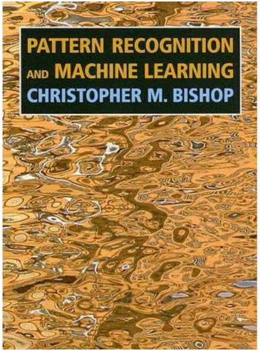
Probability Theory Refresher for Pattern Recognition Students

Dennis Madsen

Pattern Recognition vs Machine Learning



Bishop, Preface: *"Pattern recognition has its origins in engineering, whereas machine learning grew out of computer science. However, these activities can be viewed as two facets of the same field"*.

Motivation

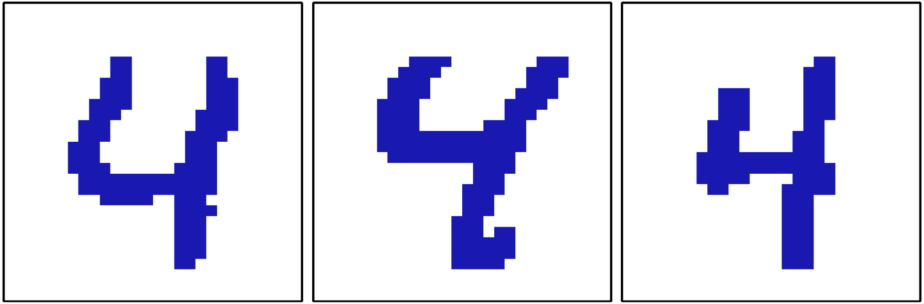
Why do we need probability theory???

Probability and Statistics

To model

- Variability of pattern itself
- Variability of measurement (noise)
- Uncertainty in our model

Variability of a pattern - Digit 4



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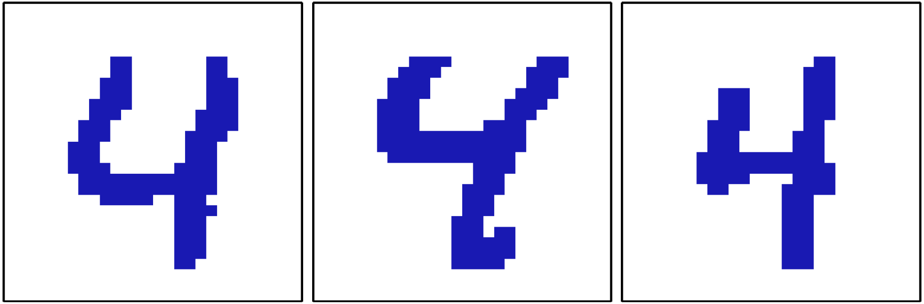
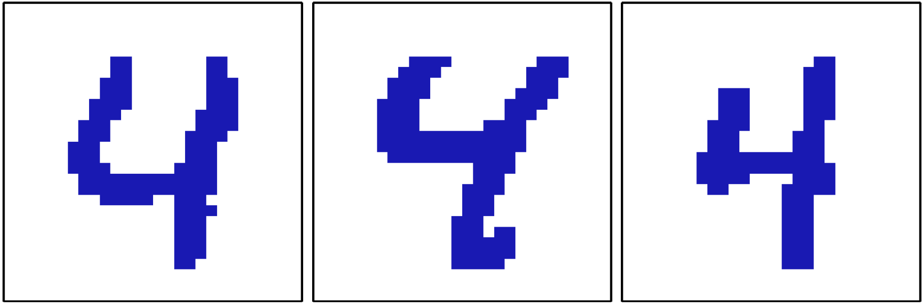


$$(10x10)^2 = 10.000$$

Variability of a pattern - Digit 4

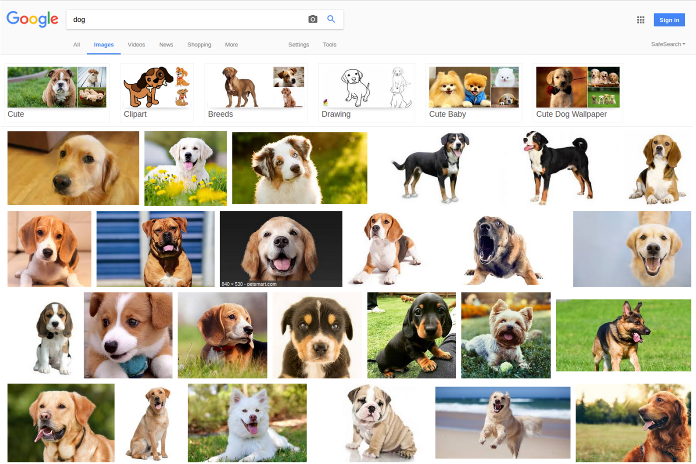


$$(10x10)^2 = 10.000$$

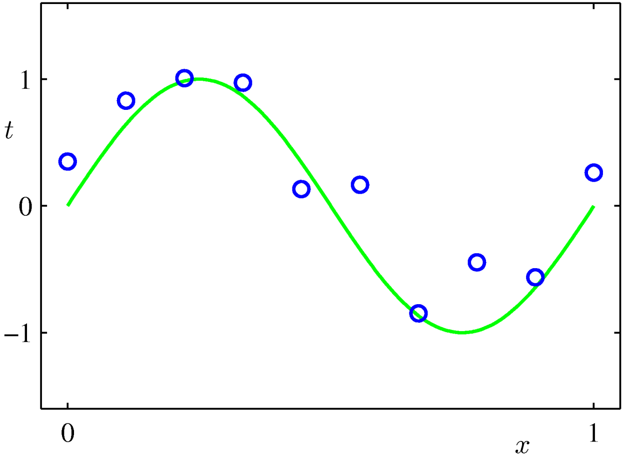
$$(200x200)^2 = 1.600.000.000$$

Bishop 2009

Variability of a pattern - Dog

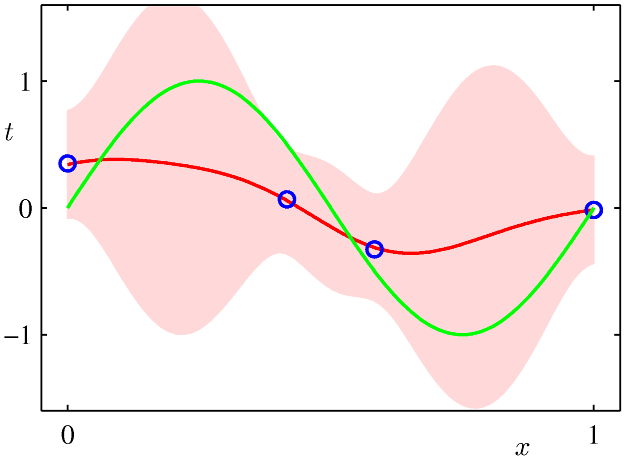


Variability of measurement (noise)



Bishop 2009

Uncertainty in the model



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$\Rightarrow$ A short repetition of probability theory in the context of pattern recognition

- First Part: Theory $\rightarrow$ quick reference for you
- Second Part: Multivariate Gaussian as an example

Basic Probability

Probability theory → chance

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Coin flip

$$P(Head) = \frac{\text{number of favourable outcoms}}{\text{total possible outcomes}} = \frac{1}{2}$$

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$$P(6) = \frac{1}{6}$$

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$$P(6) = \frac{1}{6} \qquad P(\tilde{6}) = 1 - P(6) = 1 - \frac{1}{6} = \frac{5}{6}$$

Sample space

Coin flip

$$coin \in \{head, tail\}$$

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Rolling a die and doing a Coin flip

$$mix \in \{1H, 2H, 3H, 4H, 5H, 6H, 1T, 2T, 3T, 4T, 5T, 6T\}$$

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Joint probability distribution $P(die, coin)$

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Joint probability distribution $P(die, coin)$

$$P(2T) = \frac{1}{12}, P(2) = \frac{2}{12} = \frac{1}{6}, P(H|5) = 0.5$$

Discrete Random Variables

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

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Probability Mass Function

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Normalization and Positivity

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

Binomial – A coin flip

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

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

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

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Probability Density Function (pdf)

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

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Normalisation and Positivity

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

Continuous Random Variables — Examples

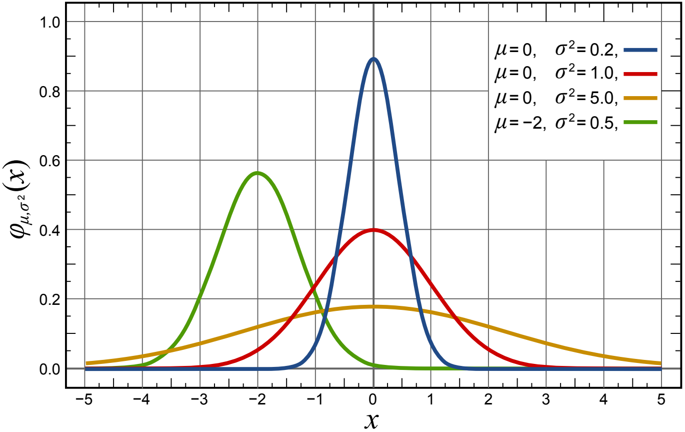
Gaussian (normal)

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

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

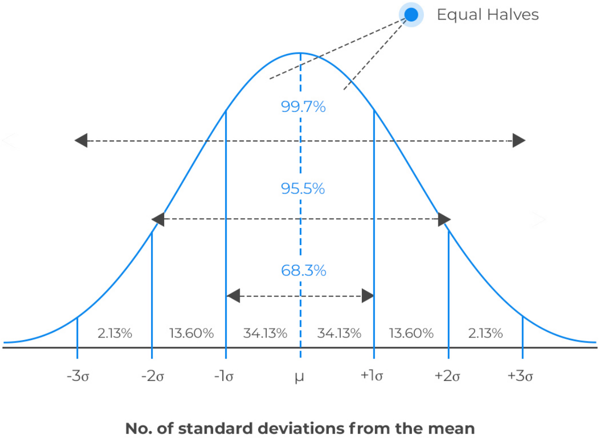
Mean μ, Variance σ^2

Example: Gaussian



wikipedia.org

Example: Gaussian Shape



analystprep.com

Mean

- The mean is a measure for **central tendency**

Expected Value, Mean, Expectation

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

Variance

- The variance is a measure for **spread**

Variance / Standard Deviation

$$V[X] = E[(X - E[X])^2]$$

$$\mathrm{sd}[X] = \sigma_X = \sqrt{V[X]}$$

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

Multivariate Case

Multiple Random Variables

Example

More than one Random Variable, e.g.

Length L and Weight W of an object

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

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Joint Probability

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

$$p(x, y)$$

Marginals and Conditionals

Marginalisation

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

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

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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:

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

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$$\Rightarrow \qquad P(\omega_i \mid \underline{x}) = \frac{p(\underline{x} \mid \omega_i) P(\omega_i)}{p(\underline{x})}$$

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

Covariance and Independence

Covariance

$$\mathrm{Cov}(X, Y) = E[(X - E[X])\,(Y - E[Y])]$$

$$\boldsymbol{\Sigma}(\mathbf{X}) = E[(\mathbf{X} - E[\mathbf{X}])(\mathbf{X} - E[\mathbf{X}])^\top]$$

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Independence

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

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Covariance $\neq$ Independence

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

Multivariate Gaussian (normal) Distribution

- This distribution occurs very frequently
- Simple enough to demonstrate these concepts

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Multivariate Gaussian Distribution

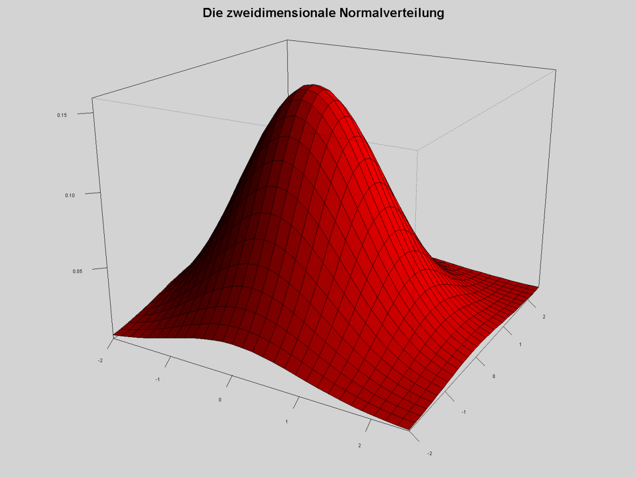
$$p(\vec{x}) = \frac{1}{\sqrt{(2\pi)^d \, |\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}(\vec{x}-\vec{\mu})^\top \mathbf{\Sigma}^{-1} (\vec{x}-\vec{\mu})\right)$$

$\vec{\mu}$	Mean
$\mathbf{\Sigma}$	Covariance Matrix ($d \times d$, positive definite, symmetric)
$\lvert\mathbf{\Sigma}\rvert$	Determinant of Σ
d	Number of dimensions

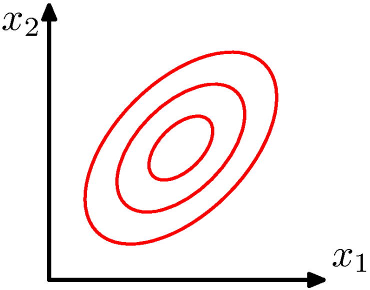
$$\vec{X} \sim \mathcal{N}(\vec{\mu}, \mathbf{\Sigma})$$

For the Multivariate normal distribution, $Cov(X, Y) = 0 \iff X \perp Y$.

2D Gaussian — Surface Plot



2D Gaussian — Contour Plot

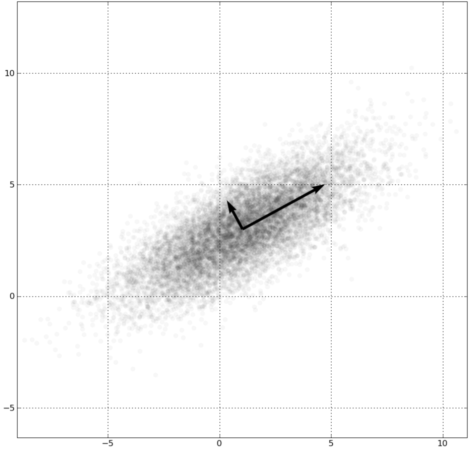


(a)

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

Figure: Bishop 2009

2D Gaussian — Samples / Scatter



Equidensity lines are Ellipsoids

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- Center at $\vec{\mu}$
- Eigenvectors and eigenvalues of $\boldsymbol{\Sigma}$

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

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

Moments of a Multivariate Gaussian Distribution

Mean

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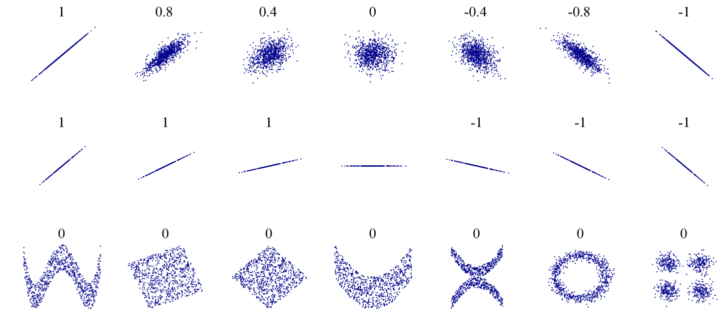
Correlation

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

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
- Covariance is in units obtained by multiplying the units of the two variables

Example



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- $p(x) = \int p(x, y) dy$

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Marginal of a Gaussian

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

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

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

Conditionals

- Conditional distribution
- Fixing a variable to a certain value — **"slices"**
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$$p(\vec{x}_a \mid \vec{X}_b = \vec{x}_b) = \mathcal{N}(\vec{x}_a \mid \vec{\mu}_{a|b}, \mathbf{\Sigma}_{a|b})$$

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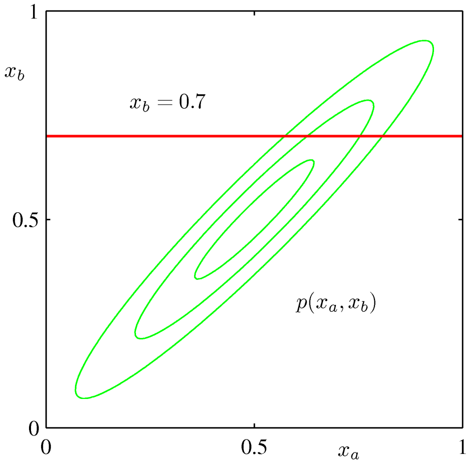
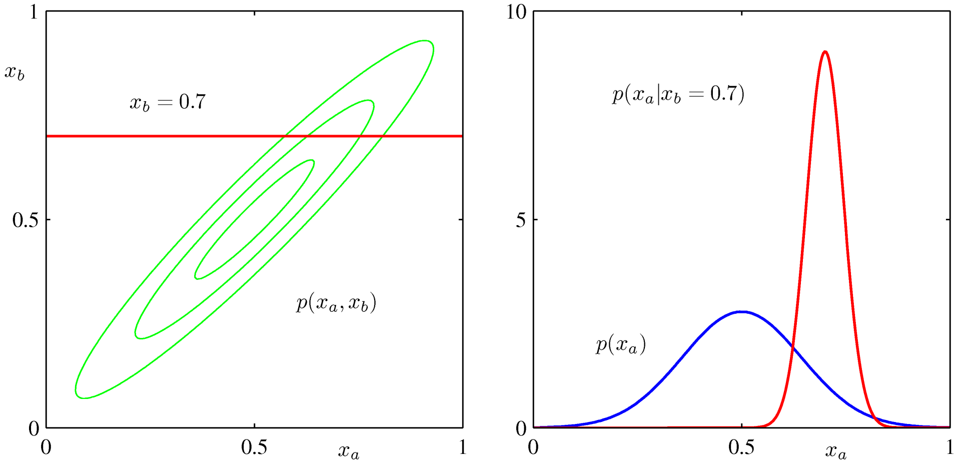
$$\begin{aligned} \vec{\mu}_{a|b} &= \vec{\mu}_a + \mathbf{\Sigma}_{ab}\mathbf{\Sigma}_{bb}^{-1}(\vec{x}_b - \vec{\mu}_b) \\ \mathbf{\Sigma}_{a|b} &= \mathbf{\Sigma}_{aa} - \mathbf{\Sigma}_{ab}\mathbf{\Sigma}_{bb}^{-1}\mathbf{\Sigma}_{ba} \end{aligned}$$

Marginal and Conditional of a Gaussian



Marginal and Conditional of a Gaussian



Bishop 2009

Affine Transformations

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

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Affine Transform

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

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

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

$$\vec{\mu}_Y = \mathbf{A}\vec{\mu} + \vec{b}$$
$$\boldsymbol{\Sigma}_Y = \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top$$

Standard Normal

Univariate Standard Normal

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

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

Multivariate Standard Normal

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

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

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- Transform a normal distributed variable X into a standard normal Z:
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Univariate

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

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- 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 $\mathbf{\Sigma} = \mathbf{U}\mathbf{D}^2\mathbf{U}^\top \Rightarrow \mathbf{\Sigma}^{\frac{1}{2}} = \mathbf{U}\mathbf{D}$

When to Stop using Gaussians

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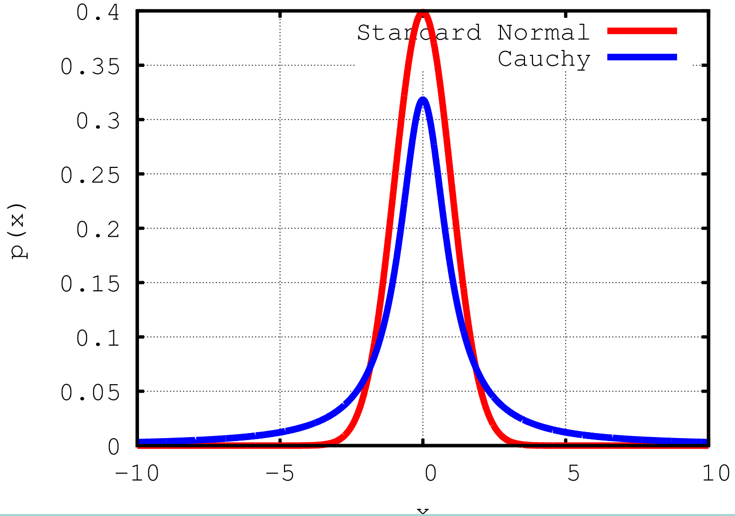
  - Can use a mixture of Gaussians here
- Gaussians do not have heavy tails
  - In many real world (empirical) distributions extreme events occur far more often than a Gaussian would allow

Heavy Tails



Standard Normal
Cauchy
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
p(x)
−10
−5
0
5
10
x

Credits:

- Sandro Schöenborn
- Adam Kortylewski