Statistical Geometry Processing

Winter Semester 2011/2012



Bayesian Statistics







Bayesian Statistics

Summary

- Importance
 - The only sound tool to handle uncertainty
 - Manifold applications: Web search to self-driving cars
- Structure
 - Probability: *positive, additive, normed* measure
 - Learning is density estimation
 - Large dimensions are the source of (almost) all evil
 - No free lunch: There is no universal learning strategy

Motivation

Modern Al

Classic artificial intelligence:

- Write a complex program with enough rules to understand the world
- This has been perceived as *not very successful*

Modern artificial intelligence

- Machine learning
- Learn structure from data
 - Minimal amount of "hardwired" rules
 - "Data driven approach"
- Mimics human development (training, early childhood)

Data Driven Computer Science

Statistical data analysis is everywhere:

- Cell phones (transmission, error correction)
- Structural biology
- Web search
- Credit card fraud detection
- Face recognition in point-and-shoot cameras

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Probability Theory

(a very brief summary)

Probability Theory

(a very brief summary)

Part I: Philosophy

What is Probability?

Question:

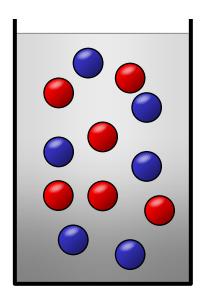
• What is probability?

Example:

- A bin with 50 red and 50 blue balls
- Person A takes a ball
- Question to Person B: What is the probability for *red*?

What happened:

- Person A took a blue ball
- Not visible to person B



Philosophical Debate...

An old philosophical debate:

- What does *"probability"* actually mean?
- Can we assign probabilities to events for which the outcome is already fixed? (but we do not know it for sure)

"Fixed outcome" examples:

- Probability for life on mars
- Probability for J.F. Kennedy having been assassinated by a intra-government conspiracy
- Probability that the code you wrote is correct

Two Camps

Frequentists' (traditional) view:

- Well defined experiment
- Probability is the relative number of positive outcomes
- Only meaningful as a mean of many experiments

Bayesian view:

- Probability expresses a degree of belief
- Mathematical model of uncertainty
- Can be subjective



Mathematical Point of View

Mathematics:

- Math does not tell you what is true
- It only tells you the *consequences* if you accept other assumptions (axioms) to be true
- Mathematicians don't do philosophy.

Mathematical definition of probability:

- Properties of probability measures
- Consistent with both views
- Defines rules for computing with probabilities
- Setting up probabilities is not a math problem

Probability Theory

(a very brief summary)

Part II: Probability Measures

Kolmogorov's Axioms

Discrete probability space:

- Elementary events:
- General *events*: Subsets $A \subseteq \Omega$
- *Probability* measure: $\Pr: \mathcal{P}(\Omega) \to \mathbb{R}$

A valid probability measure must ensure:

- Positive: $Pr(A) \ge 0$
- Additive: $[A \cap B = \emptyset] \Rightarrow [Pr(A) + Pr(B) = Pr(A \cup B)]$

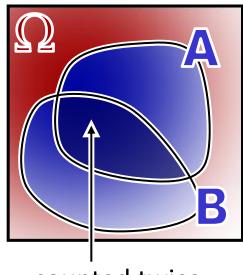
 $\Omega = \{\omega_1, ..., \omega_n\}$

• Normed: $Pr(\Omega) = 1$

Other Properties Follow

Properties derived from Kolmogorov's Axioms:

- $P(A) \in [0..1]$
- $P(\overline{A}) = P(\Omega \setminus A) = 1 P(A)$
- P(∅) = 0
- $Pr(A \cup B) = Pr(A) + Pr(B) Pr(A \cap B) \implies$



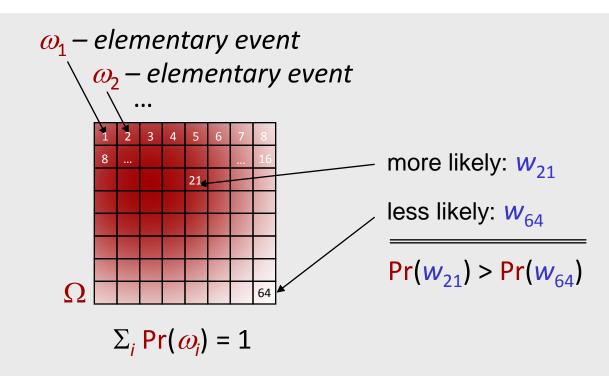
counted twice

Mathematical probability is a

- *non-negative, normed, additive* measure.
 - Always ≥ 0
 - Sums to 1
 - Disjoint pieces add up

Mathematical probability is a

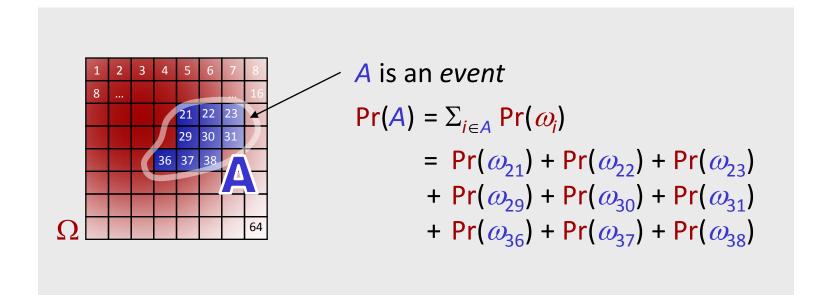
• non-negative, normed, additive measure.



• Think of a *density* on some domain Ω

Mathematical probability is a

• non-negative, normed, additive measure.



• Think of a *density* on some domain Ω

Mathematical probability is a

- non-negative, normed, additive measure.
 - Always ≥ 0
 - Sums to 1
 - Disjoint pieces add up

What does this model?

- You can always think of an area with density.
- All pieces are positive.
- Sum of densities is 1.

Discrete Models

Discrete probability space:

- Elementary events:
- General *events*: Subsets $A \subseteq \Omega$
- *Probability* measure: $\Pr: \mathcal{P}(\Omega) \to \mathbb{R}$

 $\Omega = \{ \omega_1, ..., \omega_n \}$

Probability measures:

• Sum of elementary probabilities

 $\Pr(A) = \sum_{\omega_i \in A} \Pr(\omega_i)$

Continuous Probability Measures

Continuous probability space:

- Elementary events: $\Omega \subseteq \mathbb{R}^d$
- General *events*:
- *Probability* measure:

"reasonable" $^{*)}$ subsets $A \subseteq \Omega$

measure: $\Pr: \sigma(\Omega) \to \mathbb{R}$ assigns probability to subsets^{*)} of Ω

*) not "all" subsets: Borel sigma algebra (details omitted)

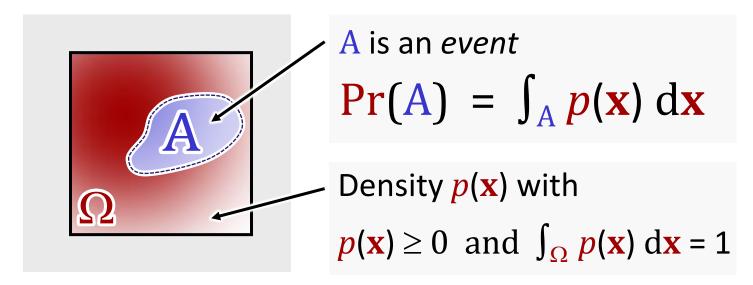
The same axioms:

- Positive: $Pr(A) \ge 0$
- Additive: $[A \cap B = \emptyset] \Rightarrow [Pr(A) + Pr(B) = Pr(A \cup B)]$
- Normed: $P(\Omega) = 1$

Continuous Density

Density model

- No elementary probabilities
- Instead: density $p: \mathbb{R}^d \rightarrow \mathbb{R}^{\geq 0}$

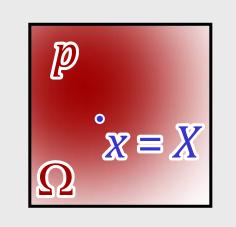


Random Variables

Random Variables

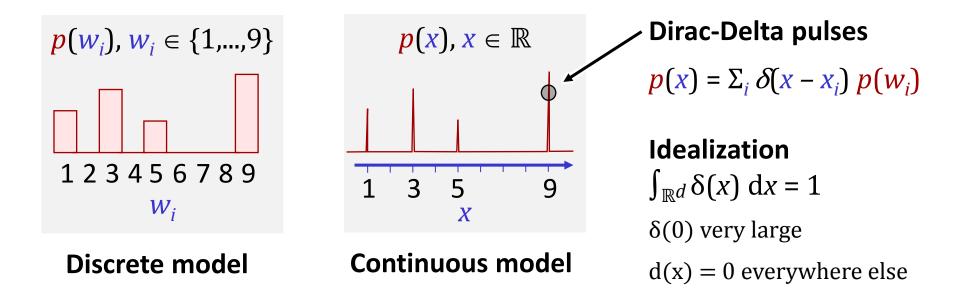
- Assign numbers or vectors from \mathbb{R}^d to outcomes
- Notation:
 - random variable X
 - density $p(x) = \Pr(X = x)$
- Usually:

Variable = domain of the density



Unified View

Discrete models as special case



Probability Theory

(a very brief summary)

Part III: Statistical Dependence

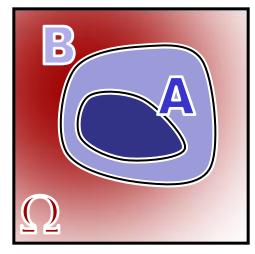
Conditional Probability

Conditional Probability:

- Pr(A | B) = Probability of A given B [is true]
- Easy to show:
 Pr(A∩B) = Pr(A | B) · Pr(B)

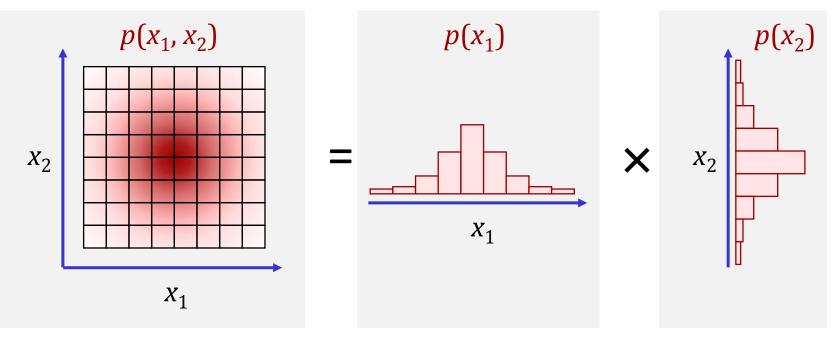
Statistical Independence

- A and B independent
 :⇔ Pr(A∩B) = Pr(A) · Pr(B)
- Knowing the value of A does not yield information about B (and vice versa)



Factorization

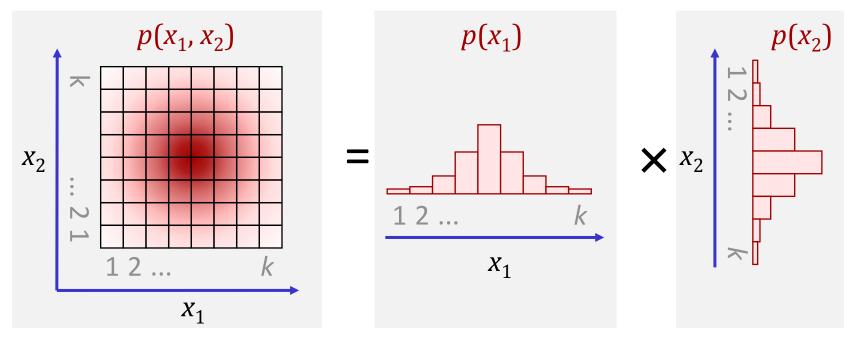
Independence = Density Factorization



 $p(x_1, x_2) = p(x_1) \times p(x_2)$

Factorization

Independence = Density Factorization



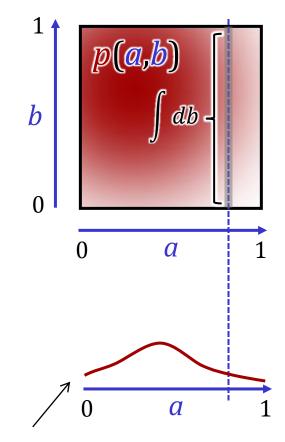
 $p(x_1, x_2) = p(x_1) \times p(x_2)$ $O(k^d) \qquad O(d \cdot k)$

Marginals

Example

- Two random variables
 a, *b* ∈ [0,1]
- Joint distribution p(a, b)
- We do not know b (could by anything)
- What is the distribution of *a*?

 $p(a) = \int p(a,b) db \, \mathbb{R}$

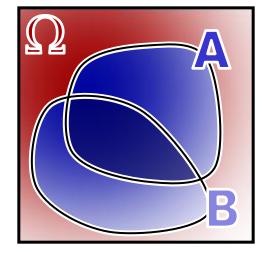


"Marginal Probability"

Conditional Probability

Bayes' Rule:

$$Pr(A | B) = \frac{Pr(B | A) \cdot Pr(A)}{Pr(B)}$$



Derivation

Pr(A∩B) = Pr(A | B) · Pr(B)
 Pr(A∩B) = Pr(B | A) · Pr(A)

 $\Rightarrow \Pr(A \mid B) \cdot \Pr(B) = \Pr(B \mid A) \cdot \Pr(A)$

Bayesian Inference

Example: Statistical Inference

- Medical test to check for a medical condition
- A: Medical test positive?
 - 99% correct if patient is ill
 - But in 1 of 100 cases, reports illness for healthy patients
- B: Patient has disease?
 - We know: One in 10 000 people have it

A patient is diagnosed with the disease:

• How likely is it for the patient to actually be sick?

Bayesian Inference

Apply Bayes' Rule:

$$Pr(B | A) = \frac{Pr(A | B) \cdot Pr(B)}{Pr(A)}$$

A: Medical test positive?B: Patient has disease?

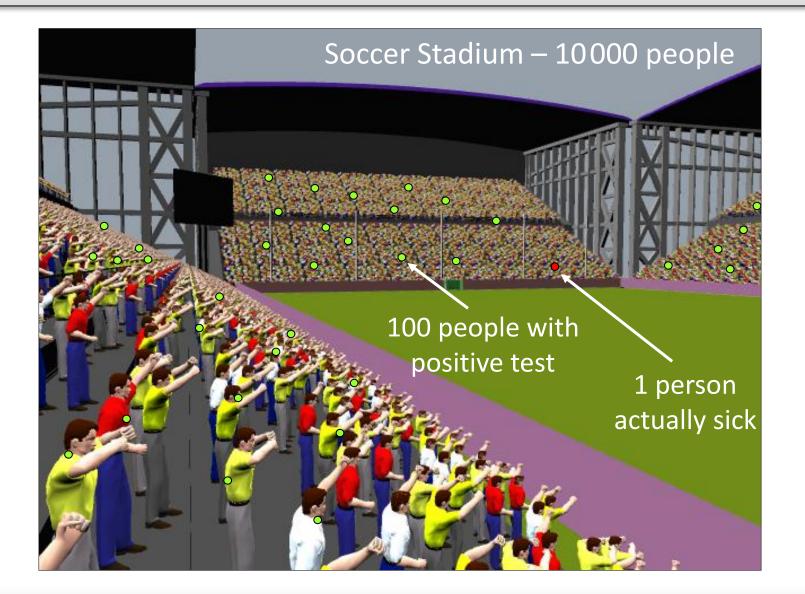
Pr(test pos. | disease) · Pr(deasease)

Pr(disease | test positive) = Pr(test pos. | disease)Pr(disease) + Pr(test pos. | disease)Pr(disease)

$$= \frac{0.99 \cdot 0.0001}{0.99 \cdot 0.0001 + 0.01 \cdot 0.9999} = \frac{0.000099}{0.0100979901}$$

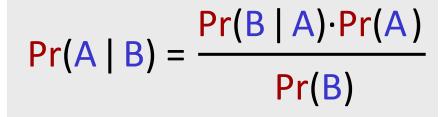
$$\approx 0.0098 \approx \frac{1}{100} \leftarrow \text{most likely healthy}$$

Intuition



Conclusion

Bayes' Rule:



- Used to fuse knowledge
 - "Prior" knowledge (prevalence of disease)
 - "Measurement": tests, sensor data, new information
 - Can be used repeatedly to add more information
- Standard tool for interpreting sensor measurements (Sensor fusion, reconstruction)
- Examples:
 - Image reconstruction (noisy sensors)
 - Face recognition

Chain Rule

Incremental update

Probability can be split into chain of conditional probabilities:

 $\Pr(X_n, ..., X_2, X_1)$

 $= \Pr(X_n | X_{n-1}, X_{n-2}, \dots, X_1) \cdots \Pr(X_3 | X_2, X_1) \Pr(X_2 | X_1) \Pr(X_1)$

- Example application:
 - X_i is measurement at time i
 - Update probability distribution as more data comes in
- Attention although it might look like, this does not reduce the complexity of the joint distribution

Probability Theory

(a very brief summary)

Part IV: Uniqueness – Philosophy Again...

Cox Axioms

Are there alternatives?

- Is this the right way to define probabilities?
- Are there no other uncertainty measures?

Answer (short):

- Yes.
- Any reasonable^{*} probability measure has the same properties
 - Up to normalization constant; we can have $Pr \in [0..42]$ if we like

*) reasonable – Cox axioms: ordering Pr(A) > Pr(B) > Pr(C) well defined, $Pr(\overline{A}) = f(Pr(A))$, $Pr(A \cap B) = g(Pr(A|B), Pr(B))$ for arbitrary, fixed f, g.

What is Probability?

Principle #1: [Hertzman 2004]

"Probability theory is nothing more than common sense reduced to calculation"

Pierre-Simon Laplace, 1814

Principle #2,3: [Hertzman 2004]

- Given a complete model, we can compute any other probability
- Use Bayes rule to infer unknown variables from observations

Probability Theory

(a very brief summary)

Part IV: Characteristics of Probability Measures

Moments of Distributions

Density Function (1D)

• $p: \mathbb{R} \to \mathbb{R}^{\geq 0}$

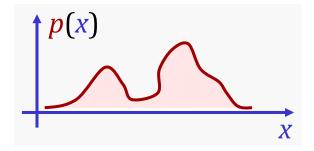
Expected Value / Mean:

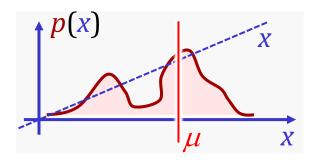
•
$$E(p) = \mu := \langle p, x \rangle$$

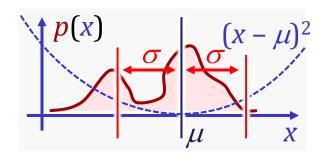
$$=\int_{\mathbb{R}}p(x)\cdot x\,dx$$

Variance:

•
$$Var(p) = \sigma^2 := \langle p, (x - \mu)^2 \rangle$$
$$= \int_{\mathbb{R}} p(x) \cdot (x - \mu)^2 dx$$







Standard Deviation

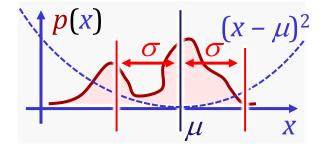
Bounds on spread

Standard deviation

 $\boldsymbol{\sigma} = \sqrt{Var(\boldsymbol{p})}$

- Expected range of variations
- Bounds spread of the distribution
- Formal bound: Chebyshev's inequality

$$\Pr(|X - \mu| \ge k\sigma) \le \frac{1}{k^2}$$



Remark: Other Moments

Higher order moments:

•
$$m_k(p) \coloneqq \langle p, (x-\mu)^k \rangle = \int_{\mathbb{R}} p(x) \cdot (x-\mu)^k dx$$

- Skewness: m_3 (asymetry of the distribution)
- Kurtosis: m_4 (peakedness)

More general

- $\langle p, f_i \rangle$ with basis functions f_i , for example:
 - Fourier basis ("characteristic function")

We will not use any of this in this lecture...

$p(x_1, x_2)$ X_2

•
$$E(p) = \mu := \langle p, x \rangle = \int_{\mathbb{R}^d} p(x) \cdot x \, dx$$

Moments of Distributions

•
$$\operatorname{Cov}(x_i, x_j) := \langle p, (x_i - \mu_i)(x_j - \mu_i) \\ = \int_{\mathbb{R}^d} p(x) (x_i - \mu_i)(x_j - \mu_i) dx$$

•
$$\sum_{i=1}^{\infty} = \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & \text{Cov}(x_i, x_j) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Multi-variate density function

Density
$$p: \mathbb{R}^d \to \mathbb{R}^{\geq 0}$$

 $E(p) = \mu := \langle p, x \rangle = \int_{\mathbb{R}^d} p(x) \cdot x \, dx$
 $\operatorname{Cov}(x_i, x_j): = \langle p, (x_i - \mu_i)(x_j - \mu_i) \rangle$



 $|p(x_1, x_2)|$

*x*₁

*x*₁

Properties

Expected Value:

- E(X+Y) = E(X) + E(Y)
- $E(\lambda X) = \lambda E(X)$

Variance:

- $Var(\lambda X) = \lambda^2 Var(X)$
- Let X, Y be *independent*, then: Var(X + Y) = Var(X) + Var(Y)

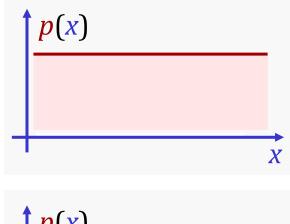
Entropy

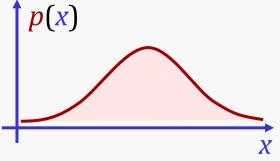
How random is the randomness?

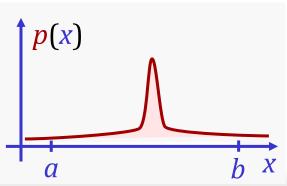
- Measure of unorderliness
- How much information remains in the events, knowing the distribution?

Idea

- Try to code the events
- Binary codes
 - short codes for frequent events
 - long codes for infrequent events







Entropy

Best solution

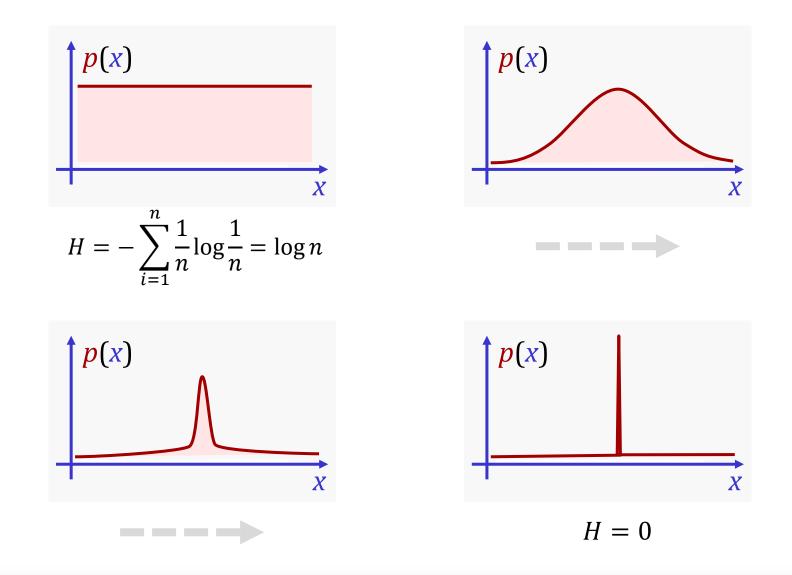
- Use codes of $\mathcal{O}(\log \frac{1}{p})$ bits for events with probability p
- Can be implemented: Huffman coding, arithmetic coding

Definition: Entropy

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log p(x_i)$$

Coding efficiency of independent events

Examples



Probability Theory

(a very brief summary)

Part V: Large numbers

Law of Large Numbers

Intuition for Probabilities:

- Single outcomes are random
- But on average over a larger number of trials, the behavior is known
- It can be shown that probability measures naturally have this property

Law of Large Numbers

Let

 X₁, X₂, ..., X_n be i.i.d. random variables (independent, identically distributed)

We look at the mean

$$\bar{X}_n = \frac{1}{n} \left(\sum_{i=1}^n X_i \right)$$

(Weak) law of large numbers

$$\lim_{n \to \infty} \Pr(|\bar{X}_n - \mu| > \epsilon) = 0$$

Proof

Proof:

- Additionally assumption: finite variance $Var(X_i) = \sigma^2$
- The theorem then follows from
 - Additivity of variances
 - Chebyshev's bound

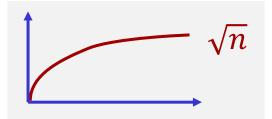
$$\operatorname{Var}(\bar{X}_n) = \operatorname{Var}\left(\frac{1}{n}\left(\sum_{i=1}^n X_i\right)\right) = \frac{1}{n^2}\left(\sum_{i=1}^n \operatorname{Var}(X_i)\right) = \frac{n\sigma}{n^2} = \frac{\sigma}{n}$$
$$\Rightarrow \sigma(\bar{X}_n) = \frac{\sigma}{\sqrt{n}}$$

• Chebyshev: $\Pr(|X - \mu| \ge k\sigma) \le \frac{1}{k^2}$

Additional Insight

Averaging of independent trials

- Reduces the variance
- For independent sampling, convergence rate is $\frac{1}{\sqrt{n}}$
- This is usually lousy...
 - Rapid progress first
 - Then takes forever to converge



Central Limit Theorem

Why are so many phenomena normal-distributed?

- Let $X_1, ..., X_n$ be real (1D) random variables with means μ_i and *finite* variances σ_i^2 .
- Then the distribution of the mean

$$\frac{\sum_{i=1}^{n} X_{i} - \sum_{i=1}^{n} \mu_{i}}{\sqrt{\sum_{i=1}^{n} \sigma_{i}^{2}}} \rightarrow \mathcal{N}(0,1)$$

converges to a normal distribution.

Multi-dimensional variant

• Similar result for multi-dimensional case

Probability Theory

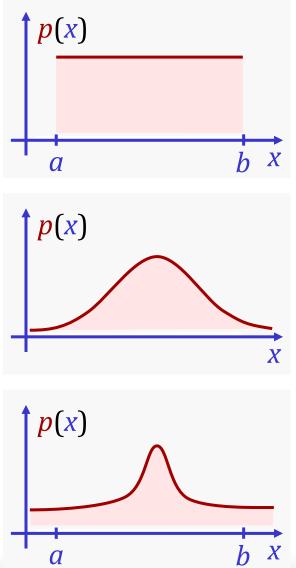
(a very brief summary)

Part VI: Gaussian Distributions

Well-known probability distributions

Important distributions

- Uniform distribution
 - Only defined for finite domains
 - Maximum entropy among all distributions
- Gaussian / normal distribution
 - Infinite domains
 - Maximizes entropy for fixed variance
- Heavy tail distributions
 - "Outlier robust"



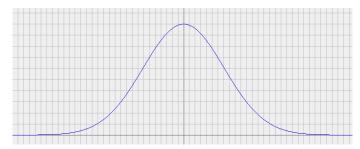
Gaussians

Gaussian Normal Distribution

- Two parameters: μ , σ
- Density:

$$\mathcal{N}_{\mu,\sigma}(x) \coloneqq \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- Mean: **µ**
- Variance: σ^2



Gaussian normal distribution

Log Space

Neg-log-density:

$$\log \mathcal{N}_{\mu,\sigma}(x) \coloneqq \frac{(x-\mu)^2}{2\sigma^2} + \frac{1}{2}\ln(2\pi\sigma^2)$$
$$\sim \frac{1}{2\sigma^2}(x-\mu)^2$$

Calculations in log-space:

- Densities of products of Gaussians are Sums of quadratic polynomials
- Calculations simplified in log-space
 - Exception: Sum of Gaussians do not work

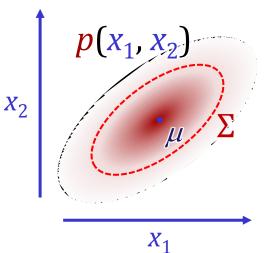
Multi-Variate Gaussians

Gaussian Normal Distribution in d Dimensions

- Two parameters: μ (*d*-dim-vector), Σ (*d*×*d* matrix)
- Density:

$$\mathcal{N}_{\boldsymbol{\mu},\boldsymbol{\Sigma}}(\mathbf{x}) \coloneqq \left(\frac{1}{(2\pi)^{-\frac{d}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}}}\right) e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$

- Mean: **µ**
- Covariance Matrix: Σ



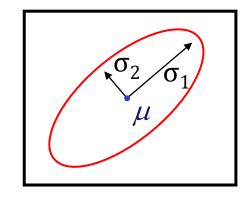
Log Space

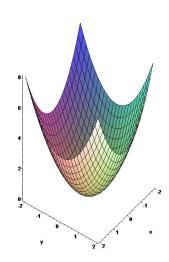
Neg-Log Density:

- $\frac{1}{2}(\mathbf{x} \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x} \boldsymbol{\mu}) + const$
- Quadratic multivariate polynomial

Consequences:

- Optimization (maximum probability density) by solving a linear system
- Gaussians are ellipsoids
 - Eigenvectors of Σ are main axes (principal component analysis, PCA)
 - Eigenvalues are extremal variances





More Rules for Computations with Gaussians

- Products of Gaussians are Gaussians
 - Algorithm: Add quadratic polynomials
 - Variance can only decrease
- Marginals ("projections") of Gaussians are Gaussians
 - Unknown values: Leave out dimensions in μ , Σ
 - Known values: Schur complement
- Affine mappings of Gaussians are Gaussians
 - Algorithm: apply map to argument x, yields different quadric
- General sums of Gaussians do not have closed-form log-densities

Coordinate Transforms

• General Gaussians as affine transforms of unit Gaussians

• Quadric
$$\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}) + c$$

• Main axis transform:

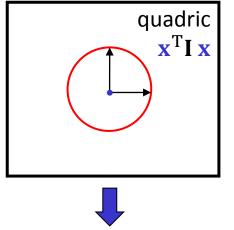
$$\boldsymbol{\Sigma}^{-1} = \mathbf{U}\mathbf{D}\mathbf{U}^{\mathrm{T}} = \mathbf{U}\begin{pmatrix}\boldsymbol{\sigma_{1}^{-2}} & & \\ & \boldsymbol{\sigma_{2}^{-2}} & \\ & & \ddots \end{pmatrix}\mathbf{U}^{\mathrm{T}}$$
$$\boldsymbol{\Sigma}^{-\frac{1}{2}} = \mathbf{U}\mathbf{D}^{\frac{1}{2}}\mathbf{U}^{\mathrm{T}} = \mathbf{U}\begin{pmatrix}\boldsymbol{\sigma_{1}^{-1}} & & \\ & \boldsymbol{\sigma_{1}^{-1}} & \\ & & \ddots \end{pmatrix}\mathbf{U}^{\mathrm{T}}$$

Unit Gaussian:

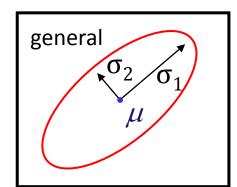
• We get:

$$\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} (\boldsymbol{\Sigma}^{-\frac{1}{2}})^{\mathrm{T}} (\boldsymbol{\Sigma}^{-\frac{1}{2}}) (\mathbf{x} - \boldsymbol{\mu}) + c$$

$$=\frac{1}{2}\left(\left(\sum^{-\frac{1}{2}}\right)_{\mathbf{X}}-\left(\sum^{-\frac{1}{2}}\right)_{\mathbf{\mu}}\right)^{T}\left(\left(\sum^{-\frac{1}{2}}\right)_{\mathbf{X}}-\left(\sum^{-\frac{1}{2}}\right)_{\mathbf{\mu}}\right)+c$$



- This is a unit Quadric / Gaussian $\boldsymbol{x}^T\boldsymbol{I}\,\boldsymbol{x}$
 - rotated to Coordinate frame $\Sigma^{-\frac{1}{2}}$
 - and translated accordingly by $(\Sigma^{-\frac{1}{2}})_{\mu}$



Unit Gaussian:

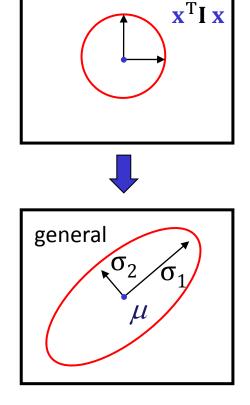
 In addition, we have to recompute the (log) normalization factor

$$c = \ln\left(\frac{1}{(2\pi)^{-\frac{d}{2}}\det(\mathbf{\Sigma})^{-\frac{1}{2}}}\right)$$

to ensure a unit integral

Rule of thumb:

- All Gaussians are related by
 - Translation
 - Rotation & non-uniform scaling
 - Adapting the density to integrate to 1



quadric

Mahalanobis Distance

Given:

- A Gaussian distribution with parameters μ , Σ
- Sample point $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

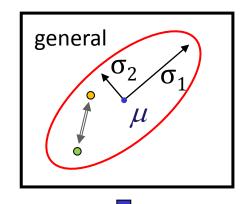
Mahalanobis distance of x:

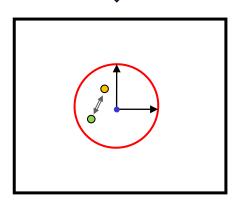
$$D_M(\mathbf{x}) = \sqrt{(\mathbf{x} - \mathbf{\mu})^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \mathbf{\mu})}$$

$$D_M(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \mathbf{y})}$$

Interpretation:

- Measures distances in "unit Gaussian space"
- One unit = one standard deviation

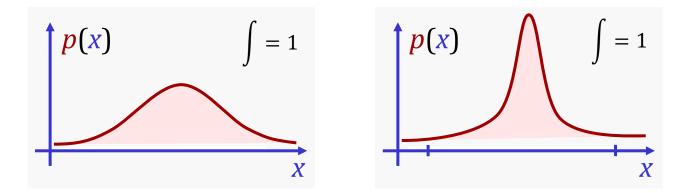




Applications

Example

- Given a sample from and a Gaussian distribution
- How likely is this sample from that distribution?
- Density value not a good measure
 - Absolute density depends on breadth



Estimation from Data

Task

- Data d₁, ..., d_n generated w/Gaussian distribution (i.i.d.)
- Estimate parameters

Maximum Likelihood Estimation

• Most likely parameters: $\operatorname{argmax}_{\mu,\Sigma} P(\mu, \Sigma | \mathbf{d}_1, \dots, \mathbf{d}_n)$

$$\boldsymbol{\mu}_{ml} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{d}_{i} \qquad \boldsymbol{\Sigma}_{ml} = \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{d}_{i} - \boldsymbol{\mu}) (\mathbf{d}_{i} - \boldsymbol{\mu})^{\mathrm{T}}$$

mean covariance

Mahalanobis Distance

Given:

- A Gaussian distribution with parameters μ , Σ
- Sample point $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

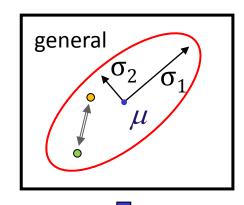
Mahalanobis distance of x:

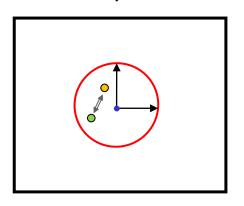
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Interpretation:

- Measures distances in "unit Gaussian space"
- One unit = one standard deviation





Conclusions

Bayesian Statistics

- Uncertain captured in numbers
- Mathematics gives us the rules to derive consequences of our assumptions

The rest of the theory

• Formal tools to work with uncertainty