LTAT.02.004 Machine Learning II

Affine data projections

based on normal distribution

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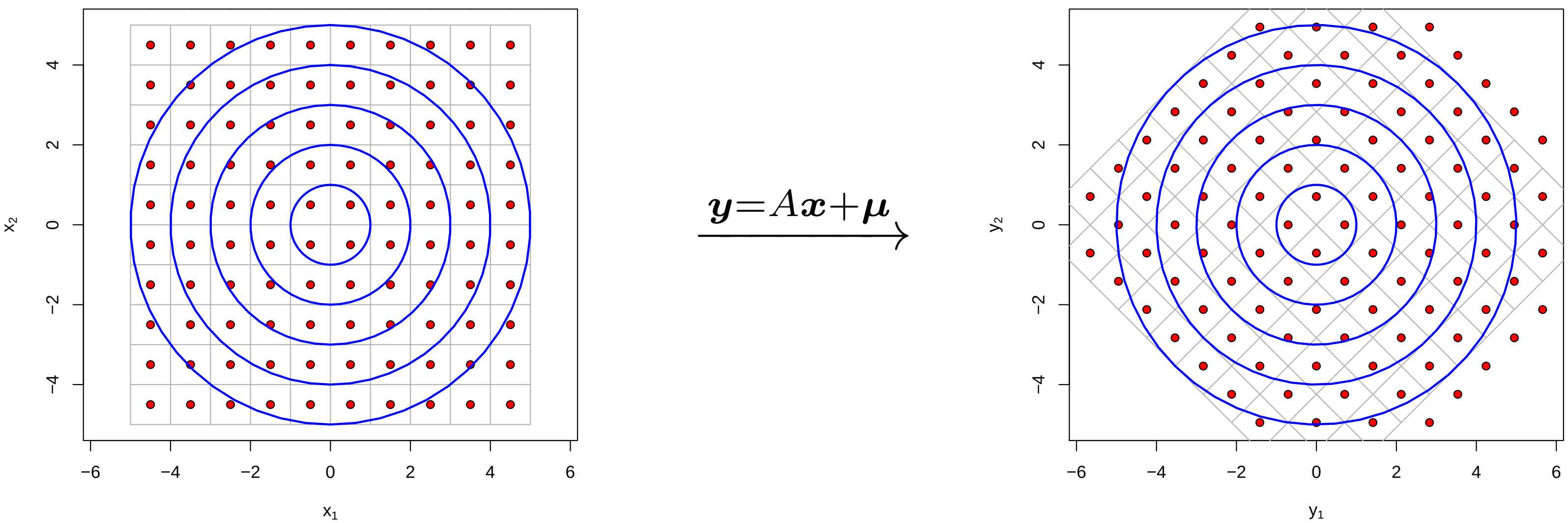
Principal component analysis

Distribution reconstruction task

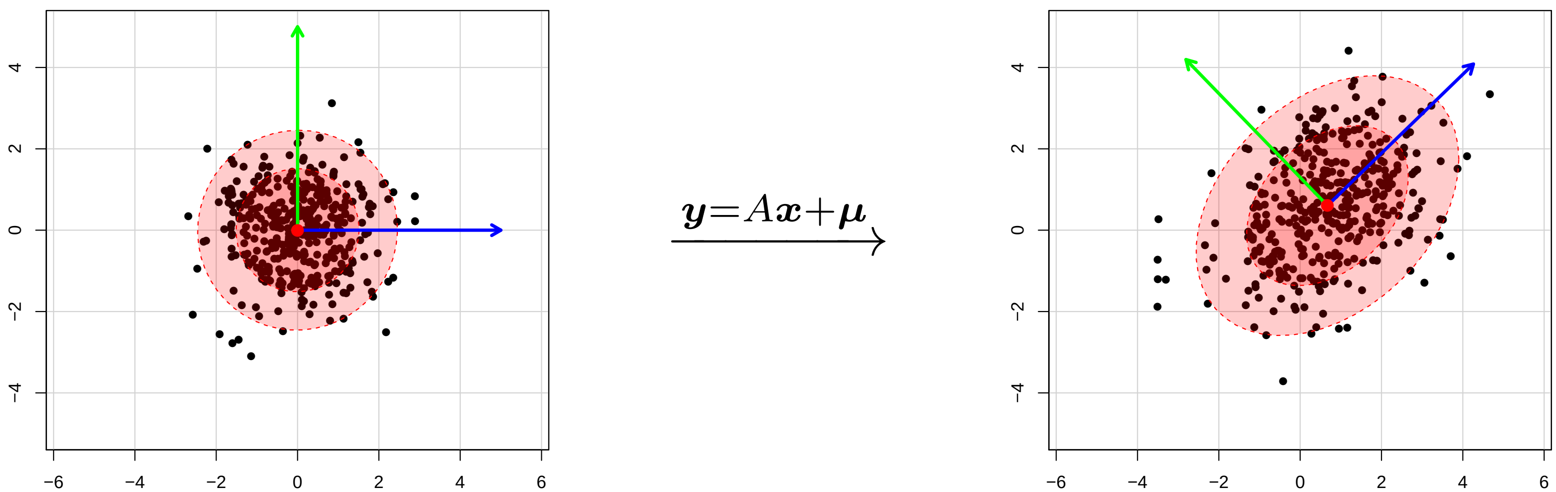
Original goal. Given the set of observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ determine the affine transformation $\boldsymbol{y} = A\boldsymbol{x} + \boldsymbol{\mu}$ and original source signals $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$.

Impossibility result. The matrix A can be recovered *only* up to rotations.



Simplified distribution reconstruction task

Achievable goal. Given the set of observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ determine the affine transformation by fixing the centre and axis of the ellipsoid.



- ▷ We need to find the origin and semi-axes $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ of the ellipsoid.
- ▷ Unit vectors $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n$ are mapped to semi-axes $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ of ellipsoid.

Variance for a fixed direction

Fact. Ortogonal projection onto a unit vector $\boldsymbol{w}$ is given by scalar product.

Question. What is the direction $\boldsymbol{w}$ that maximises the variance for ellipsoid?

$$\mathbf{Var}(\boldsymbol{w}^T \operatorname{diag}(\boldsymbol{a})\boldsymbol{x}) = \mathbf{Var}\left(\sum_{i=1}^{n} w_i a_i x_i\right) = \sum_{i=1}^{n} w_i^2 a_i^2 \ .$$

The variance is maximised in the direction of the longest ellipse axis a_1.

Question. How is the center of the ellipsoid and mean values connected?

$$\mathbf{E}(A\boldsymbol{x} + \boldsymbol{\mu}) = \mathbf{E}(A\boldsymbol{x}) + \mathbf{E}(\boldsymbol{\mu}) = \boldsymbol{\mu} \ .$$

Principal component analysis

- ▷ Compute the average value of the observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$:

$$\hat{\boldsymbol{\mu}} \leftarrow \frac{\boldsymbol{y}_1 + \cdots + \boldsymbol{y}_m}{m} \enspace .$$

- ▷ Centre the data by substituting $\hat{\boldsymbol{\mu}}$:

$$\boldsymbol{y}_i \leftarrow \boldsymbol{y}_i - \hat{\boldsymbol{\mu}}, \qquad i \in \{1, \ldots, m\} \enspace .$$

- ▷ Find the unit direction $\boldsymbol{w}_1$ that has *a maximal empirical* variance:

$$F(\boldsymbol{w}) = \mathbf{Var}(\boldsymbol{w}^T \boldsymbol{y}_1, \ldots, \boldsymbol{w}^T \boldsymbol{y}_n) = \frac{(\boldsymbol{w}^T \boldsymbol{y}_1)^2 + \cdots + (\boldsymbol{w}^T \boldsymbol{y}_m)^2}{m} \enspace .$$

- ▷ Find unit directions $\boldsymbol{w}_i$ orthogonal to previous directions that maximise the empirical variance of the corresponding the projection onto $\boldsymbol{w}_i$.

Covariance matrix and optimisation goal

We can use matrix algebra to simplify the variance estimate

$$\begin{aligned} F(\boldsymbol{w}) &= \frac{1}{m} \cdot \Bigl(\boldsymbol{w}^T \boldsymbol{y}_1 \boldsymbol{y}_1^T \boldsymbol{w} + \cdots + \boldsymbol{w}^T \boldsymbol{y}_m \boldsymbol{y}_m^T \boldsymbol{w}\Bigr) \\ &= \boldsymbol{w}^T \left(\frac{\boldsymbol{y}_1 \boldsymbol{y}_1^T + \cdots + \boldsymbol{y}_m \boldsymbol{y}_m^T}{m}\right) \boldsymbol{w} \end{aligned}$$

The $n \times n$ matrix in the middle is known as a *covariance matrix* Σ.

Due to the restriction $\|\boldsymbol{w}\|_2^2 = \boldsymbol{w}^T \boldsymbol{w} = 1$, we have to use Lagrange' trick:

$$F_*(\boldsymbol{w}) = \boldsymbol{w}^T \Sigma \boldsymbol{w} - 2\lambda \boldsymbol{w}^T \boldsymbol{w} \qquad \Rightarrow \qquad \frac{\partial F_*(\boldsymbol{w})}{\partial \boldsymbol{w}} = 2\Sigma \boldsymbol{w} - 2\lambda \boldsymbol{w} = \boldsymbol{0}.$$

Principal components as eigenvectors

The $F_*(\boldsymbol{w})$ is maximised only if the direction $\boldsymbol{w}$ is an *eigenvector* of Σ:

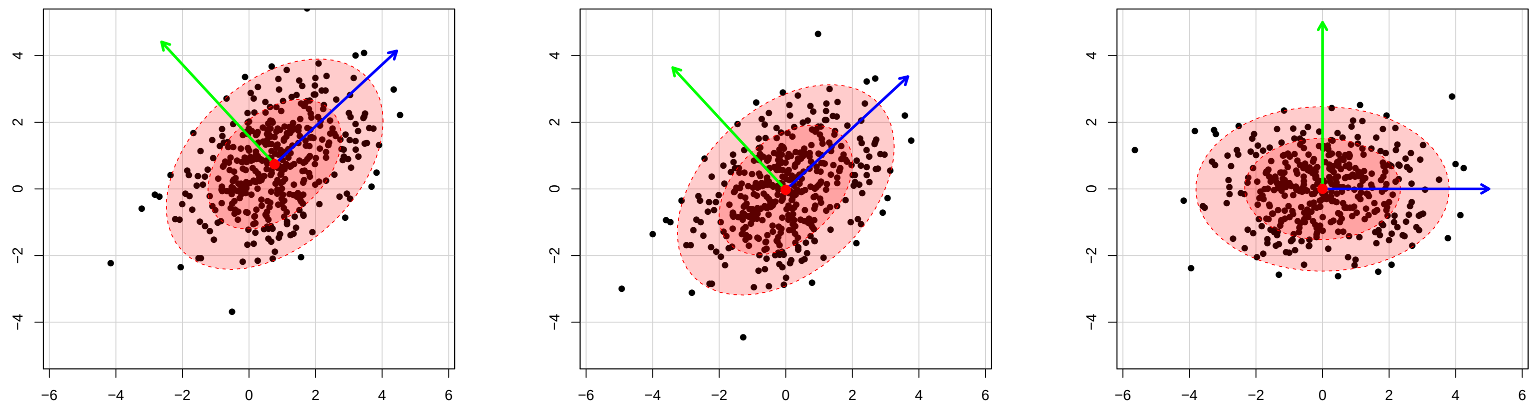
$$\Sigma\boldsymbol{w} = \lambda\boldsymbol{w} \qquad \Rightarrow \qquad \boldsymbol{w}^T\Sigma\boldsymbol{w} = \boldsymbol{w}^T\lambda\boldsymbol{w} = \lambda \ .$$

Fact. If $n \times n$ matrix is symmetric and positively definite then there exists n orthogonal eigenvectors $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_n$ with *eigenvalues* $\lambda_1 \geq \ldots \geq \lambda_n > 0$.

Corollary. Principal components corresponding to observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ are the eigenvectors of the covariance matrix Σ.

Principal component analysis as a rotation

Reconstruction of the source signal can be viewed as a *translation* followed by a *rotation* to orientate the ellipsoid wrt coordinate axis.



As vectors $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_n$ are orthogonal, the rotation can be done through computing projections (read scalar products):

$$\hat{\boldsymbol{x}}_i = (\boldsymbol{w}_1 || \cdots || \boldsymbol{w}_n)^T (\boldsymbol{y}_i - \hat{\boldsymbol{\mu}}_0) = W(\boldsymbol{y}_i - \hat{\boldsymbol{\mu}}) \ .$$

Maximum likelihood estimate

The algorithm formulated above was based on *ad hoc* reasoning:

▷ Empirical estimates for the mean and variance are not precise!

Theoretically correct way to handle the problem is

▷ obtain the maximum likelihood estimate on the model parameters,

▷ determine the translation and rotation based on the model parameters.

What are the model parameters?

▷ Parameters of the density formula Σ and $\boldsymbol{\mu}$.

▷ Parameters of the affine transformation A and $\boldsymbol{\mu}$.

Likelihood function under iid assumption

If all observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ are independent then

$$p[\boldsymbol{y}_i, \ldots, \boldsymbol{y}_m | \Sigma, \boldsymbol{\mu}] = \prod_{i=1}^{m} p[\boldsymbol{y}_i | \Sigma, \boldsymbol{\mu}]$$

where

$$p[\boldsymbol{y}_i | \Sigma, \boldsymbol{\mu}] = \frac{1}{(2\pi)^{n/2}} \cdot \frac{1}{\sqrt{\det(\Sigma)}} \cdot \exp\left(-\frac{(\boldsymbol{y}_i - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y}_i - \boldsymbol{\mu})}{2}\right)$$

The *log-likelihood* of the data $\ln p[\boldsymbol{y}_i, \ldots, \boldsymbol{y}_m | \Sigma, \boldsymbol{\mu}]$ can be expressed

$$\mathcal{L}(\Sigma, \boldsymbol{\mu}) = const + \frac{m}{2} \cdot \ln\det(\Sigma^{-1}) - \sum_{i=1}^{m} \frac{(\boldsymbol{y}_i - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y}_i - \boldsymbol{\mu})}{2}$$

Now we have to find the arrangement $(\Sigma, \boldsymbol{\mu})$ that maximises $\mathcal{L}(\Sigma, \boldsymbol{\mu})$.

Gradients of the log-likelihood function

Gradient with respect to the shift $\boldsymbol{\mu}$:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}} = -\sum_{i=1}^{m} \frac{\partial}{\partial \boldsymbol{\mu}} \frac{(\boldsymbol{y}_i - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y}_i - \boldsymbol{\mu})}{2} = -\sum_{i=1}^{m} \frac{\Sigma^{-1}(\boldsymbol{y}_i - \boldsymbol{\mu})}{2} \cdot (-1)$$

Gradient with respect to the inverse matrix Σ^{-1}:

$$\frac{\partial \mathcal{L}}{\partial (\Sigma^{-1})} = \frac{m}{2} \cdot \frac{\partial}{\partial (\Sigma^{-1})} \ln \det(\Sigma^{-1}) - \sum_{i=1}^{m} \frac{\partial}{\partial (\Sigma^{-1})} \frac{(\boldsymbol{y}_i - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y}_i - \boldsymbol{\mu})}{2}$$

$$= \frac{m}{2} \cdot \Sigma^T - \sum_{i=1}^{m} \frac{(\boldsymbol{y}_i - \boldsymbol{\mu})^T (\boldsymbol{y}_i - \boldsymbol{\mu})}{2}$$

As Σ is symmetric and Σ^{-1} exists we can derive closed form solutions.

Maximum likelihood estimates for parameters

The shift must be the mean of all observations

$$\boldsymbol{\mu} = \frac{1}{m} \cdot \sum_{i=1}^{m} \boldsymbol{y}_i \enspace .$$

The covariance matrix

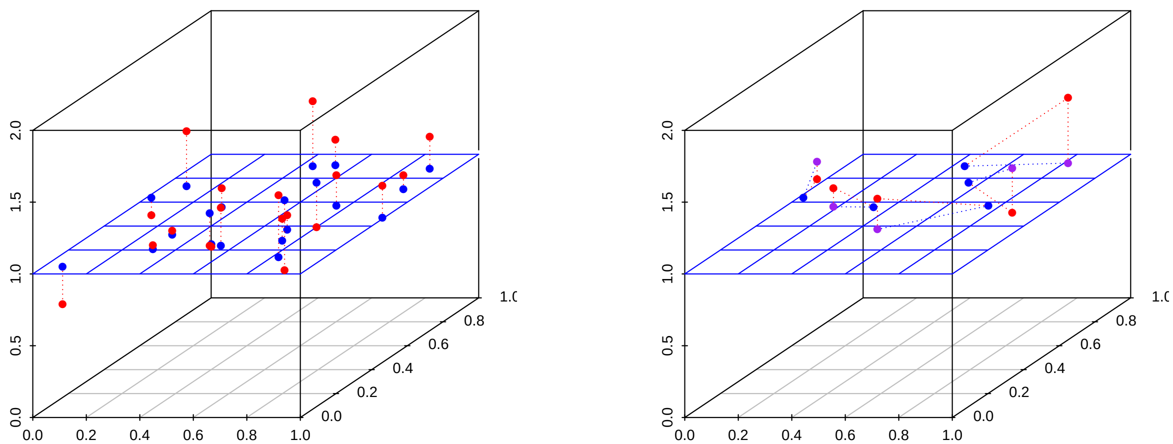
$$\Sigma = \frac{1}{m} \cdot \sum_{i=1}^{m} (\boldsymbol{y}_i - \boldsymbol{\mu})^T (\boldsymbol{y}_i - \boldsymbol{\mu})$$

Correctness of PCA. As ML estimates are exactly the same we used in principal component analysis, the method is theoretically justified!

Principal component analysis
Alternative formalisations

Dimensionality reduction

What if the actual data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$ lies in a lower-dimensional plane and the observation $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ are obtained by random shifts?



The shifts can be either orthogonal to the plane or just random. The first model is easier to analyse while the second is more plausible.

Maximum likelihood estimate

Let $\mathcal{H}$ be the plane. Assume that the random shifts ε_i are orthogonal to the plane and have a normal distribution $\mathcal{N}(0, \sigma I)$. Then

$$p[\boldsymbol{y}_i|\mathcal{H}, \sigma] = const \cdot \exp\left(-\frac{d_i^2}{2\sigma^2}\right)$$

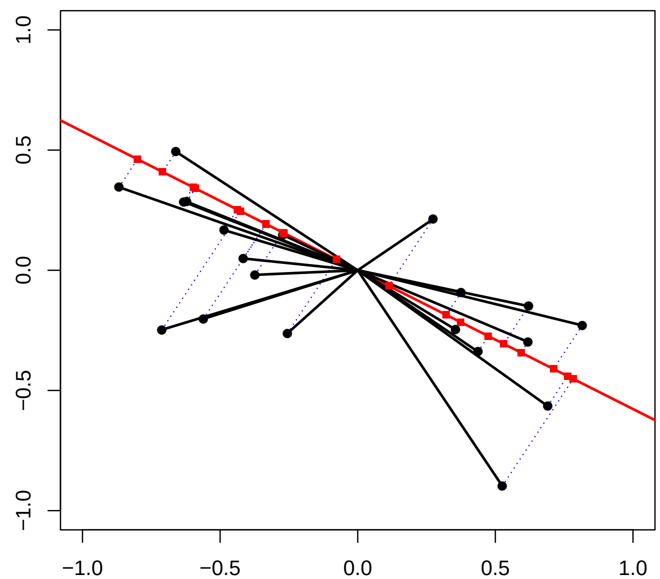
where d_i is the distance between the plane $\mathcal{H}$ and the point $\boldsymbol{y}_i$. Thus

$$p[\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m|\mathcal{H}, \sigma] = const \cdot \exp\left(-\sum_{i=1}^{m}\frac{d_i^2}{2\sigma^2}\right)$$

and the maximum likelihood estimate of the plane minimises sum of the distance squares. Corresponding estimates of $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$ are projections of $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m$ to the plane $\mathcal{H}$.

Another characterisation of PCA

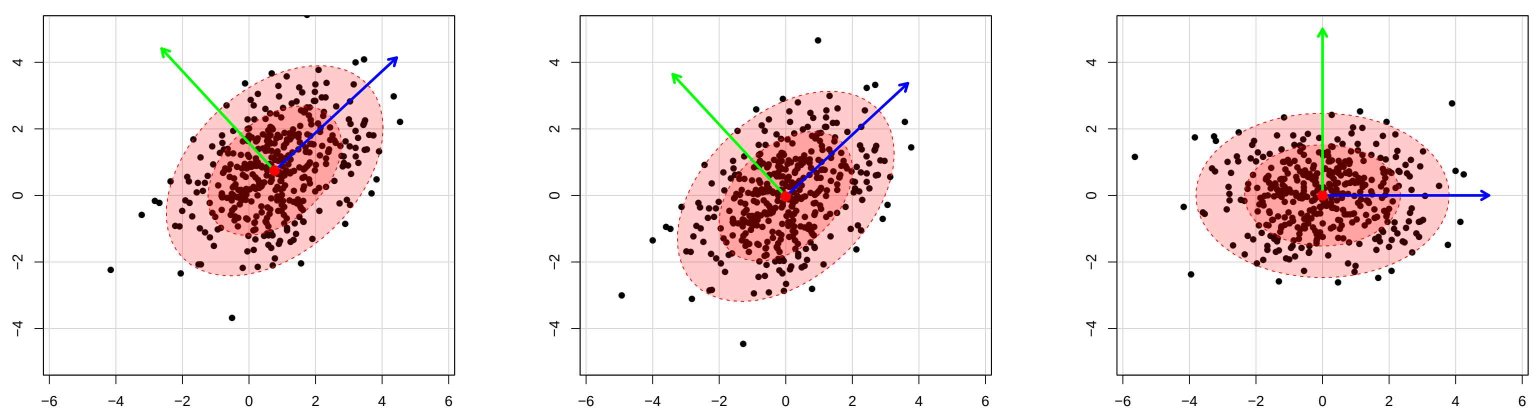
Fact. If the data is centred then PCA chooses the direction $\boldsymbol{w}_1$ such that the sum of squares of the projections $\boldsymbol{w}_1^T \boldsymbol{y}_i$ is maximal.



Corollary. PCA chooses directions $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_n$ such that the sum of distance squares from the hyperplane formed by $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_k$ is minimal.

PCA as a dimensionality reduction tool

Corollary. PCA rotates the data such way that first k coordinates of the rotated data correspond to maximum likelihood reconstructions of original vectors corrupted with white Gaussian noise $\mathcal{N}(0, \sigma I)$.



Alternatively, we can view the last components of the source signal $\boldsymbol{x}$ as the uninformative noise. The overall noise component should be small.