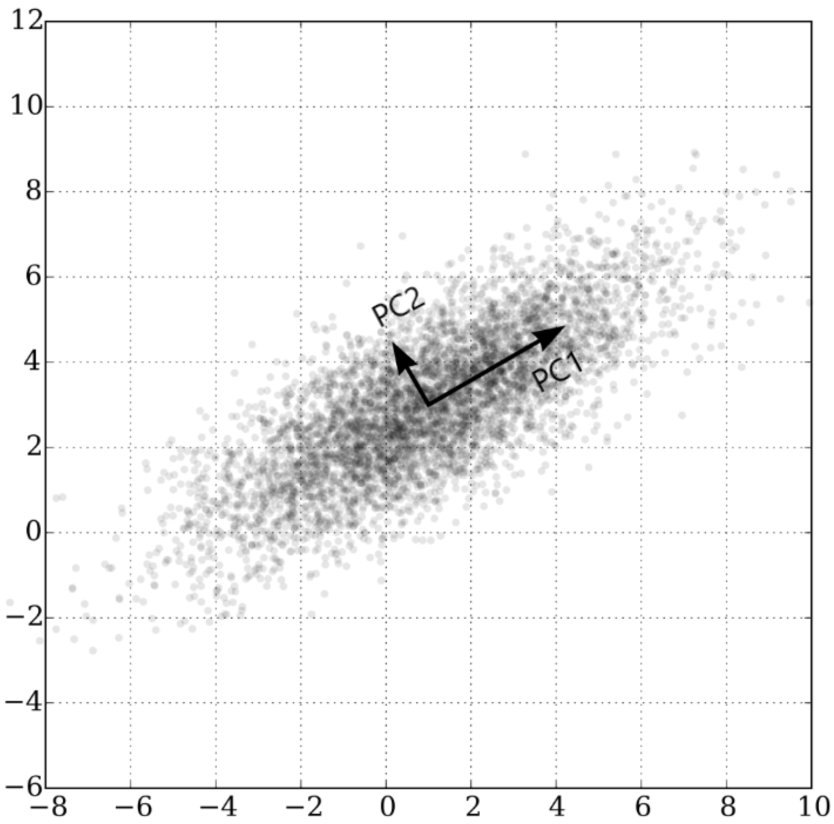
Principal Component Analysis

PCA is an unsupervised learning method which aims to *reduce* the dimensionality of an input space $\mathcal{X}$.

Formally, principal component analysis (PCA) is a statistical procedure that uses an *orthogonal transformation* to convert a set of observations of possibly correlated variables into a set of values of *linearly uncorrelated* variables called *principal components*.

To have a graphical intuition:



It is based on the principle of projecting the data onto the input subspace which accounts for most of the variance:

- Find a line such that when the data is projected onto that line, it has the maximum variance.
- Find a new line, orthogonal to the first one, that has maximum projected variance.
- Repeat until m lines have been identified and project the points in the data set on these lines.

The precise steps of *PCA* are the following (remember that $\mathbf{X}$ is an $n \times d$ matrix where n denotes the number of samples and d is the dimensionality) :

- Compute the mean of the data

$$\overline{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n \tag{1}$$

- Bring the data to zero-mean (by subtracting $\overline{\mathbf{x}}$)
- Compute the covariance matrix $\mathbf{S} = \mathbf{X}^T\mathbf{X} = \frac{1}{N-1}\sum_{n=1}^{N}(\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^T$
    - Eigenvector $\mathbf{e}_1$ with largest eigenvalue λ_1 is the *first principal component*
    - Eigenvector $\mathbf{e}_k$ with k^{th} largest eigenvalue λ_k is the k^{th} *principal component*
    - $\frac{\lambda_k}{\sum_i \lambda_i}$ is the proportion of variance captured by the k^{th} principal component.

Transforming the reduced dimensionality projection back into the original spaces gives a reduced dimensionality reconstruction of the data, that will have some error. This error can be small and often acceptable given the other benefits of dimensionality reduction. PCA has multiple benefits:

- Helps to reduce the computational complexity
- Can help supervised learning, because reduced dimensions allow simpler hypothesis spaces and less risk of overfitting
- Can be used for noise reduction

But also some drawbacks:

- Fails when data consists of multiple clusters
- The directions of greatest variance may not be the most informative
- Computational problems with many dimensions
- PCA computes linear combination of features, but data often lies on a nonlinear manifold. Suppose that the data is distributed on two dimensions as a circumference: it can be actually represented by one dimension, but PCA is not able to capture it.