

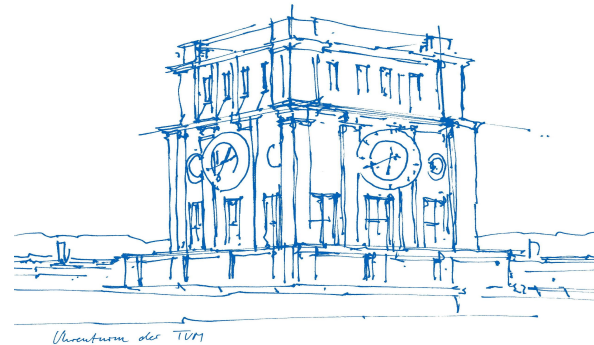
The multivariate normal distribution

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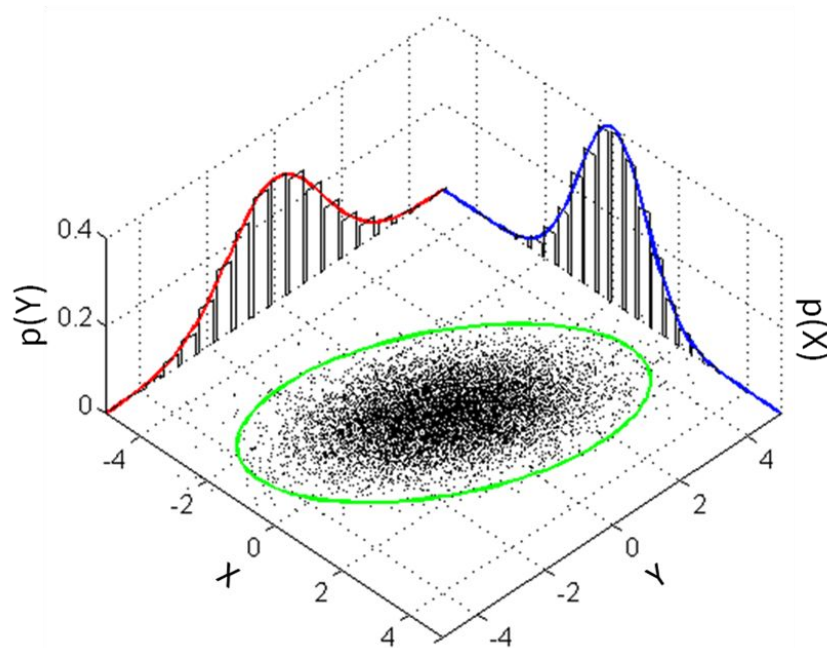
www.gagneurlab.in.tum.de

To understand the genetic basis of gene regulation and its implication in diseases



An important distribution

- The multivariate normal distribution (MVN, also called multivariate Gaussian) is the multivariate generalization of the normal distribution
- It often arises due to the central limit theorem
- It is the workhorse of a large set of statistical methods
- This lecture overviews its most important properties



Multivariate Normal Distribution (source: Wikipedia)

Definition

- We consider the joint distribution of p scalar random variables

$$\mathbf{x} = (x_1, \dots, x_p)^\top$$

- MVN probability density

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\}$$

- Mean vector

$$\boldsymbol{\mu} = (\mu_1, \dots, \mu_p)^\top$$

- Covariance matrix

$$\begin{aligned} \sigma_{i,j} &= \mathbb{E}[(x_i - \mu_i)(x_j - \mu_j)] \\ &= \rho_{i,j} \sigma_i \sigma_j \end{aligned}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & & & & \\ & \ddots & & & \\ & & \sigma_{i,j} & \sigma_i^2 & \\ & & & \ddots & \\ & & & & \sigma_p^2 \end{pmatrix}$$

Special case: Independent Gaussian variables

- For MVNs, Pearson correlation = 0 is equivalent to independence

$$\rho_{i,j} = 0 \iff x_i \perp\!\!\!\perp x_j$$

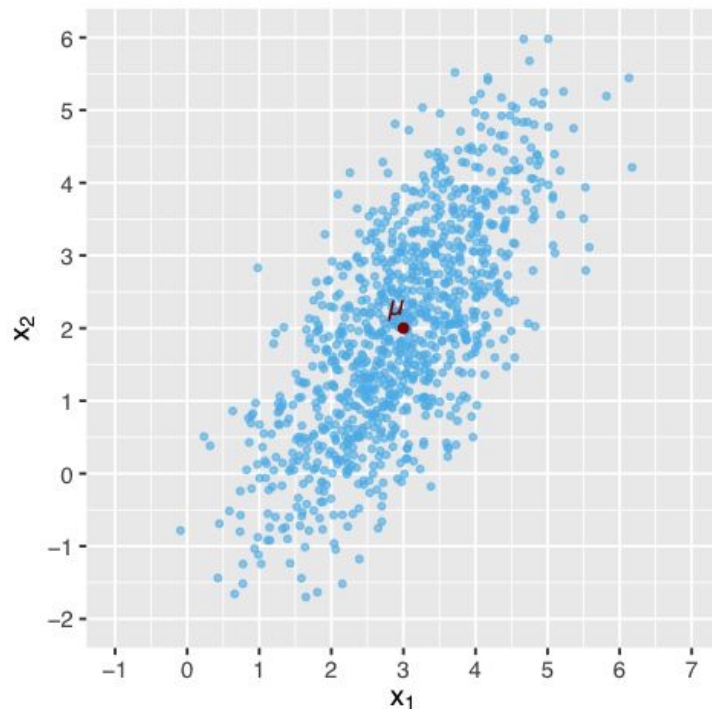
- Independent univariate Gaussian can be jointly modeled as:

$$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & \\ & & \ddots & \\ & & & \sigma_n^2 \end{pmatrix}$$

Density

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\}$$



1,000 random draws with

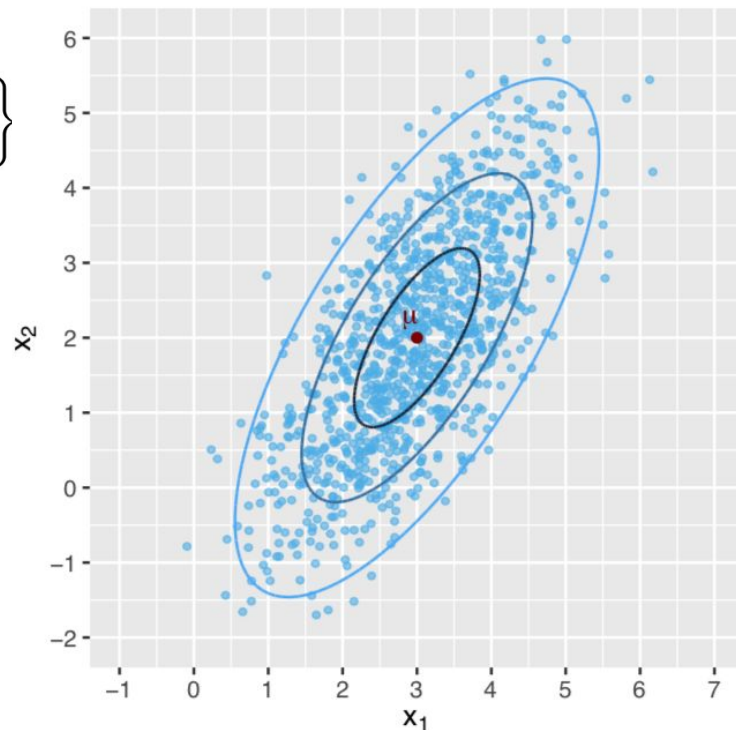
$$\boldsymbol{\mu} = (3, 2)^\top \quad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$$

Surfaces of equi-likelihood are ellipsoids

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\}$$

- Squared Mahalanobis distance

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})$$



1,000 random draws with

$$\boldsymbol{\mu} = (3, 2)^\top \quad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$$

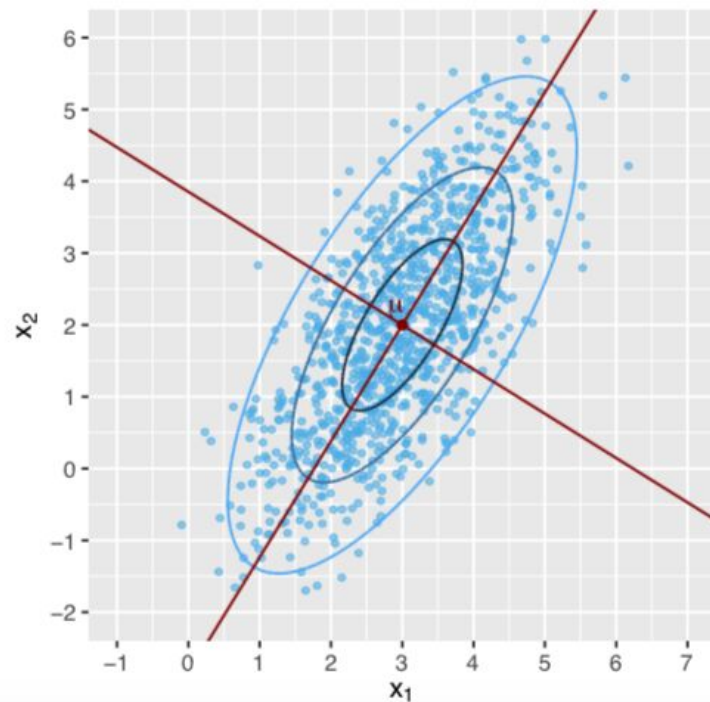
Eigendirections of the covariance

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\}$$

- Squared Mahalanobis distance

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})$$

- The covariance matrix is symmetric positive definite
- The axes are the eigendirections of the covariance



1,000 random draws with

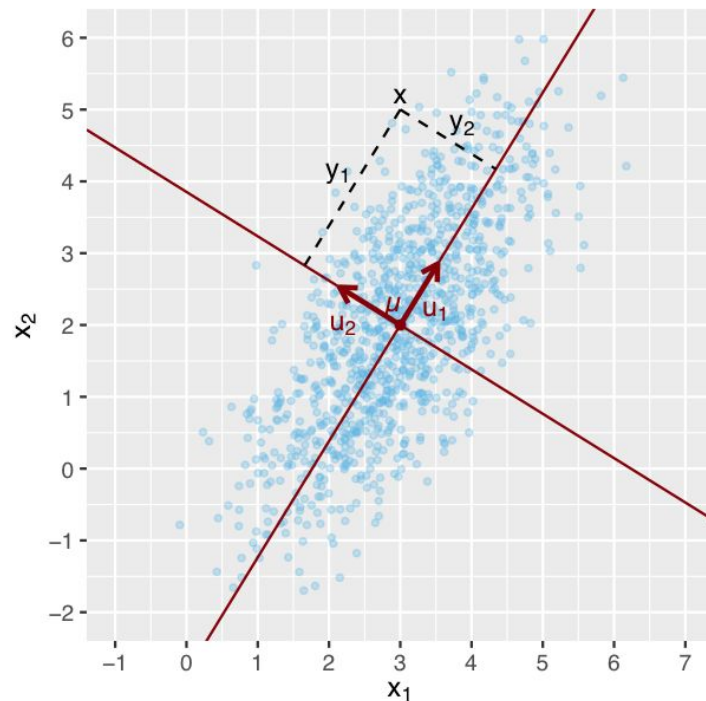
$$\boldsymbol{\mu} = (3, 2)^\top \quad \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$$

Independence of transformed coordinates

- Eigenvalues $\lambda_1 > \dots > \lambda_p$
- Eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_p$
- Transformed coordinates $y_i = \mathbf{u}_i^\top (\mathbf{x} - \boldsymbol{\mu})$
- MVN and independence

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y} | \mathbf{0}, \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_p \end{pmatrix})$$

- This transformation is used in data analysis (Principal Component Analysis), even for non-Gaussian data



Conclusion

- MVN probability density $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{p/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right\}$
- Geometry
- Transformed variables
- Details in Bishop, CM. 2007 (Springer)
Pattern Recognition and Machine Learning

