Pattern Recognition: Probability Theory

Sandro Schönborn

Department of Mathematics and Computer Science
University of Basel

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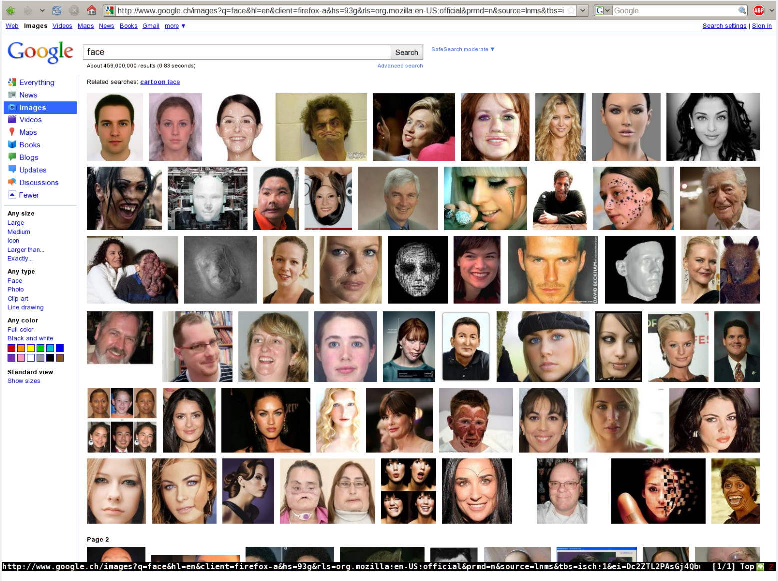
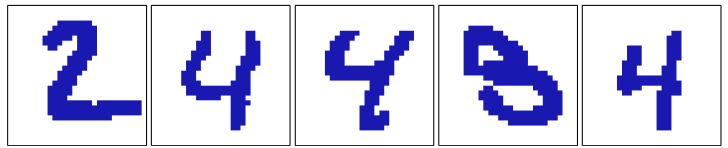
Variability

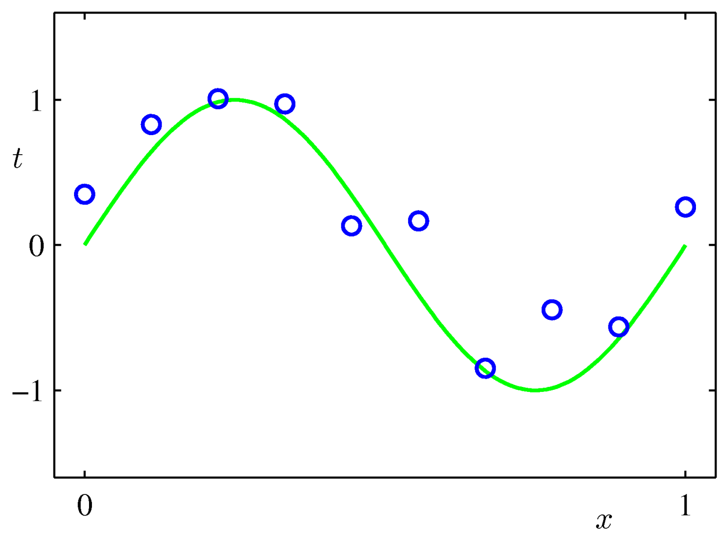


Variability



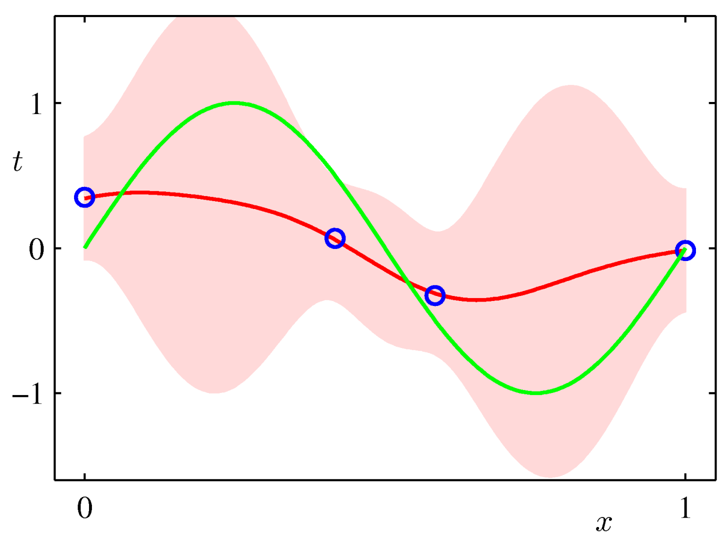
Bishop 2009

Noise



Bishop 2009

Uncertainty



Bishop 2009

Motivation

Why do we need probability theory??

Probability and Statistics

To model

- Variability of pattern itself
- Variability of measurement / context (noise)
- Uncertainty in our models and methods

$\Rightarrow$ A short repetition of probability theory

- First Part: Dry theory $\rightarrow$ quick reference for you
- Second Part: Multivariate Gaussian serving as example

Discrete Random Variables

Random Variable X with possible Realisations $x \in \{1, 2, 3, \ldots\}$:

Cummulative Distribution Function (cdf)

$$P[X < x] = F(x)$$

Probability Mass Function

$$P[X = x] = P_x$$

Normalisation and Positivity

$$\sum_x P_x = 1 \qquad P_x \geq 0$$

Discrete Random Variables — Examples

Binomial – A coin flip

$$x \in \{0, 1\}$$

$$P_0 = P[X = 0] = p, \qquad P_1 = P[X = 1] = q$$

$$p \in [0, 1], \quad q = 1 - p$$

Poisson – Rare events

$$x \in \{0, 1, 2, \ldots\}$$

$$P_x = P[X = x] = \frac{\lambda^x e^{-\lambda}}{x!}$$

$\lambda > 0$: Rate of events occuring per interval

Continouos Random Variables

Random Variable X with possible Realisations $x \in \mathbb{R}$:

Cummulative Distribution function (cdf)

$$F(x): \qquad P[X < x] = F(x)$$

Probability Density Function (pdf)

$$p(x): \qquad P[x < X < x + \mathrm{d}x] = p(x)\,\mathrm{d}x \qquad = \mathrm{d}F(x)$$

Normalisation and Positivity

$$\int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1 \qquad p(x) \geq 0$$

Continuous Random Variables — Examples

Gaussian

$$X \sim \mathcal{N}(\mu, \sigma^2), \quad x \in \mathbb{R}$$

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Mean μ, Variance σ^2 ▸ Examples

Gamma Distribution

$$X \sim \Gamma(k, \theta), \quad x \in [0, \infty)$$

$$p(x) = x^{k-1} \frac{e^{-\frac{x}{\theta}}}{\Gamma(k)\theta^k}$$

Shape $k > 0$, Scale $\theta > 0$

Mean

- The mean is a measure for *central tendency*

Expected Value, Mean, Expectation

$$E[X] = \sum_x x P_x \qquad E[X] = \int x p(x)\,\mathrm{d}x$$

Linearity

$$E[aX + bY] = a\ E[X] + b\ E[Y]$$

a, b Real *constants*,
X, Y Random variables (same space)

Variance

- The variance is a measure for *spread*

Variance / Standard Deviation

$$V[X] = E[(X - E[X])^2]$$
$$\mathrm{sd}[X] = \sigma_X = \sqrt{V[X]}$$

Hint: $V[X] = E[X^2] - E[X]^2$

Properties

$$V[aX + bY] = a^2 V[X] + b^2 V[Y] + 2ab\ \mathrm{Cov}(X, Y)$$

Mean and Variance — Examples

Binomial

$$E[X] = q$$

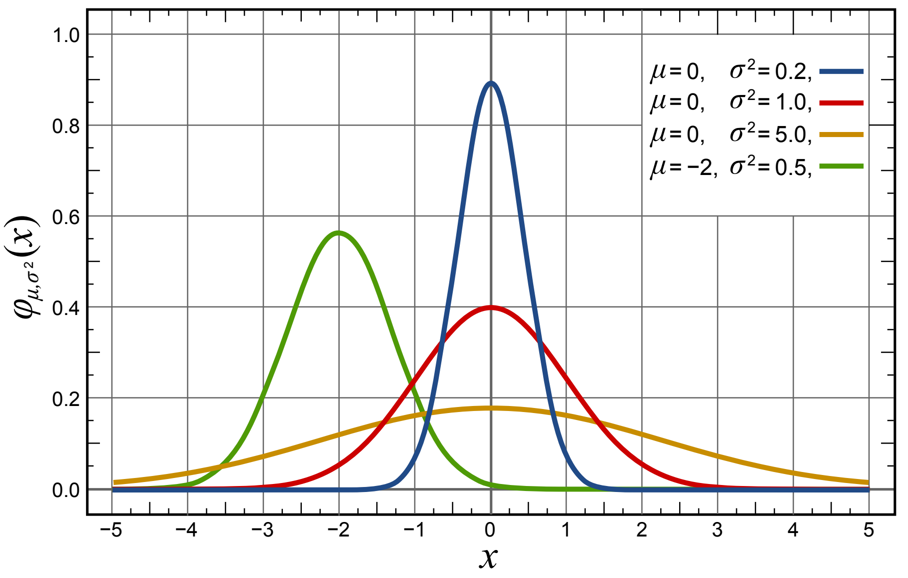
$$V[X] = q(1-q) = p(1-p)$$

Gaussian

$$E[X] = \mu$$

$$V[X] = \sigma^2$$

Example: Gaussian



Example

More than one Random Variable, e.g.

Length L and Weight W of a fish

$$\vec{X} = [L, W]^{\mathsf{T}}$$

Joint Probability

$$P[X = x \ \wedge \ Y = y] = P_{xy}$$

$$P[x < X < x + \mathrm{d}x \ \wedge \ y < Y < y + \mathrm{d}y] = p(x, y)\,\mathrm{d}x\,\mathrm{d}y$$

Marginals and Conditionals

Marginalisation

$$P[X = x] = \sum_y P[X = x, Y = y]$$

$$p(x) = \int p(x, y) \, \mathrm{d}y$$

Conditional Probability

$$P[X = x \mid Y = y] = \frac{P[X = x, Y = y]}{P[Y = y]} \qquad P[Y = y] > 0$$

$$p(x \mid y) := \frac{p(x, y)}{p(y)}$$

Bayes' Rules

Use the factorization for the joint probability density / distribution:

$$p(x, y) = p(x \mid y)\; p(y)$$

$$p(x, y) = p(y \mid x)\; p(x)$$

Bayes' Rule

$$P_{x|y} = \frac{P_{y|x} P_x}{P_y}$$

$$p(x \mid y) = \frac{p(y \mid x) p(x)}{p(y)}$$

- *Bayesian talk*: "Prior adapted to data leads to posterior"

Covariance and Independence

Covariance

$$\mathrm{Cov}(X,Y) = E[(X - E[X])\ (Y - E[Y])]$$
$$\mathbf{\Sigma}(\mathbf{X}) = E[(\mathbf{X} - E[\mathbf{X}])(\mathbf{X} - E[\mathbf{X}])^{\mathsf{T}}]$$

Independence

$$p(x,y) = p(x)p(y) \iff X \text{ and } Y \text{ are independent}$$

Covariance $\neq$ Independence

$$X \text{ and } Y \text{ are independent, } X \perp Y \implies \mathrm{Cov}(X,Y) = 0$$

Multivariate Gaussian Distribution

- This distribution occurs very frequently
  - Central Limit Theorem
  - Maximum Entropy Principle
  - Ease of use
- Simple enough to demonstrate these concepts

Multivariate Gaussian Distribution

$$p\left(\vec{x}\right) = \frac{1}{\sqrt{(2\pi)^d \det\left(\mathbf{\Sigma}\right)}} \exp\left(-\frac{1}{2}\left(\vec{x}-\vec{\mu}\right)^{\mathsf{T}} \mathbf{\Sigma}^{-1} \left(\vec{x}-\vec{\mu}\right)\right)$$

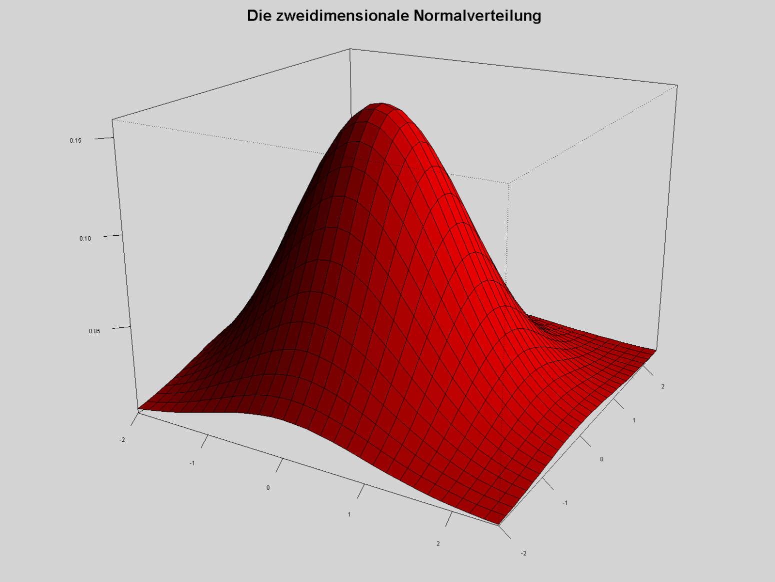
$\vec{\mu}$ Mean

$\mathbf{\Sigma}$ Covariance Matrix ($d \times d$, positive definite, symmetric)

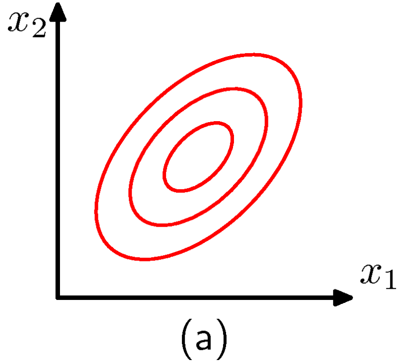
d Number of dimensions

$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$

2D Gaussian — Surface Plot



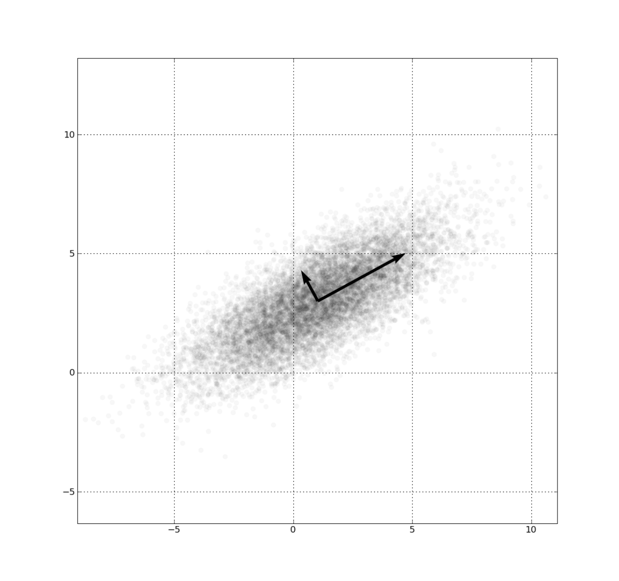
2D Gaussian — Contour Plot



- Points on a contour have equal probability density - *equidensity* lines
- Contours are ellipsoids

Figure: Bishop 2009

2D Gaussian — Samples / Scatter



Equidensity lines are Ellipsoids

- The ellipsoids are determined by the quadratic form

$$(\vec{x} - \vec{\mu})^{\mathsf{T}} \mathbf{\Sigma}^{-1} (\vec{x} - \vec{\mu})$$

- $\mathbf{\Sigma}$ is positive definite and symmetric $\Rightarrow$ Ellipsoid
- Center at $\vec{\mu}$
- Eigenvectors and eigenvalues of Σ

$$\mathbf{\Sigma}\vec{e}_i = \lambda_i \vec{e}_i$$

- Direction of semi-axes is determined by eigenvectors $\vec{e}_i$
- λ_i measures the variance along the corresponding eigendirection $\vec{e}_i$

Moments

Mean

$$E[\vec{X}] = \vec{\mu} \qquad E[X_i] = \mu_i$$

Covariance

$$V[\vec{X}] = \mathbf{\Sigma} \qquad \mathrm{Cov}(X_i, X_j) = \Sigma_{ij}$$

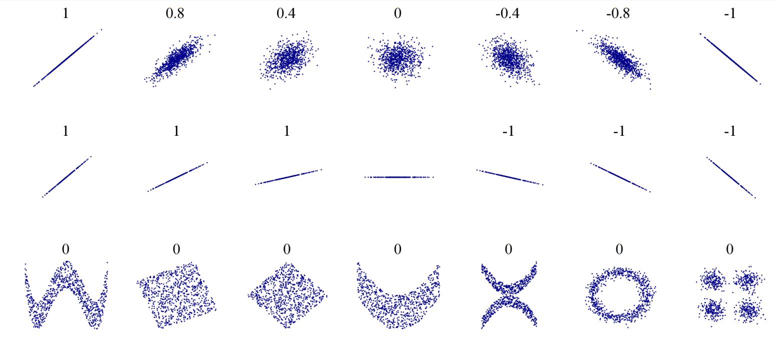
Correlation

$$\mathrm{Cor}(X_i, X_j) = \rho_{ij} = \frac{\mathrm{Cov}(X_i, X_j)}{\sigma_i \sigma_j} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}, \qquad \sigma_i = \sqrt{\Sigma_{ii}}$$

Correlation and Covariance

- Correlation measures strength of linear relations between variables
- It does not measure independence
- It does not tell you anything about causal relations
- Correlation is normalized and dimensionless

Example



Marginals

- Marginal: *Randverteilung*
- Removing unknown variables — *"projection"*
- $p(x) = \int p(x,y)dy$

Marginal of a Gaussian

$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$

$$\vec{X} = \begin{bmatrix} \vec{X}_a \\ \vec{X}_b \end{bmatrix}, \quad \vec{\mu} = \begin{bmatrix} \vec{\mu}_a \\ \vec{\mu}_b \end{bmatrix}, \quad \mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Sigma}_{aa} & \mathbf{\Sigma}_{ab} \\ \mathbf{\Sigma}_{ba} & \mathbf{\Sigma}_{bb} \end{bmatrix}$$

$$p(\vec{x}_a) = \mathcal{N}(\vec{x}_a \mid \vec{\mu}_a, \mathbf{\Sigma}_{aa})$$

Conditionals

- Conditional: *Bedingte Verteilung*
- Fixing a variable to a certain value — *"slices"*
- $p(x \mid y) = \dfrac{p(x, y)}{p(y)}$

Conditional of a Gaussian

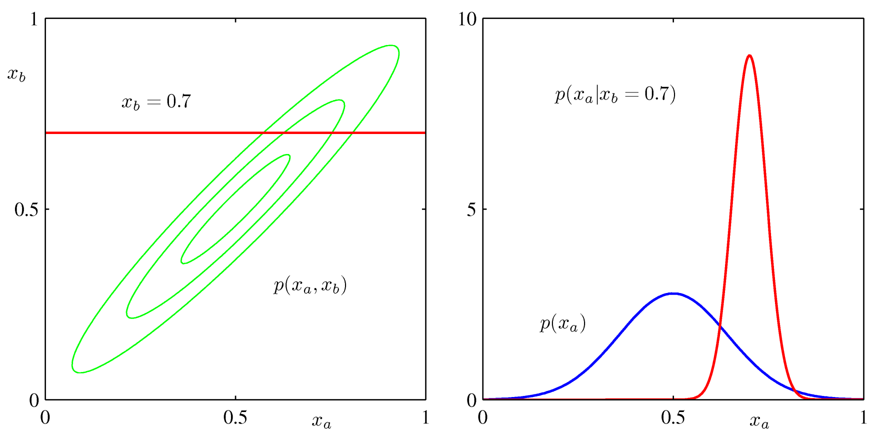
$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$

$$\vec{X} = \begin{bmatrix} \vec{X}_a \\ \vec{X}_b \end{bmatrix}, \quad \vec{\mu} = \begin{bmatrix} \vec{\mu}_a \\ \vec{\mu}_b \end{bmatrix}, \quad \mathbf{\Sigma} = \begin{bmatrix} \mathbf{\Sigma}_{aa} & \mathbf{\Sigma}_{ab} \\ \mathbf{\Sigma}_{ba} & \mathbf{\Sigma}_{bb} \end{bmatrix}$$

$$p(\vec{x}_a \mid \vec{X}_b = \vec{x}_b) = \mathcal{N}(\vec{x}_a \mid \vec{\mu}_{a|b}, \mathbf{\Sigma}_{a|b})$$

$$\begin{aligned} \vec{\mu}_{a|b} &= \vec{\mu}_a + \mathbf{\Sigma}_{ab}\mathbf{\Sigma}_{bb}^{-1}(\vec{x}_b - \vec{\mu}_b) \\ \mathbf{\Sigma}_{a|b} &= \mathbf{\Sigma}_{aa} - \mathbf{\Sigma}_{ab}\mathbf{\Sigma}_{bb}^{-1}\mathbf{\Sigma}_{ba} \end{aligned}$$

Marginal and Conditional of a Gaussian



Bishop 2009

Affine Transformations

- Gaussians are stable under affine transforms
- Affine transformation: $\vec{Y} = \mathbf{A}\vec{X} + \vec{b} \quad (\mathbf{A}$ and $\vec{b}$ are constant)

Affine Transform

$$\begin{aligned} \vec{X} &\sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma}) && \vec{X} \in \mathbb{R}^d \\ \vec{Y} &= \mathbf{A}\vec{X} + \vec{b} && \vec{Y} \in \mathbb{R}^n,\ \mathbf{A} \in \mathbb{R}^{n \times d},\ \vec{b} \in \mathbb{R}^n \end{aligned}$$

$$\vec{Y} \sim \mathcal{N}(\vec{y} \mid \vec{\mu}_Y, \Sigma_Y)$$

$$\begin{aligned} \vec{\mu}_Y &= \mathbf{A}\vec{\mu} + \vec{b} \\ \mathbf{\Sigma}_Y &= \mathbf{A}\mathbf{\Sigma}\mathbf{A}^{\mathsf{T}} \end{aligned}$$

Standard Normal

Univariate Standard Normal

$$X \;\sim \mathcal{N}(0, 1)$$

$$\mu = 0 \qquad \sigma = 1$$

Multivariate Standard Normal

$$\vec{X} \;\sim \mathcal{N}(0, \mathbf{I}_d)$$

$$\vec{\mu} = 0 \qquad \sigma = \mathbf{I}$$

Standardizing

- Transform a normal distributed variable X into a standard normal Z:
- Also called *whitening* or *Z transform / score*

Univariate

$$X \sim \mathcal{N}(\mu, \sigma^2) \quad \rightarrow \quad Z = \frac{X - \mu}{\sigma} \quad \rightarrow \quad Z \sim \mathcal{N}(0, 1)$$

Multivariate

$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma}) \quad \rightarrow \quad \vec{Z} = \mathbf{\Sigma}^{-\frac{1}{2}}(\vec{X} - \vec{\mu}) \quad \rightarrow \quad \vec{Z} \sim \mathcal{N}(0, \mathbf{I})$$

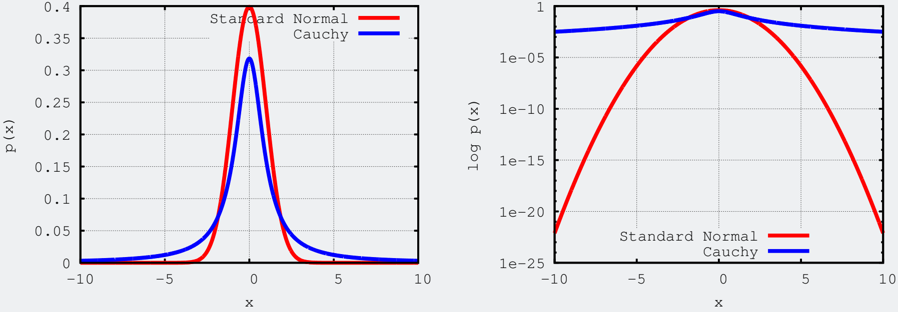
use $\mathbf{\Sigma} = \mathbf{U}\mathbf{D}^2\mathbf{U}^\mathsf{T} \Rightarrow \mathbf{\Sigma}^{\frac{1}{2}} = \mathbf{U}\mathbf{D}$

When to Stop using Gaussians

Gaussians are very handy and can be used in a lot of situations, but be careful if one of the these points applies to your problem:

- Gaussians do not have heavy tails
  - In many real world (empirical) distributions extreme events occur far more often than a Gaussian would allow
- Gaussians have only a single mode
  - Can use a mixture of Gaussians here (see lecture)
- The central limit theorem is only valid for sums of independent random variables
  - For products use a log-normal distribution
  - The variables need to have finite mean and variance
- If you only know the mean and you know nothing about the variance
  - Use an exponential distribution in this case (maximum entropy)

Heavy Tails



Standard Normal
Cauchy
p(x)
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−10
−5
0
5
10
x
log p(x)
1
1e−05
1e−10
1e−15
1e−20
1e−25
Standard Normal
Cauchy
−10
−5
0
5
10
x