Seminar Explainable AI

Module 00

Primer on Probability, Information and Learning from Data

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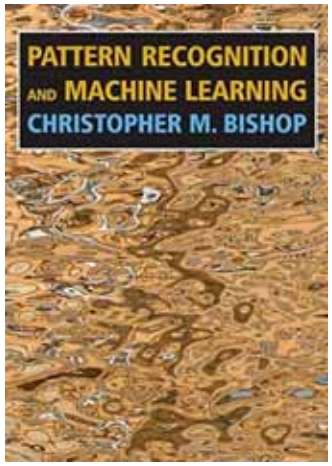
This is the version for printing and reading. The lecture version is didactically different.

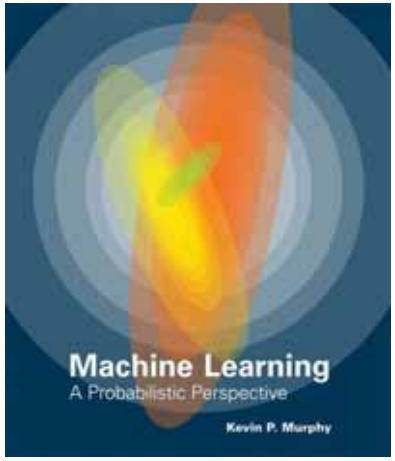
- Probability Distribution
- Probability Density
- Frequentist/Bayesian
- Continuous/Discrete
- Independent/Dependent
- Identical/Non-Identical
- Correlation/Causation
- Joint Probability
- Conditional Probability

- Information Entropy
- Mutual Information
- Kullback-Leibler Divergence
- Maximum Likelihood Estimation
- Maximum a Posteriori Estimate
- Bayesian Estimate
- Bayesian Learning
- Fisher Information
- Marginal Likelihood

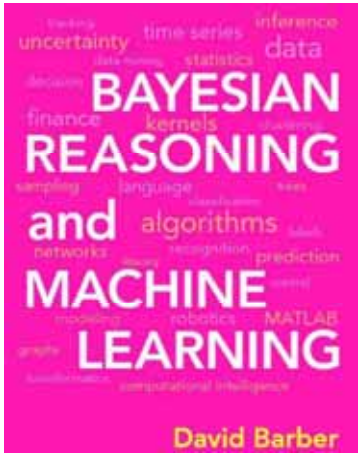
Book recommendations (selection)



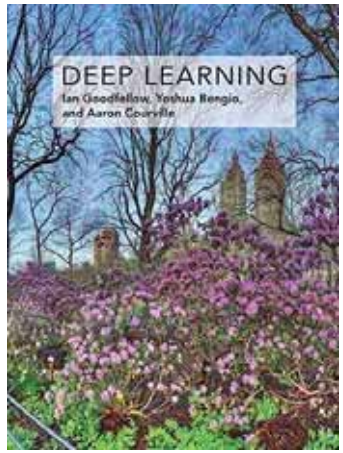
Christopher M. Bishop 2006. Pattern Recognition and Machine Learning, New York, Springer.



Kevin P. Murphy 2012. Machine learning: a probabilistic perspective, Cambridge (MA), MIT press.

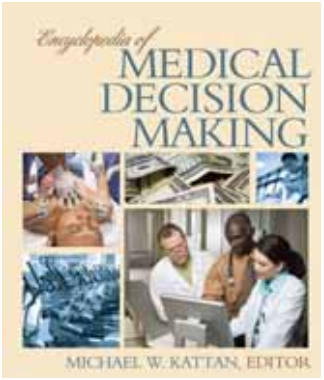


David Barber 2012. Bayesian reasoning and machine learning, Cambridge, Cambridge University Press.



Ian Goodfellow, Yoshua Bengio & Aaron Courville 2016. Deep Learning, Cambridge (MA), MIT Press.

For those students who are interested in decision making, this is a Standard: Michael W. Kattan (ed.) 2009. Encyclopedia of medical decision making, London: Sage.



- 00 Mathematical Notations
- 01 Probability Distribution and Density
- 02 Expectation and Expected Utility Theory
- 03 Joint Probability/Conditional Probability
- 04 Independent, identically distributed (iid)
- 05 Bayes and Laplace
- 06 Information Theory & Entropy

00 Mathematical Notations

We denote random and fixed scalars by lower case, random and fixed vectors by bold lower case, and random and fixed matrices by bold upper case. Occasionally we use non-bold upper case to denote scalar random variables. Also, we use $p()$ for both discrete and continuous random variables

Most used – at a glance

$\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}, ...$	"Calligraphic" font generally denotes sets or lists, e.g., data set $\mathcal{D} = x_1, ..., x_n$
$x \in \mathcal{D}$	x is an element of set $\mathcal{D}$
$x \notin \mathcal{D}$	x is not an element of set $\mathcal{D}$
$\mathcal{D} \cup \mathcal{D}$	x union of two sets, i.e., the set containing all elements of $\mathcal{D}$ and $\mathcal{D}$
$\lvert\mathcal{D}\rvert$	cardinality of set $\mathcal{D}$, i.e., the number of (possibly non-distinct) elements in it
$\max_x[\mathcal{D}]$	the maximum x value in set $\mathcal{D}$
$dom(x)$	Domain of variable x
$x = x$	The variable x is in the state x
$dim(x)$	For a discrete variable x, this denotes the number of states x can take
$x_{a:b}$	$x_a, x_{a+1}, ..., x_b$
$\not<, \not>$	not less than; not greater than
$\neq$	not equal to
$\ll, \gg$	much less than; much greater than
d/dx	the derivative with respect to x
$\mathcal{M} \subset \mathcal{N}$	$\mathcal{M}$ is a subset of $\mathcal{N}$
$\mathcal{M} \supset \mathcal{N}$	$\mathcal{M}$ contains $\mathcal{N}$
$\mathcal{M} \bigcap \mathcal{N}$	intersection of $\mathcal{M}$ and $\mathcal{N}$
$\Longrightarrow$	implies
$\longleftrightarrow$	equivalent to
$\exists$	there exists
$\forall$	for every

Linear algebra notations

We use boldface lower-case to denote vectors, such as $\vec{x}$, and boldface upper-case to denote matrices, such as $\vec{X}$. We denote entries in a matrix by non-bold upper case letters, such as X_{ij}.

Vectors are assumed to be column vectors, unless noted otherwise. We use $(x_1, \cdots, x_D)$ to denote a column vector created by stacking D scalars. If we write $\vec{X} = (\vec{x}_1, \cdots, \vec{x}_n)$, where the left hand side is a matrix, we mean to stack the $\vec{x}_i$ along the columns, creating a matrix.

$\|\|\vec{x}\|\| = \|\|\vec{x}\|\|_2$	Euclidean or ℓ_2 norm $\sqrt{\sum_{j=1}^{d} x_j^2}$
$\|\|\vec{x}\|\|_1$	ℓ_1 norm $\sum_{j=1}^{d} \|x_j\|$
$\vec{X}_{:,j}$	j'th column of matrix
$\vec{X}_{i,:}$	transpose of i'th row of matrix (a column vector)
$\vec{X}_{i,j}$	Element (i, j) of matrix $\vec{X}$

Probability notations (1/3)

X, Y	Random variable
$P()$	Probability of a random event
$F()$	Cumulative distribution function(CDF), also called distribution function
$p(x)$	Probability mass function(PMF)
$f(x)$	probability density function(PDF)
$F(x, y)$	Joint CDF
$p(x, y)$	Joint PMF
$f(x, y)$	Joint PDF
$p(X\|Y)$	Conditional PMF, also called conditional probability
$f_{X\|Y}(x\|y)$	Conditional PDF
$X \perp Y$	X is independent of Y
$X \not\perp Y$	X is not independent of Y
$X \perp Y\|Z$	X is conditionally independent of Y given Z
$X \not\perp Y\|Z$	X is not conditionally independent of Y given Z
$X \sim p$	X is distributed according to distribution p
$\vec{\alpha}$	Parameters of a Beta or Dirichlet distribution
$\mathrm{cov}[X]$	Covariance of X
$\mathbb{E}[X]$	Expected value of X
$\mathbb{E}_q[X]$	Expected value of X wrt distribution q
$\mathbb{H}(X)$ or $\mathbb{H}(p)$	Entropy of distribution $p(X)$
$\mathbb{I}(X; Y)$	Mutual information between X and Y
$\mathbb{KL}(p\|\|q)$	KL divergence from distribution p to q

Probability notations (2/3)

$\ell(\vec{\theta})$	Log-likelihood function
$L(\theta, a)$	Loss function for taking action a when true state of nature is θ
λ	Precision (inverse variance) $\lambda = 1/\sigma^2$
Λ	Precision matrix $\Lambda = \Sigma^{-1}$
$\text{mode}[\vec{X}]$	Most probable value of $\vec{X}$
μ	Mean of a scalar distribution
$\vec{\mu}$	Mean of a multivariate distribution
Φ	cdf of standard normal
ϕ	pdf of standard normal
$\vec{\pi}$	multinomial parameter vector, Stationary distribution of Markov chain
ρ	Correlation coefficient
$\text{sigm}(x)$	Sigmoid (logistic) function, $\frac{1}{1+e^{-x}}$
σ^2	Variance
Σ	Covariance matrix

Probability notations (3/3)

$\text{var}[x]$	Variance of x
ν	Degrees of freedom parameter
Z	Normalization constant of a probability distribution
$\sim$	has the distribution, e.g., $p(x) \sim N(\mu, \sigma^2)$
$N(\mu, \sigma^2)$	multidimensional normal or Gaussian distribution with mean μ and variance σ^2
$O(h(x))$	big oh order of $h(x)$
$\Theta(h(x))$	big theta order of $h(x)$
$\Omega(h(x))$	big omega order of $h(x)$
$\sup_x f(x)$	the supremum value of $f(x)$-the global maximum of $f(x)$ over all values of x
$p(x = tr)$	Probability of variable x being in the state true
$p(x = fa)$	Probability of variable x being in the state false
$p(x \cap y)$	Probability of x and y
$p(x \cup y)$	Probability of x or y
$p(x\|\|y)$	Probability of x contioned on y
$\langle f(x) \rangle_{g(x)}$	The average of the function $f(x)$ with respect to the distribtioin $p(x)$
$\sigma(x)$	The logistic sigmoid $\frac{1}{(1+\exp(-x))}$
$erf(x)$	The (Gaussian) error function

Note: parameter θ (theta) credit to Zoubin Ghahramani

http://mlg.eng.cam.ac.uk/zoubin

Weather Prediction

Assume that the weather in London is independent and identically distributed across days. It can either rain (R) or be cloudy (C).

Data: $\mathcal{D} = (RCCRRCR\ldots)$

Parameters: $\theta \stackrel{\text{def}}{=}$ Probability of rain

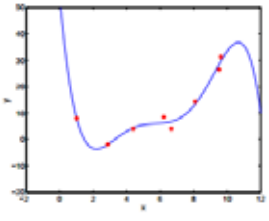
$$P(R|\theta) = \theta$$
$$P(C|\theta) = 1 - \theta$$

Goal: To infer θ from the data and predict future outcomes $P(R|\mathcal{D})$.

Polynomial Regression

Data: $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}$ for $n = 1, \ldots, N$

$$x^{(n)} \in \Re$$
$$y^{(n)} \in \Re$$



Parameters: $\boldsymbol{\theta} = (a_0, \ldots, a_m, \sigma)$

Model:

$$y^{(n)} = a_0 + a_1 x^{(n)} + a_2 {x^{(n)}}^2 \ldots + a_m {x^{(n)}}^m + \epsilon$$

where

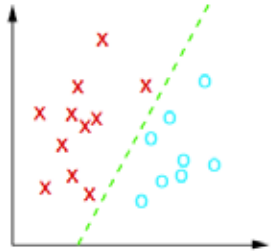
$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

Goal: To infer $\boldsymbol{\theta}$ from the data and to predict future outputs $P(y|\mathcal{D}, x, m)$

Linear Classification

Data: $\mathcal{D} = \{(\mathbf{x}^{(n)}, y^{(n)})\}$ for $n = 1, \ldots, N$ data points

$$\mathbf{x}^{(n)} \in \Re^D$$
$$y^{(n)} \in \{+1, -1\}$$



Parameters: $\boldsymbol{\theta} \in \Re^{D+1}$

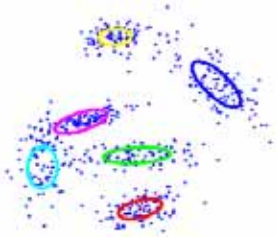
$$P(y^{(n)} = +1|\boldsymbol{\theta}, \mathbf{x}^{(n)}) = \begin{cases} 1 & \text{if } \sum_{d=1}^{D} \theta_d x_d^{(n)} + \theta_0 \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Goal: To infer $\boldsymbol{\theta}$ from the data and to predict future labels $P(y|\mathcal{D}, \mathbf{x})$

Clustering with Gaussian Mixtures (Density Estimation)

Data: $\mathcal{D} = \{\mathbf{x}^{(n)}\}$ for $n = 1, \ldots, N$

$$\mathbf{x}^{(n)} \in \Re^D$$



Parameters: $\boldsymbol{\theta} = \left((\mu^{(1)}, \Sigma^{(1)}) \ldots, (\mu^{(m)}, \Sigma^{(m)}), \boldsymbol{\pi}\right)$

Model:

$$\mathbf{x}^{(n)} \sim \sum_{i=1}^{m} \pi_i p_i(\mathbf{x}^{(n)})$$

where

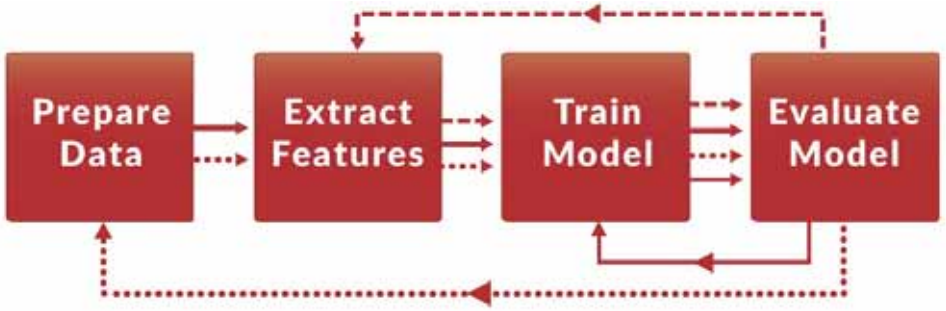
$$p_i(\mathbf{x}^{(n)}) = \mathcal{N}(\mu^{(i)}, \Sigma^{(i)})$$

Goal: To infer $\boldsymbol{\theta}$ from the data and predict the density $p(\mathbf{x}|\mathcal{D}, m)$

Machine learning builds on 3 mathematical pillars

- 1) Linear algebra,
- 2) probability/statistics, and
- 3) optimization
- typical data organization is in arrays (matrices),
- rows represent the samples (data items)
- columns represent attributes (features, representations, covariates), ML = “feature engineering”
- Simplest: each training input x_i is a d-dimensional vector of numbers, but x_i could be a complex object (image, sentence, graph, time series, molecular shape, etc.

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$$



See a typical ML-pipeline here:
https://www.datasciencecentral.com/profiles/blogs/data-version-control-iterative-machine-learning

Discussion: What makes a good feature?

https://www.youtube.com/watch?v=N9fDIAflCMY

Thus the high-level features found in primates are not expected to occur also in simpler animals, such as the fish or frog. Across species, therefore, we find an enormous spectrum of features, especially if we include those specialized trigger patterns or "innate releasing mechanisms" reported by the ethologists (Thorpe, 1963; Tinbergen, 1951). Given this vast collection, it might seem unlikely that one could abstract away some principles that define "what makes a good feature?" However, here we attempt to do just that.

Our guiding hypothesis is that "seeing" is the inference of world properties from image elements—i.e. the various patterns of intensities on the retina. A "feature" is typically viewed as a measurement of image structure, at the level for example of Marr's primal sketch (Marr, 1982). Clearly, many different kinds of measurements or "features" are possible. Intuitively, however, those most often sought after will point directly and reliably to a unique, *meaningful* event in the world. But the criterion that a feature be meaningful implies that the perceiver has some goal or context in mind. For example, for a baby gull the significance of a red spot in the image depends on whether it is seen in the context of a traffic light or as coloration on the beak of an adult gull (Figure 1). In the context of a beak, its salience is sufficient to trigger a feeding response. Somehow the gull is primed to immediately make the necessary inference. Hence we propose that "what makes a good feature" should include the property of having a ready explanation for its appearance (MacKay, 1978; MacKay, 1985).

Allan Jepson & Whitman Richards 1992. What makes a good feature. Spatial vision in humans and robots, 89-126.

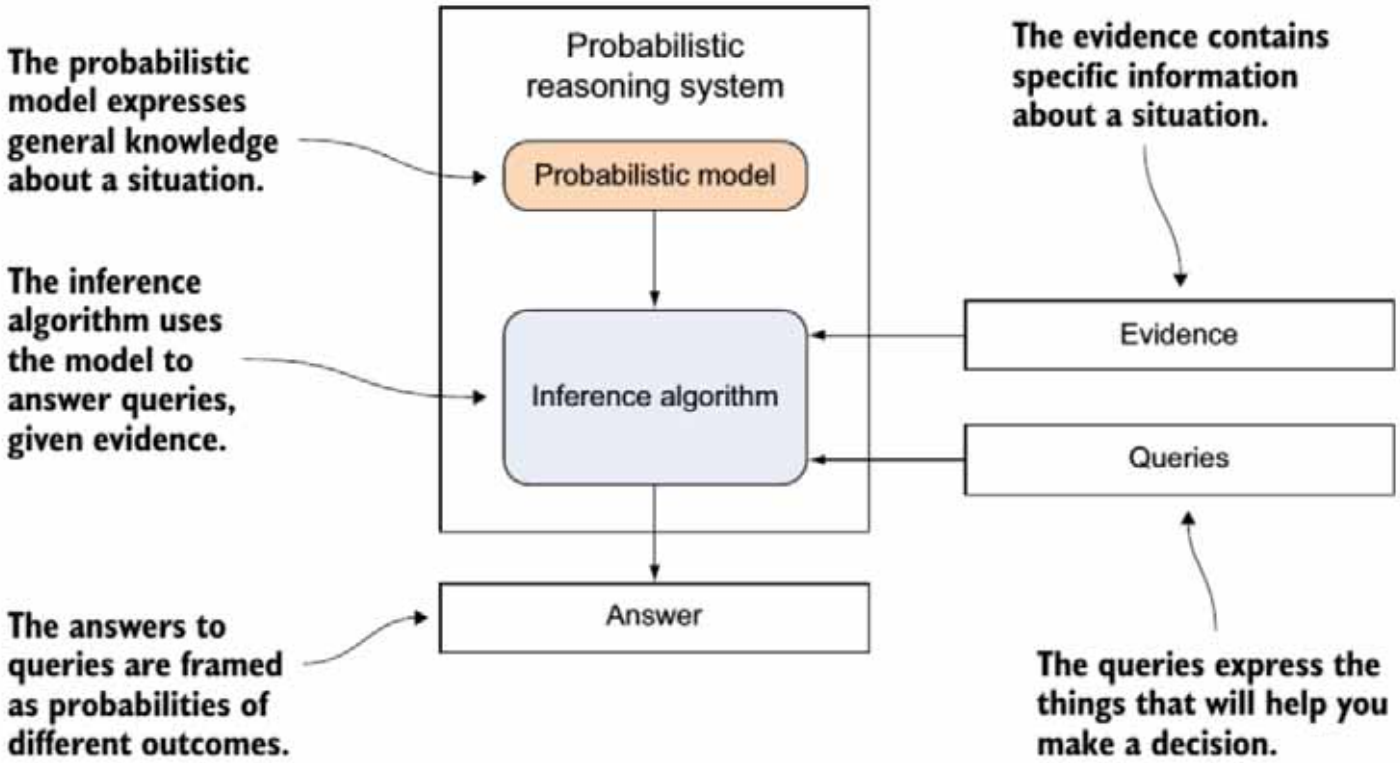
Definition 1 (*Relevant to the target*). A feature x_i is *relevant to a target concept* c if there exists a pair of examples A and B in the instance space such that A and B differ only in their assignment to x_i and $c(A) \neq c(B)$.

Definition 3 (*Weakly relevant to the sample/distribution*). A feature x_i is *weakly relevant* to sample S (or to target c and distribution D) if it is possible to remove a subset of the features so that x_i becomes strongly relevant.

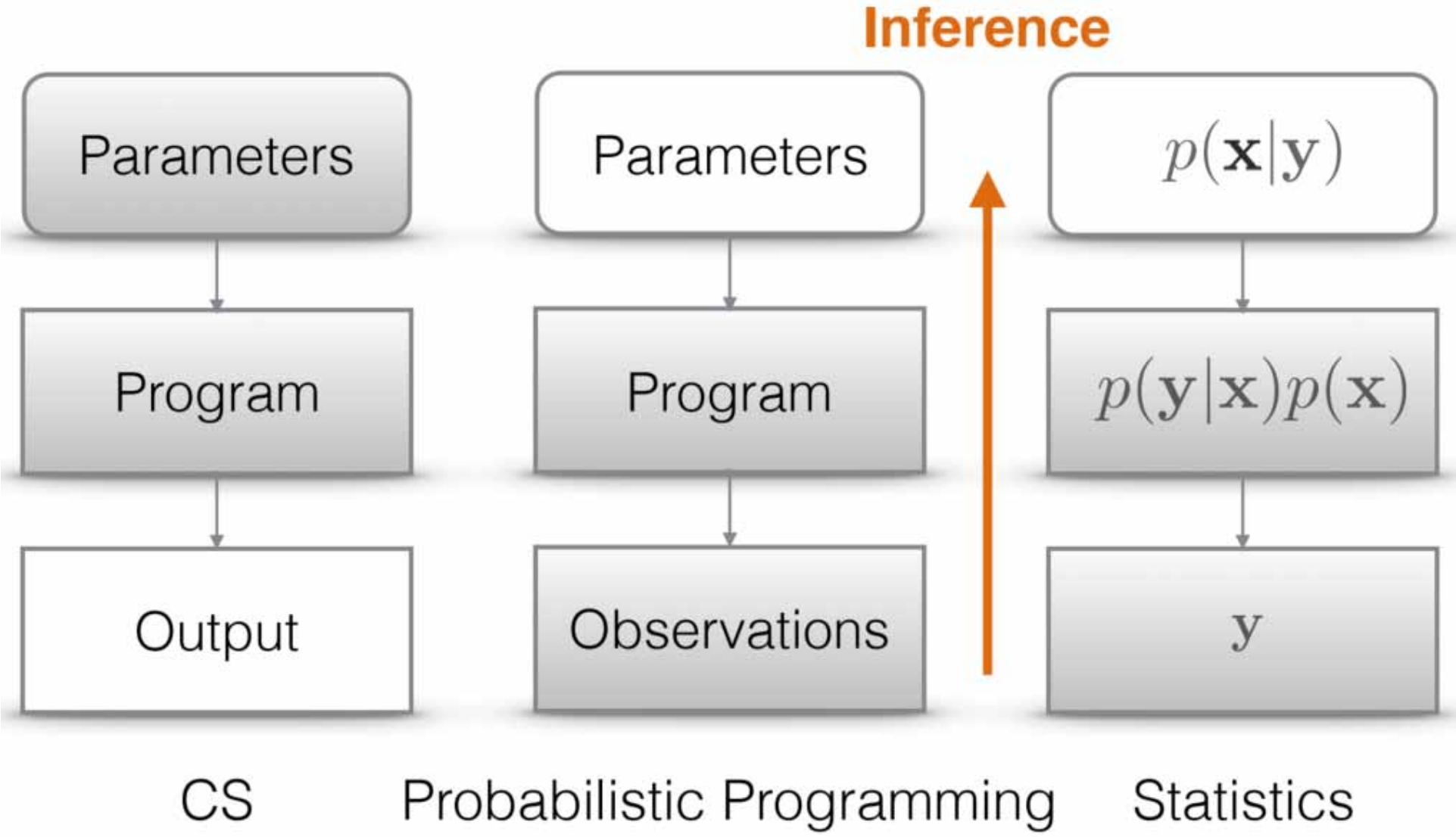
Avrim L. Blum & Pat Langley 1997. Selection of relevant features and examples in machine learning. Artificial intelligence, 97, (1), 245-271, doi:10.1016/S0004-3702(97)00063-5.

Practical Example: Probabilistic Reasoning System

Remark: compare with early Expert Systems (see module 3)



Avi Pfeffer 2016. Practical probabilistic programming, Shelter Island (NY), Manning Publications.

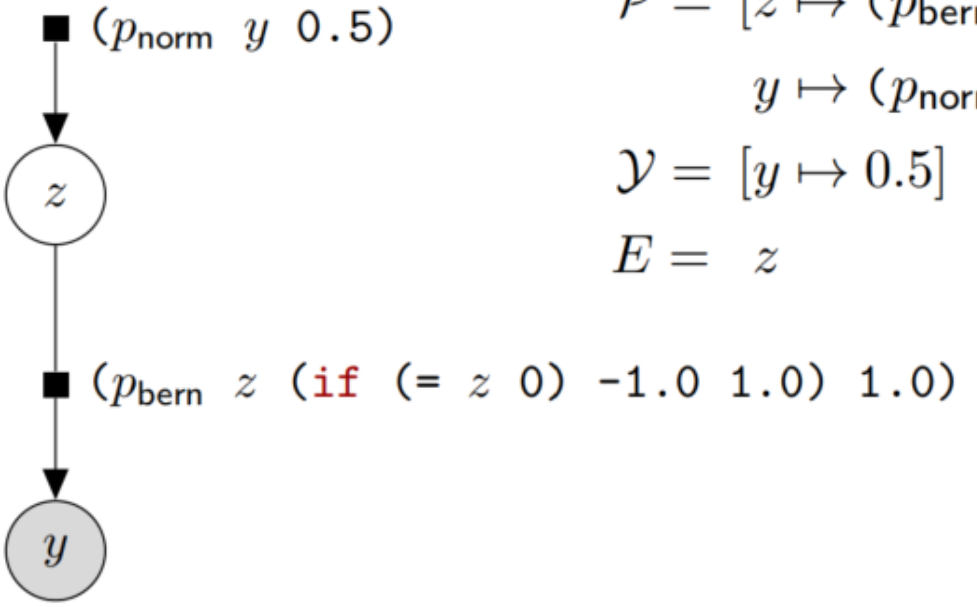


Jan-Willem Van De Meent, Brooks Paige, Hongseok Yang & Frank Wood 2018. An introduction to probabilistic programming. arXiv preprint arXiv:1809.10756.

Example for a graphical model

```
(let [z (sample (bernoulli 0.5))
      mu (if (= z 0) -1.0 1.0)
      d (normal mu 1.0)
      y 0.5]
  (observe d y)
  z)
```

$$V = \{z, y\},$$
$$A = \{(z, y)\},$$
$$\mathcal{P} = [z \mapsto (p_{\text{bern}}\ z\ 0.5),$$
$$y \mapsto (p_{\text{norm}}\ y\ (\texttt{if}\ (=\ z\ 0)\ -1.0\ 1.0)\ 1.0)],$$
$$\mathcal{Y} = [y \mapsto 0.5]$$
$$E = z$$



Jan-Willem Van De Meent, Brooks Paige, Hongseok Yang & Frank Wood 2018. An introduction to probabilistic programming. arXiv preprint arXiv:1809.10756.

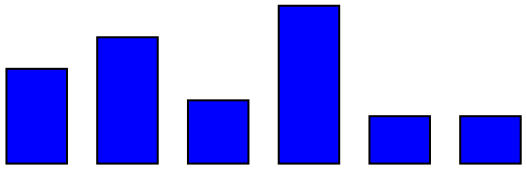
01 Probability

What is probability p(x)?

- $Probability\ p(x)$ is the formal study of laws of chance and managing uncertainty; allows to measure (many) events
  - Frequentist* view: coin toss
  - Bayesian* view: probability as a measure of belief (this is what made machine learning successful)
  - $p(x)$ = 1 means that all events occur for certain
  - Information is a measure for the reduction of uncertainty
  - If something is 100 % certain its uncertainty = 0
  - Uncertainty is max. if all choices are equally probable (I.I.D = independent and identically distributed)
  - Uncertainty (as information) sums up for independent sources: $\sum_x p(x = X) = 1$

*) Bayesian vs. Frequentist - please watch the excellent video of Kristin Lennox (2016): https://www.youtube.com/watch?v=eDMGDhyDxuY

- Discrete distributions:

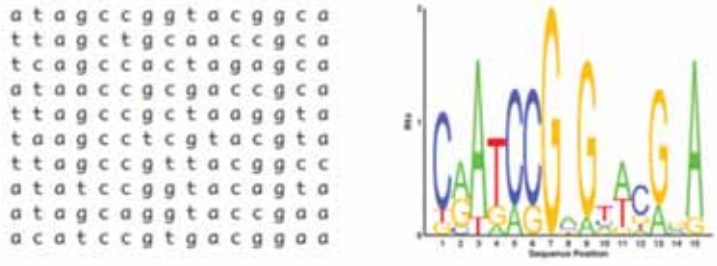


1 2 3 4 5 6

$$\sum_i P(X = x_i) = 1$$

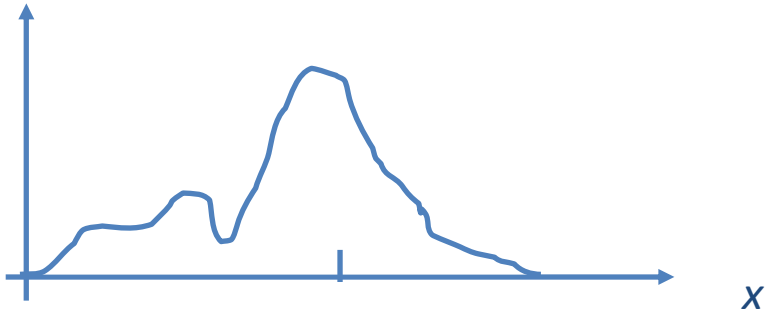
Name	n	K	x
Multinomial	-	-	$\mathbf{x} \in \{0, 1, \ldots, n\}^K, \sum_{k=1}^K x_k = n$
Multinoulli	1	-	$\mathbf{x} \in \{0, 1\}^K, \sum_{k=1}^K x_k = 1$ (1-of-K encoding)
Binomial	-	1	$x \in \{0, 1, \ldots, n\}$
Bernoulli	1	1	$x \in \{0, 1\}$

Table 2.1 Summary of the multinomial and related distributions.

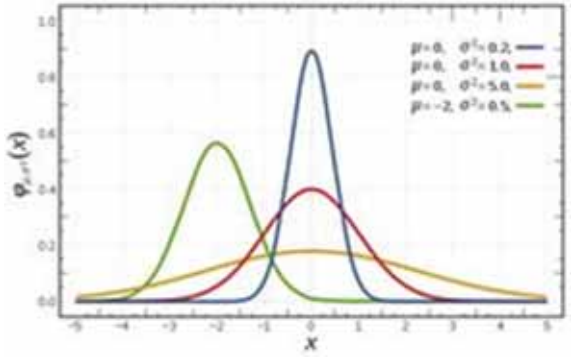


(a) (b)

- Continuous: Probability density function (PDF) vs Cumulative Density Function (CDF):

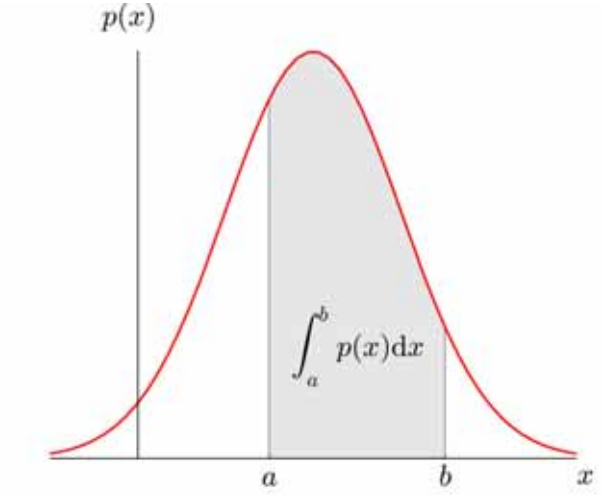


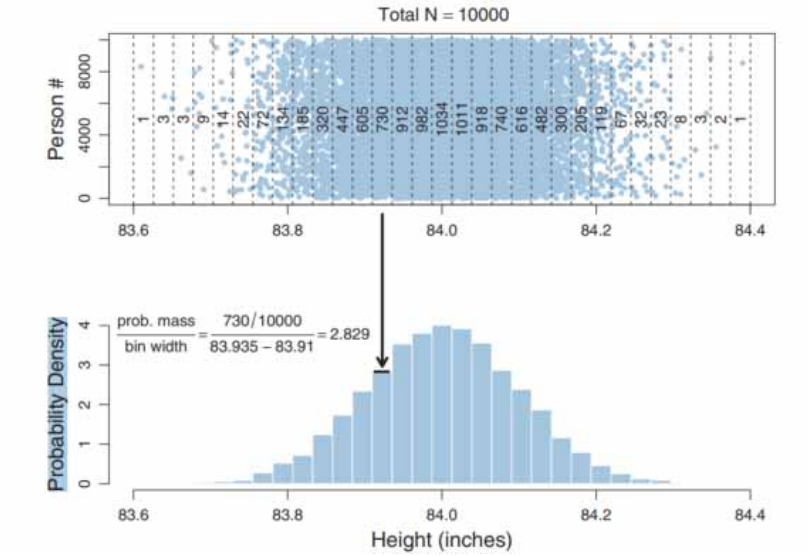
$$P(x \leq a) = \int_{-\infty}^{a} f(\tau) d\tau$$



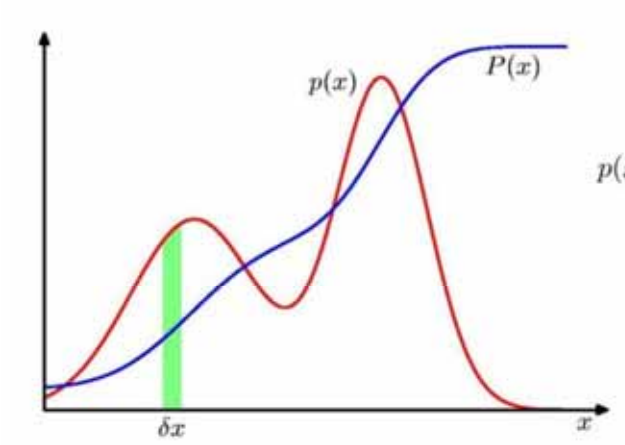
$$\mathcal{N}(x|\mu, \sigma^2) \triangleq \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Probability Density Function and Probability Distribution





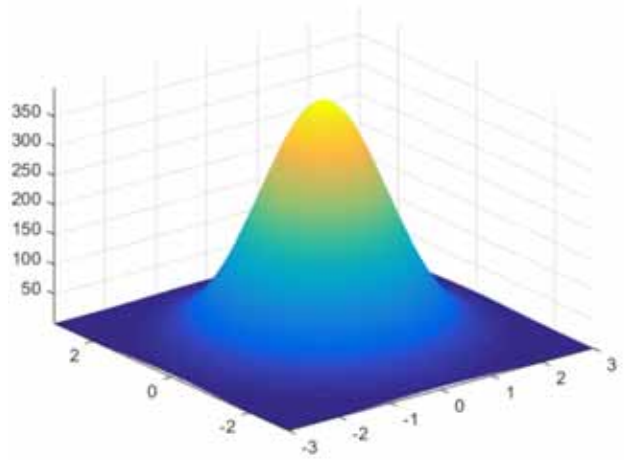
John Kruschke 2014. Doing Bayesian data analysis: A tutorial with R, JAGS, and Stan, Amsterdam et al., Academic Press.



$$p(x \in (a,b)) = \int_a^b p(x)\,\mathrm{d}x$$

$$P(z) = \int_{-\infty}^{z} p(x)\,\mathrm{d}x$$

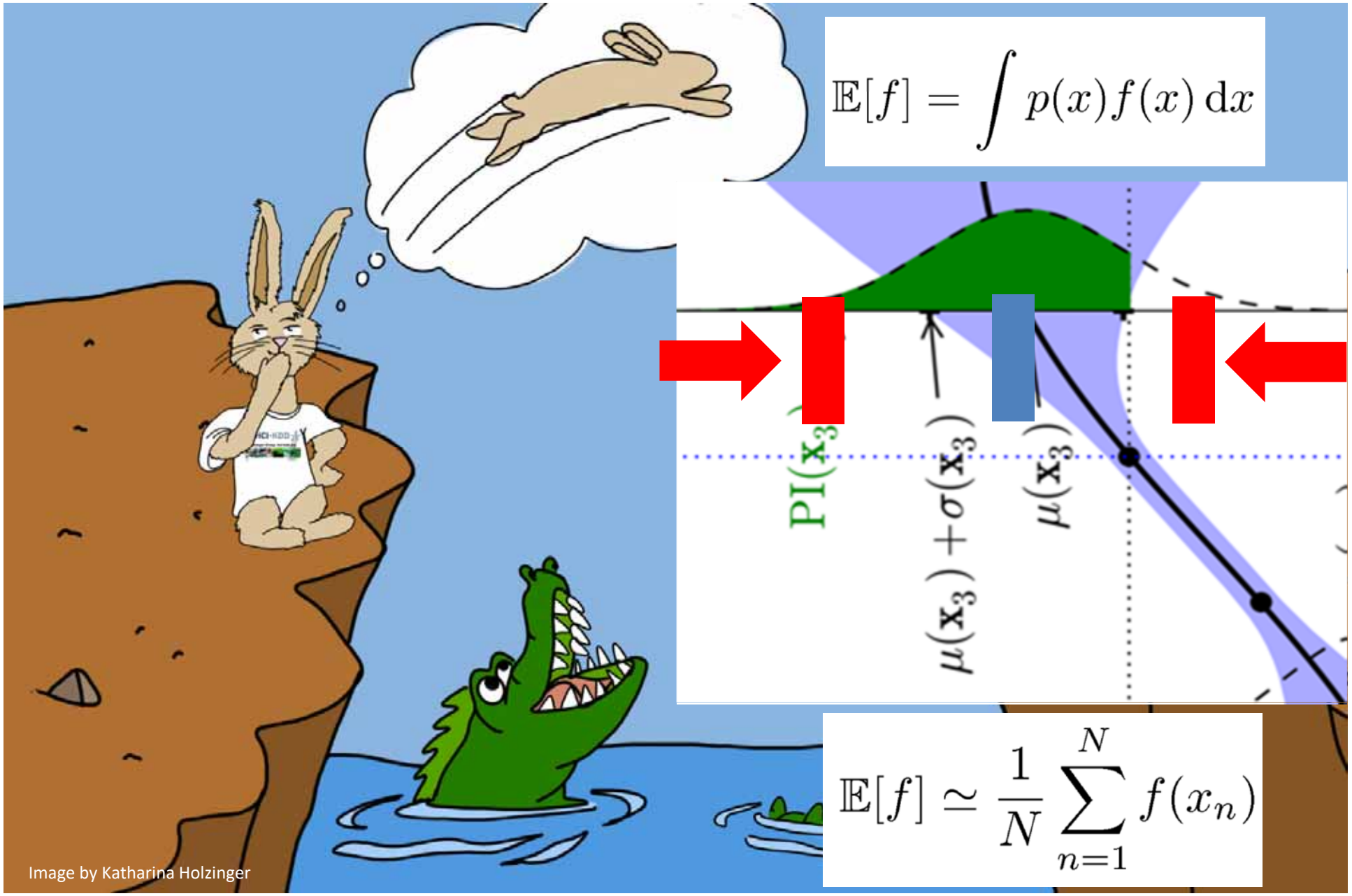
$$p(x) \geqslant 0 \qquad \int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1$$



https://brilliant.org/wiki/multivariate-normal-distribution

02 Expectation and Expected Utility Theory

Estimate Confidence Interval: Uncertainty matters !



Expected Utility Theory $E\ (U|d)$

For a single decision variable an agent can select $D = d$ for any $d \in dom(D)$.

The expected utility of decision $D = d$ is

http://www.eoht.info/page/Oskar+Morgenstern

$$E(U \mid d) = \sum_{x_1,\ldots,x_n} P(x_1,\ldots,x_n \mid d)U(x_1,\ldots,x_n,d)$$

An optimal single decision is the decision $D = dmax$ whose expected utility is maximal:

$$d_{\max} = \arg \max_{d \in \mathrm{dom}(D)} E(U \mid d)$$

John Von Neumann & Oskar Morgenstern 1944. Theory of games and economic behavior, Princeton university press.

03 Joint Probability
Conditional Probability

Independence and Conditional Independence

Please review chapter 2.2.4, page 30 of David Barbers Book, here a summary:

We say that two events are **independent** if their joint probability equals the product of their individual probabilities,

$$p(A, B) = p(A)p(B).$$

In this case we use the notation $A \perp B$. Two random variables are independent if this is true for all values that the random variables can take.

By using the product, we see that two variables are independent iff

$$p(A)p(B) = p(A, B) = p(A|B)p(B),$$

or equivalently that

$$p(A|B) = p(A).$$

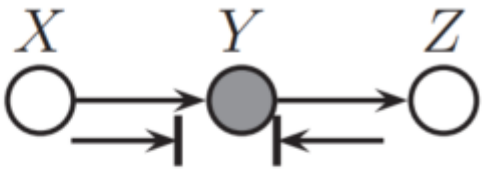
This means that knowing that B happened tells us nothing about the probability of A happening, and vice versa.

A generalization of independence is **conditional independence**, where we consider independence given that we know a third event C occurred,

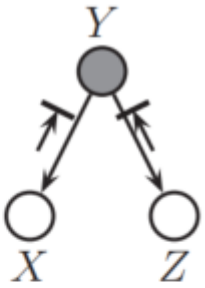
$$p(A, B|C) = p(A|C)p(B|C),$$

and in this case we use the notation $A \perp B \mid C$. Conditional independence is much weaker than marginal independence, and we often make use of it to model high-dimensional probability distributions.

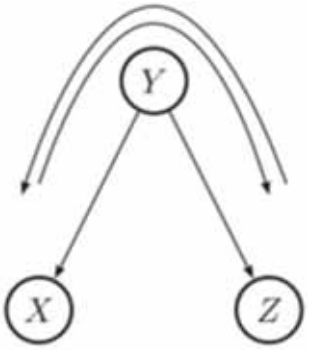
When we condition on y: Are x and z independent?



(a)

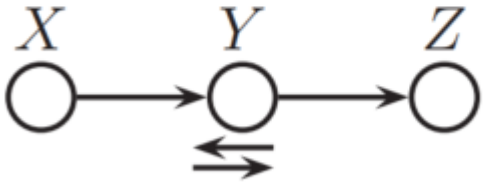


(b)

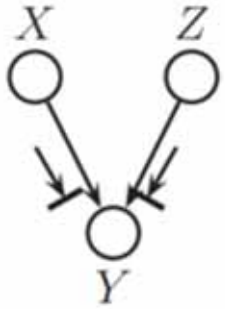


(e)

(c)



(d)



(f)

$$p(x,z|y) = \frac{p(x)p(y|x)p(z|y)}{p(y)} = \frac{p(x,y)p(z|y)}{p(y)} = p(x|y)p(z|y)$$

$$x \perp z|y \qquad X \leftarrow Y \rightarrow Z \qquad p(x,y,z) = p(y)p(x|y)p(z|y)$$

Please review chapter 10.5., page 325 of David Barbers Book

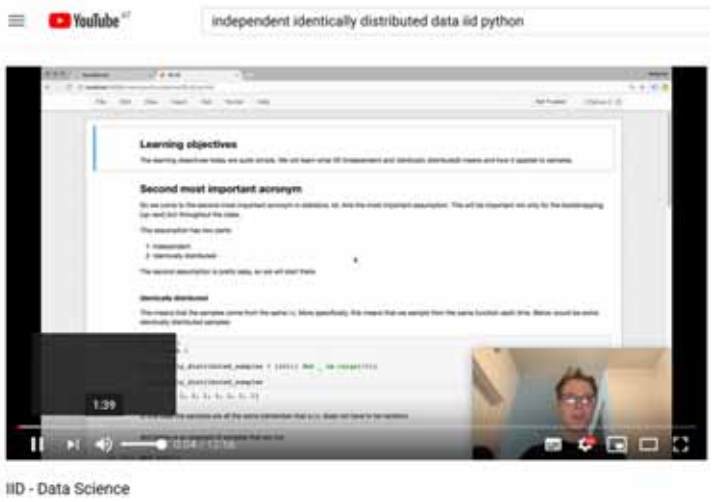
04 Independent Identically distributed (IID, i.i.d.) data

Please review chapter 8.6., page 180ff of David Barbers Book, particularly:

Definition 8.32 (Independent and Identically distributed). For a variable x, and a set of i.i.d. observations, $x^1, \ldots, x^N$, conditioned on θ, we assume there is no dependence between the observations

$$p(x^1, \ldots, x^N|\theta) = \prod_{n=1}^{N} p(x^n|\theta) \tag{8.6.7}$$

Watch these examples: https://www.youtube.com/watch?v=lhzndcgCXeo



05 Bayes and Laplace

Bayes and Laplace on one single slide

$P(x)$	probability of x	$P(\mathcal{D}\|\theta)$	likelihood of θ
$P(x\|\theta)$	conditional probability of x given θ	$P(\theta)$	prior probability of θ
$P(x,\theta)$	joint probability of x and θ	$P(\theta\|\mathcal{D})$	posterior of θ given $\mathcal{D}$

$$P(\theta|\mathcal{D}) = \frac{P(\mathcal{D}|\theta)P(\theta)}{P(\mathcal{D})}$$

$$P(x,\theta) = P(x)P(\theta|x) = P(\theta)P(x|\theta)$$

Bayes Rule:

$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

Marginalization

$$P(x) = \int P(x,\theta)\, d\theta$$

Model Comparison:

$$P(m|\mathcal{D}) = \frac{P(\mathcal{D}|m)P(m)}{P(\mathcal{D})}$$

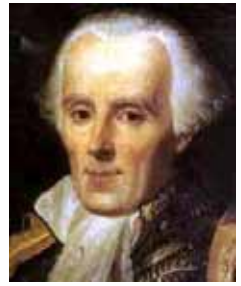
$$P(\mathcal{D}|m) = \int P(\mathcal{D}|\theta,m)P(\theta|m)\, d\theta$$

Prediction:

$$P(x|\mathcal{D},m) = \int P(x|\theta,\mathcal{D},m)P(\theta|\mathcal{D},m)d\theta$$

$$P(x|\mathcal{D},m) = \int P(x|\theta)P(\theta|\mathcal{D},m)d\theta \quad \text{(for many models)}$$

Note: This is probably not Bayes, but this image is heavily in use



Pierre Simon de Laplace (1749-1827)

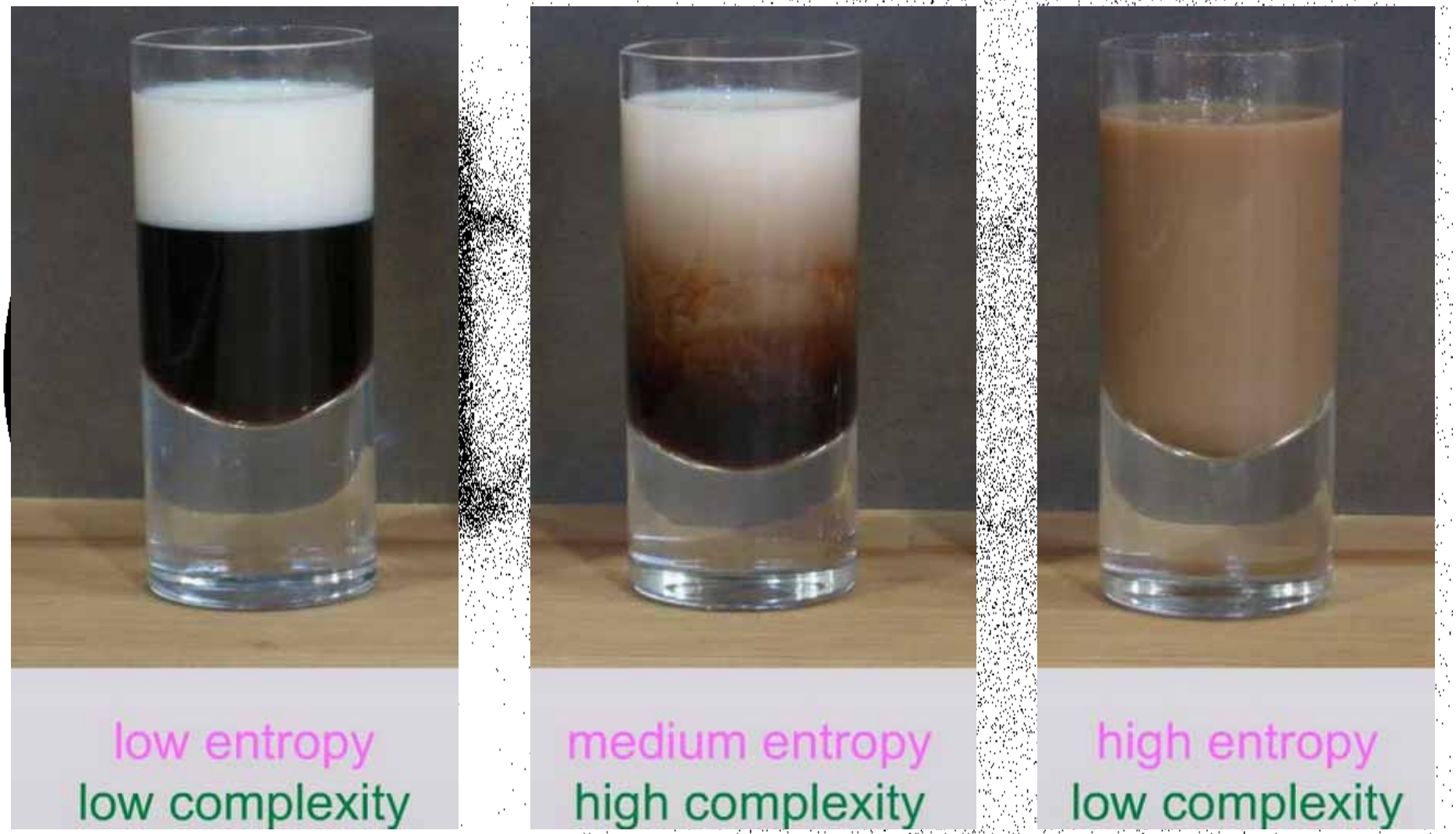
Please refer to the excellent Lectures of Zoubin Ghahramani for profound details, http://mlg.eng.cam.ac.uk/zoubin

06 Measuring Information

- Information is a measure for the reduction of uncertainty
- If something is 100 % certain its uncertainty = 0
- Uncertainty is max. if all choices are equally probable (I.I.D)
- Uncertainty (as information) sums up for independent sources

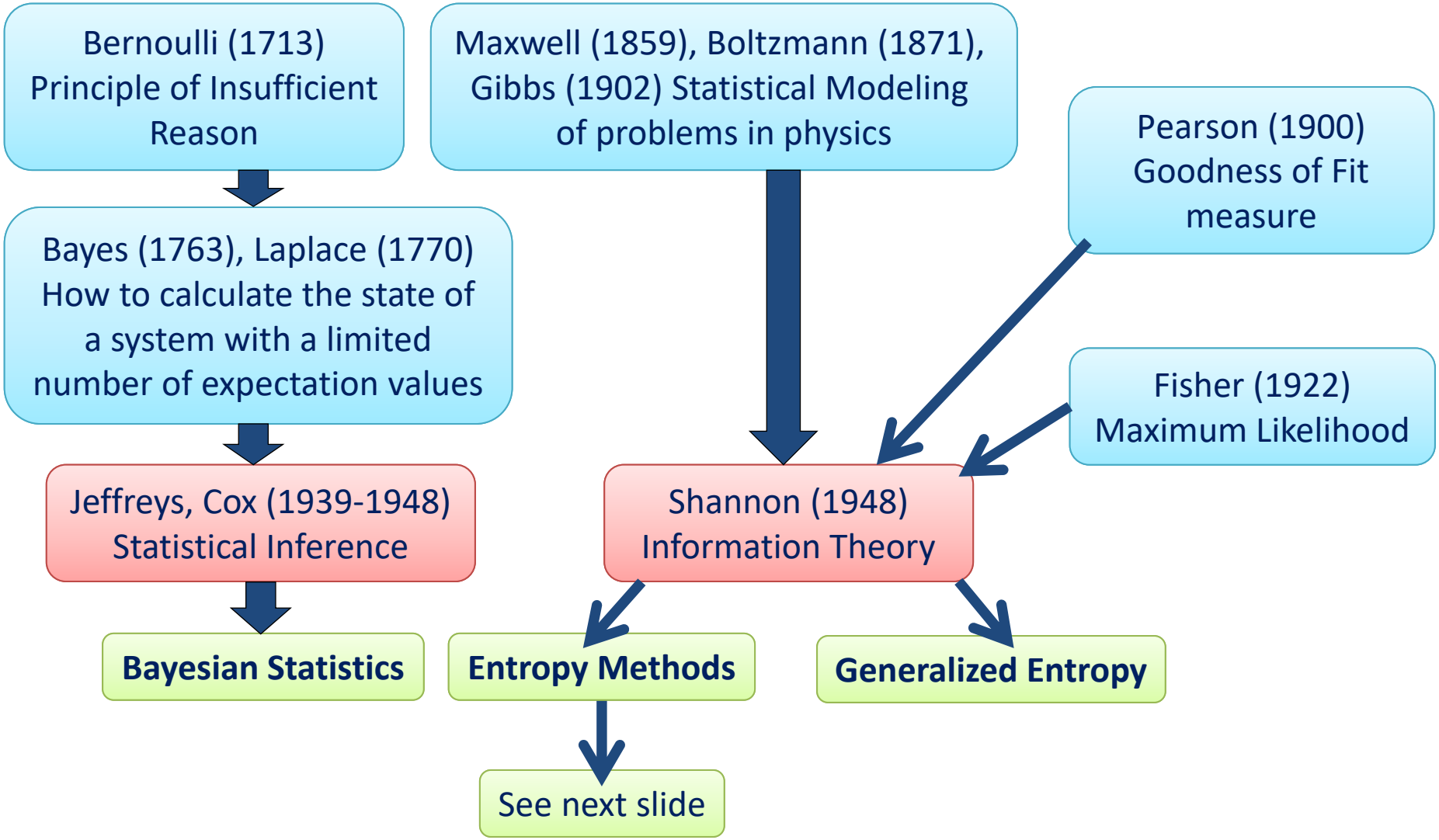
Andreas Holzinger, Matthias Hörtenhuber, Christopher Mayer, Martin Bachler, Siegfried Wassertheurer, Armando Pinho & David Koslicki 2014. On Entropy-Based Data Mining. In: Lecture Notes in Computer Science, LNCS 8401. Berlin Heidelberg: Springer, pp. 209-226, doi:10.1007/978-3-662-43968-5_12.

Entropy as measure for disorder



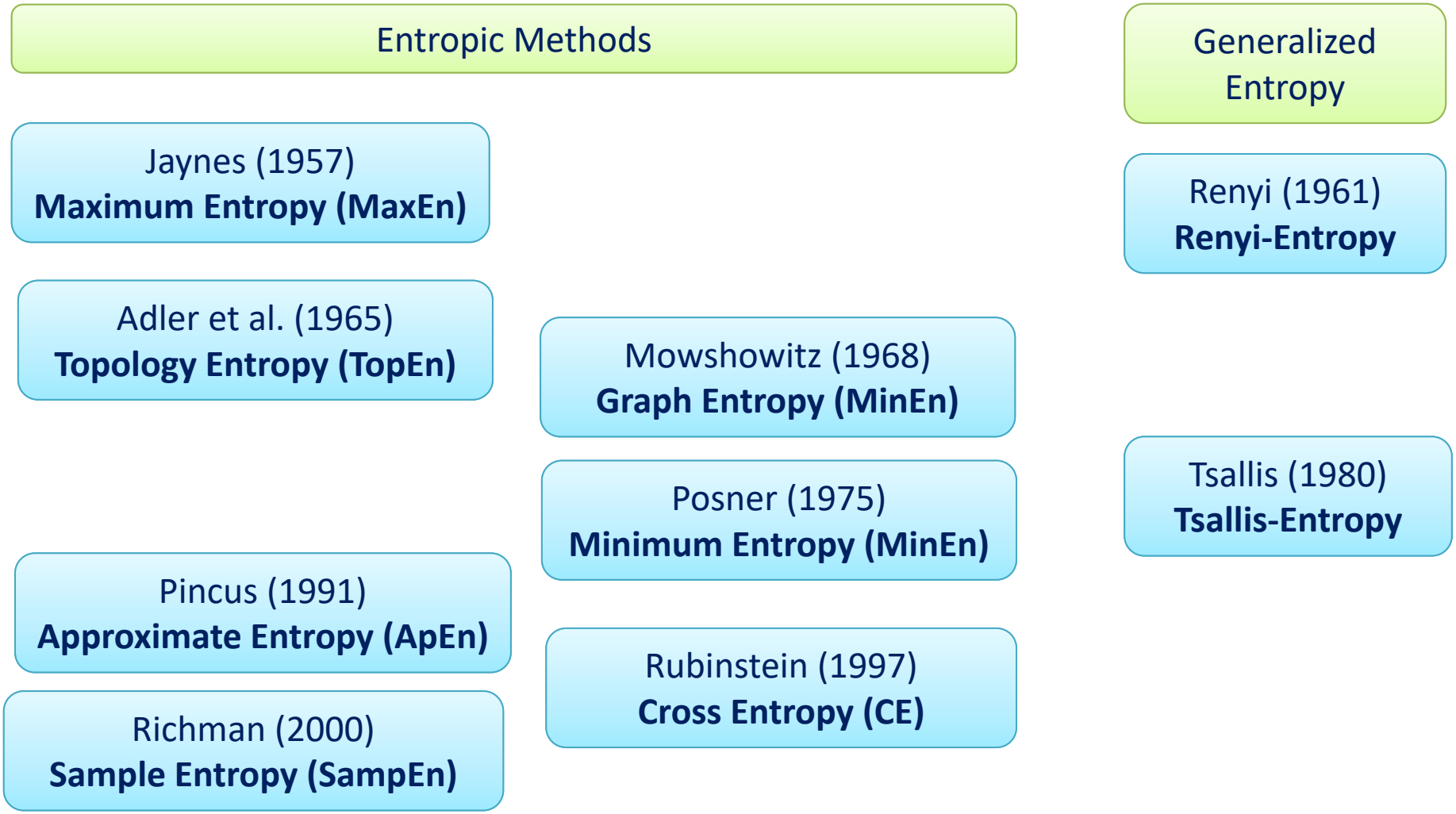
http://www.scottaaronson.com

An overview on the History of Entropy



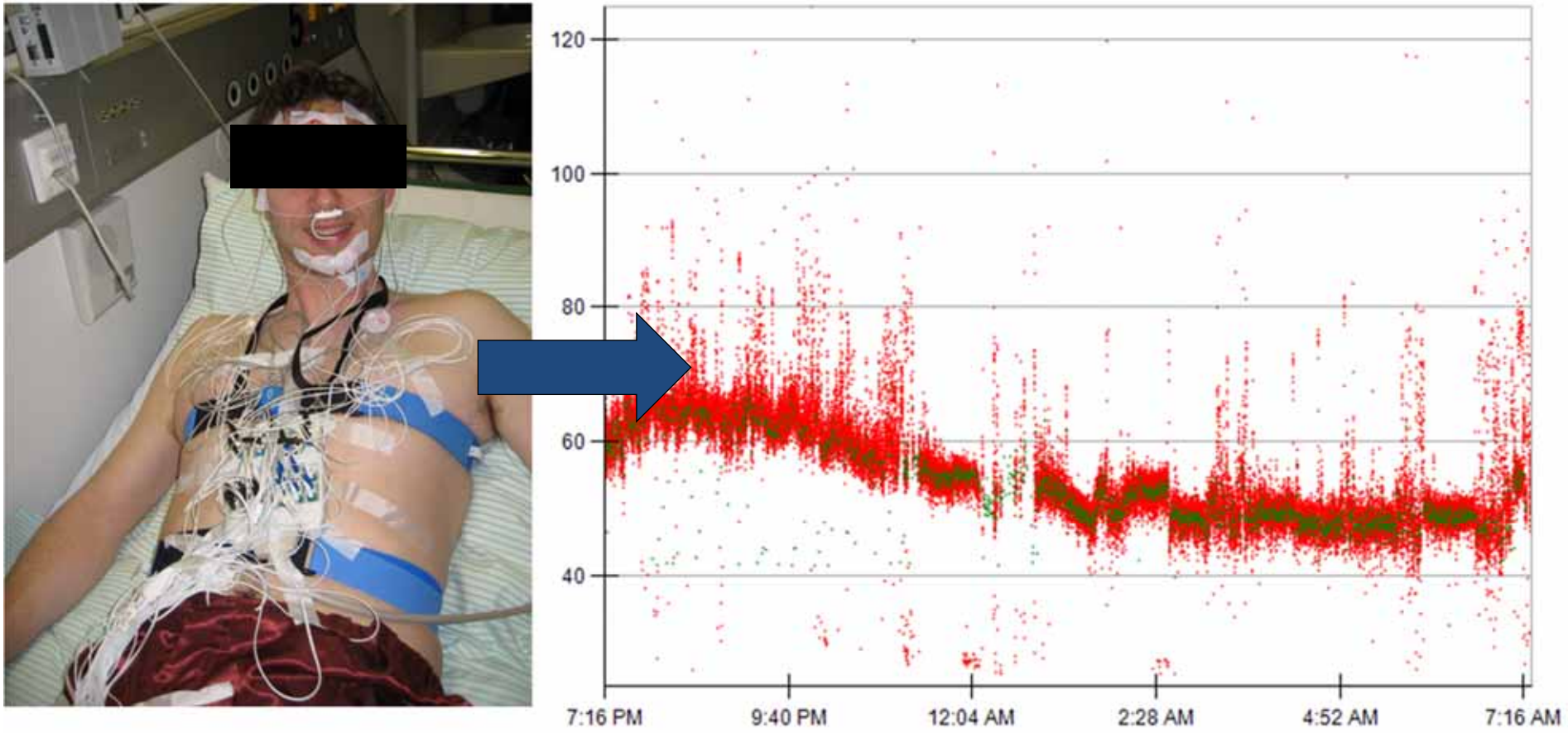
confer also with: Golan, A. (2008) Information and Entropy Econometric: A Review and Synthesis. *Foundations and Trends in Econometrics, 2, 1-2, 1-145*.

Towards a Taxonomy of Entropic Methods



Holzinger, A., Hörtenhuber, M., Mayer, C., Bachler, M., Wassertheurer, S., Pinho, A. & Koslicki, D. 2014. On Entropy-Based Data Mining. In: Holzinger, A. & Jurisica, I. (eds.) Lecture Notes in Computer Science, LNCS 8401. Berlin Heidelberg: Springer, pp. 209-226.

Example of the usefulness of ApEn (1/3)



Holzinger, A., Stocker, C., Bruschi, M., Auinger, A., Silva, H., Gamboa, H. & Fred, A. 2012. On Applying Approximate Entropy to ECG Signals for Knowledge Discovery on the Example of Big Sensor Data. *In: Huang, R., Ghorbani, A., Pasi, G., Yamaguchi, T., Yen, N. & Jin, B. (eds.) Active Media Technology, Lecture Notes in Computer Science, LNCS 7669. Berlin Heidelberg: Springer, pp. 646-657.*

EU Project EMERGE (2007-2010)

Example of the usefulness of ApEn (2/3)

$$Let: \ \langle x_n \rangle = \{x_1, x_2, \dots, x_N\}$$

$$\vec{X}_i = (x_i, x_{(i+1)}, \dots, x_{(i+m-1)})$$

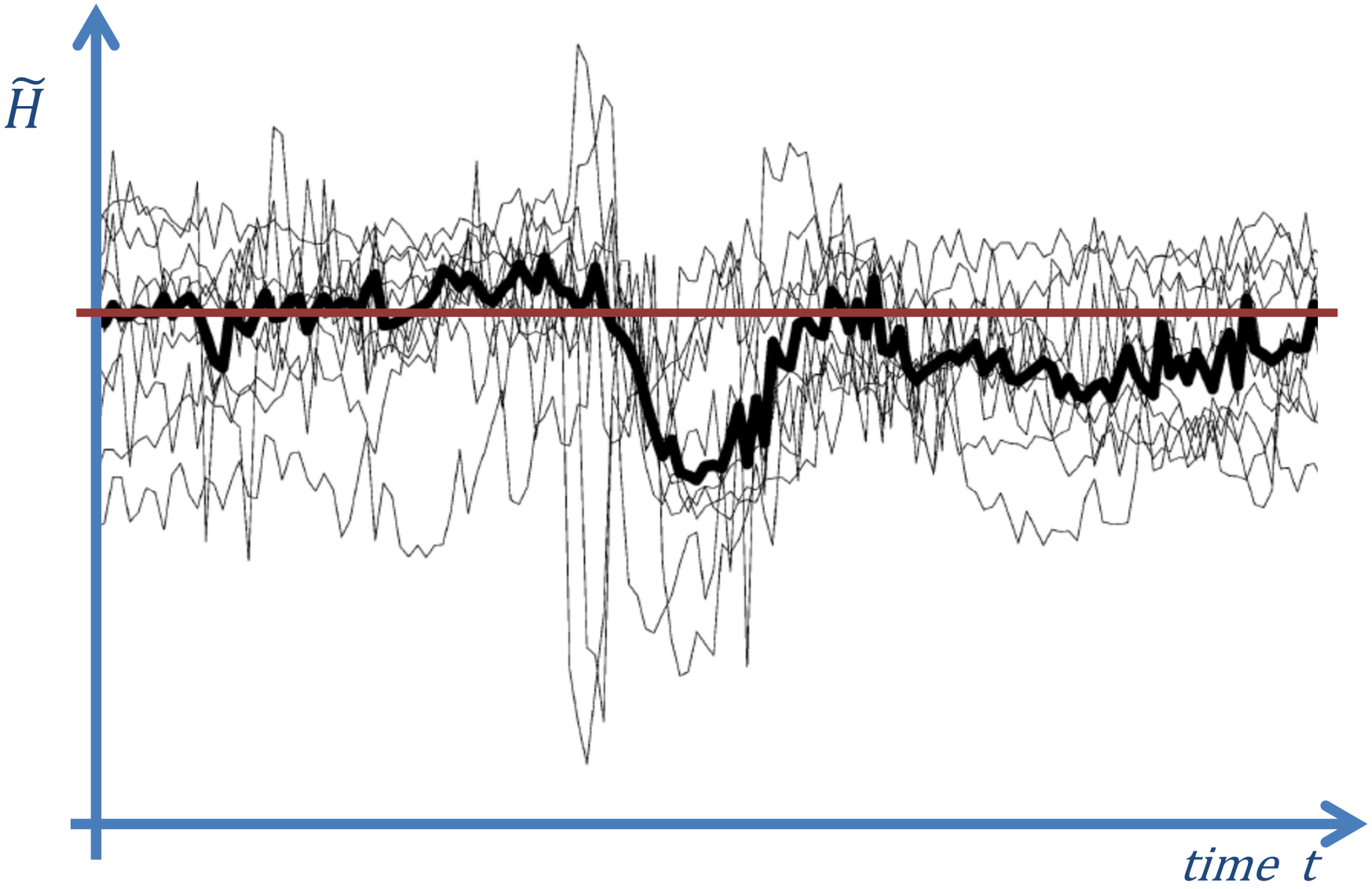
$$\left\| \vec{X}_i , \vec{X}_j \right\| = \max_{k=1,2,\dots,m} \left(\left| x_{(i+k-1)} - x_{(j+k-1)} \right| \right)$$

$$\tilde{\mathrm{H}}(m,r) = \lim_{N \to \infty} [\phi^m(r) - \phi^{m+1}(r)]$$

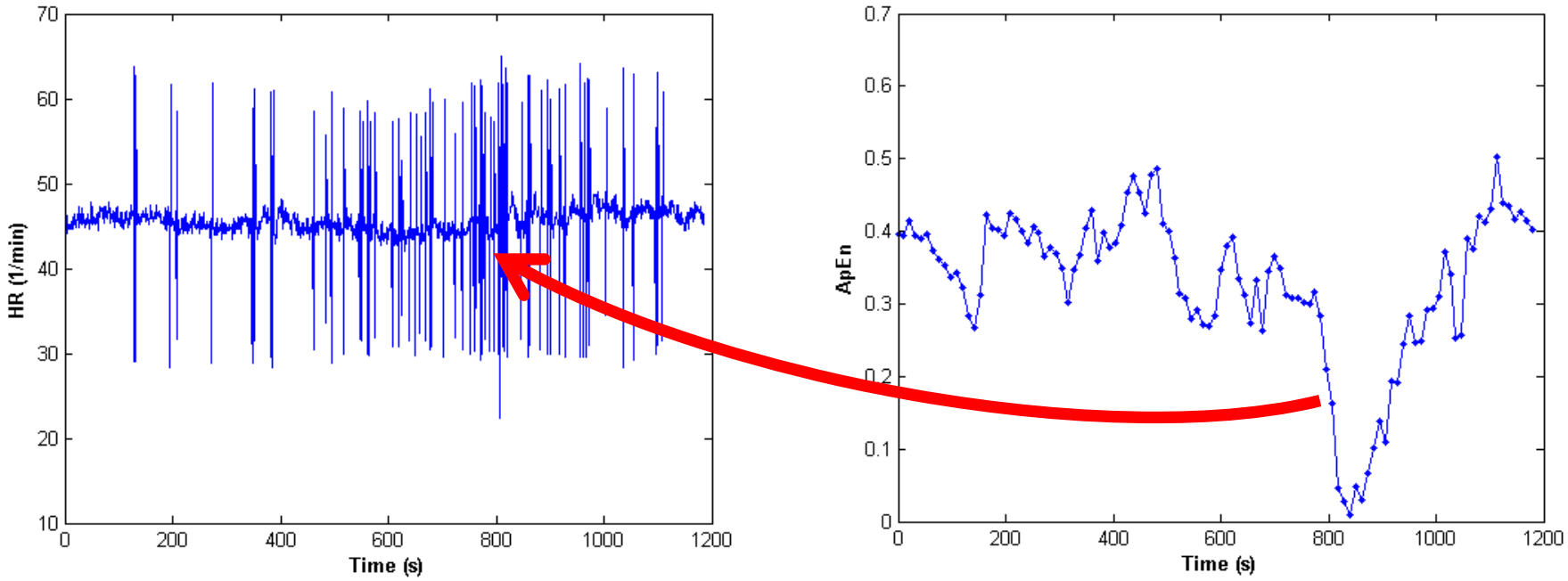
$$C_r^m(i) = \frac{N^m(i)}{N-m+1} \qquad \phi^m(r) = \frac{1}{N-m+1} \sum_{t=1}^{N-m+1} \ln C_r^m(i)$$

Pincus, S. M. (1991) Approximate Entropy as a measure of system complexity. *Proceedings of the National Academy of Sciences of the United States of America, 88, 6, 2297-2301.*

Example: ApEn (2)

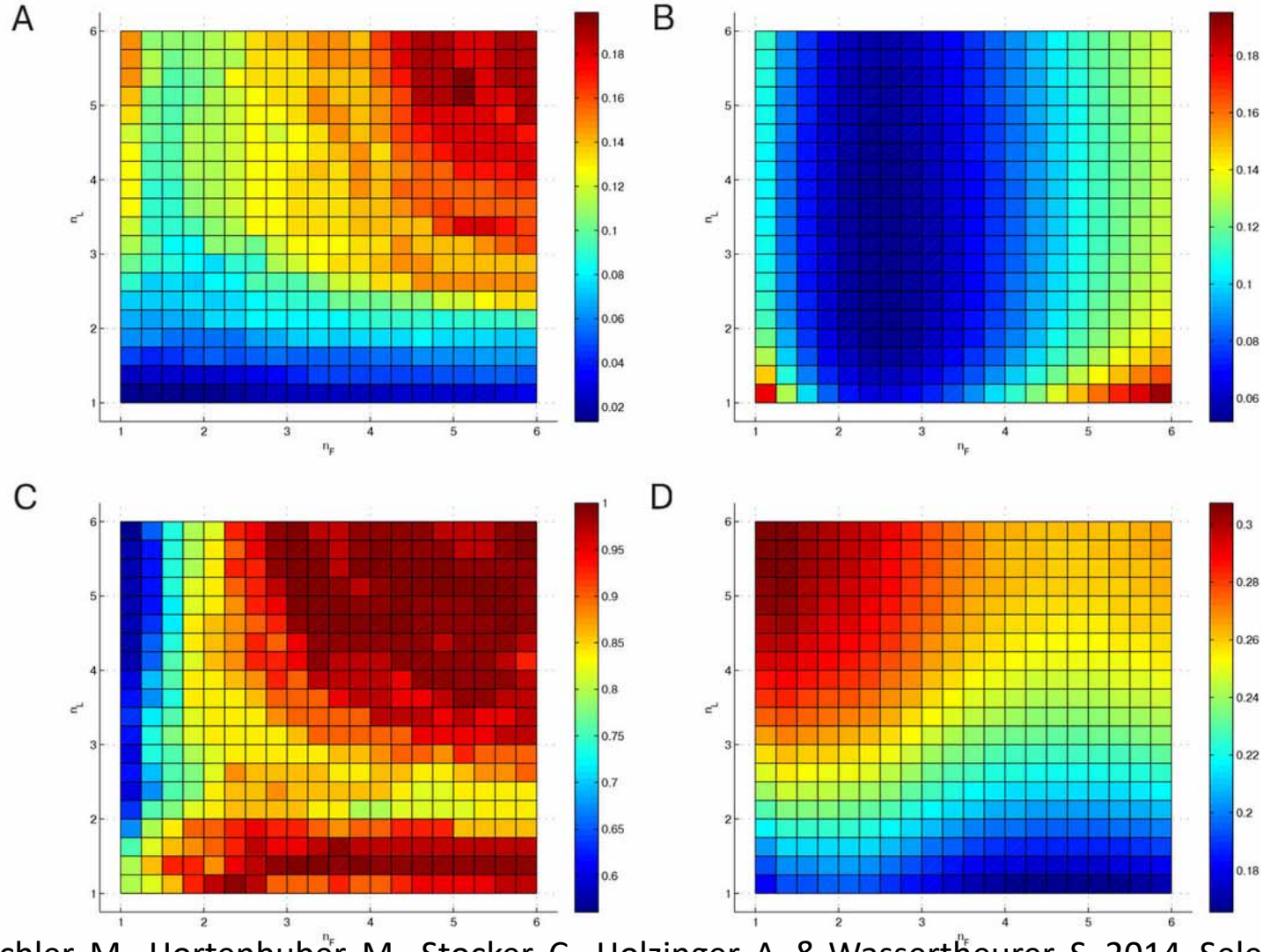


ApEn



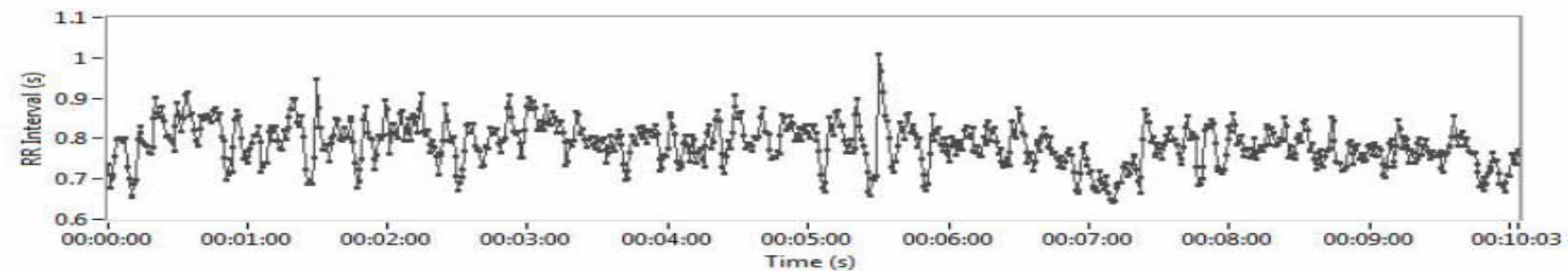
Holzinger, A., Hörtenhuber, M., Mayer, C., Bachler, M., Wassertheurer, S., Pinho, A. & Koslicki, D. 2014. On Entropy-Based Data Mining. In: Holzinger, A. & Jurisica, I. (eds.) Interactive Knowledge Discovery and Data Mining in Biomedical Informatics, Lecture Notes in Computer Science, LNCS 8401. Berlin Heidelberg: Springer, pp. 209-226.

Significance of FuzzyMEn for different nL and nF, N=1000



Mayer, C., Bachler, M., Hortenhuber, M., Stocker, C., Holzinger, A. & Wassertheurer, S. 2014. Selection of entropy-measure parameters for knowledge discovery in heart rate variability data. *BMC Bioinformatics,* 15, (Suppl 6), S2, doi:doi:10.1186/1471-2105-15-S6-S2.

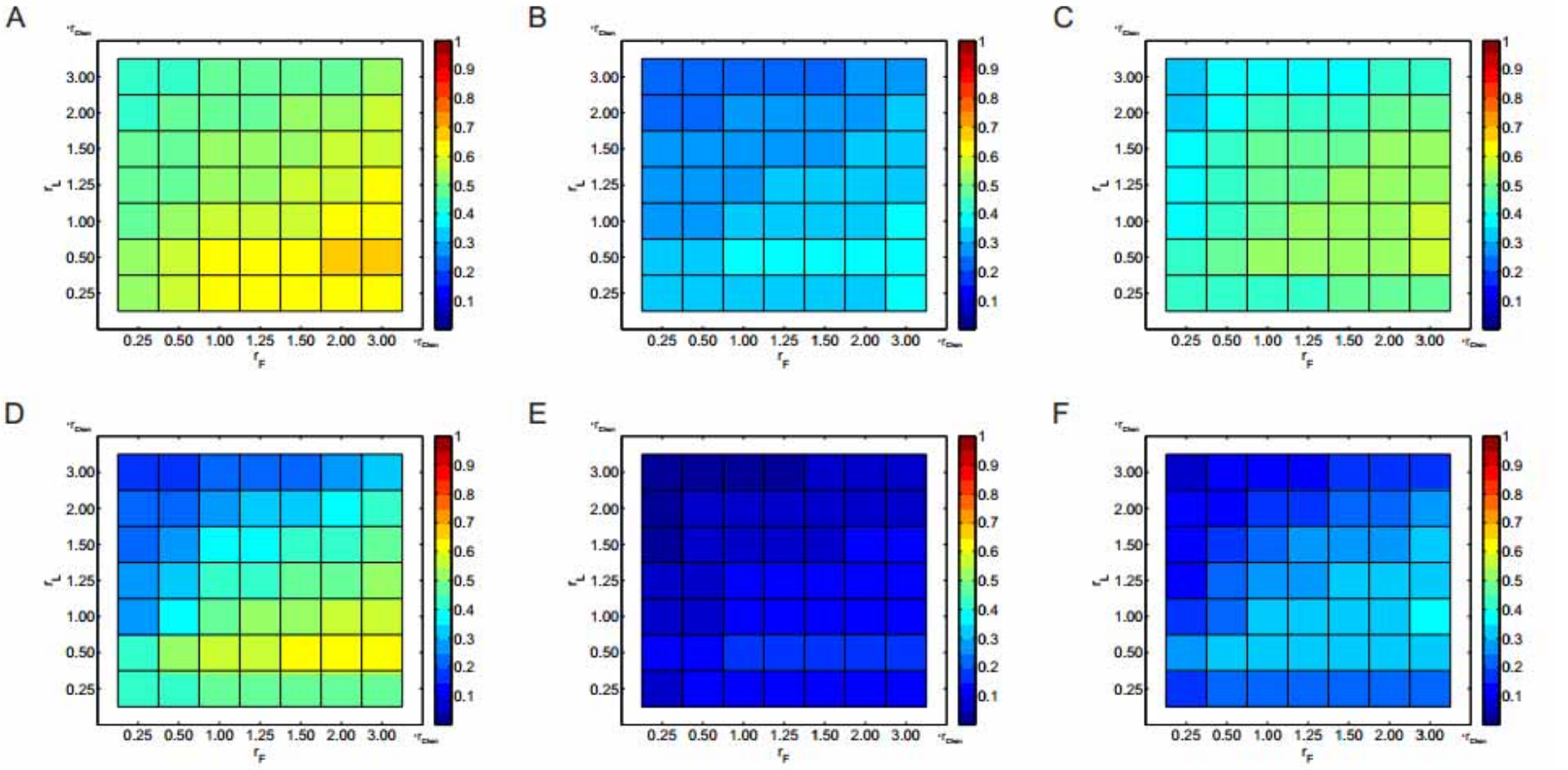
Summary: Example Heart Rate Variability



- Heart Rate Variability (HRV) can be used as a marker of cardiovascular health status.
- Entropy measures represent a family of new methods to quantify the variability of the heart rate.
- Promising approach, due to ability to discover certain patterns and shifts in the "apparent ensemble amount of randomness" of stochastic processes,
- measure randomness and **predictability of processes.**

Mayer, C., Bachler, M., Holzinger, A., Stein, P. K. & Wassertheurer, S. 2016. The Effect of Threshold Values and Weighting Factors on the Association between Entropy Measures and Mortality after Myocardial Infarction in the Cardiac Arrhythmia Suppression Trial (CAST). Entropy, 18, (4), 129, doi::10.3390/e18040129.

Baseline: A,B,C – After treatment: D,E,F N=1200



Mayer, C., Bachler, M., Holzinger, A., Stein, P. K. & Wassertheurer, S. 2016. The Effect of Threshold Values and Weighting Factors on the Association between Entropy Measures and Mortality after Myocardial Infarction in the Cardiac Arrhythmia Suppression Trial (CAST). Entropy, 18, (4), 129, doi::10.3390/e18040129.

Cross-Entropy
Kullback-Leibler
Divergence

- Entropy:
  - Measure for the **uncertainty** of random variables
- Kullback-Leibler divergence:
  - **comparing two distributions**
- Mutual Information:
  - measuring the **correlation** of two random variables

Solomon Kullback & Richard Leibler (1951)

ON INFORMATION AND SUFFICIENCY

By S. Kullback and R. A. Leibler

The George Washington University and Washington, D. C.

1. Introduction. This note generalizes to the abstract case Shannon's definition of information [15], [16]. Wiener's information (p. 75 of [18]) is essentially the same as Shannon's although their motivation was different (cf. footnote 1, p. 95 of [16]) and Shannon apparently has investigated the concept more completely. R. A. Fisher's definition of information (intrinsic accuracy) is well known (p. 709 of [6]). However, his concept is quite different from that of Shannon and Wiener, and hence ours, although the two are not unrelated as is shown in paragraph 2.

R. A. Fisher, in his original introduction of the *criterion of sufficiency*, required "that the statistic chosen should summarize the whole of the relevant information supplied by the sample," (p. 316 of [5]). Halmos and Savage in a recent paper, one of the main results of which is a generalization of the well known Fisher-Neyman theorem on sufficient statistics to the abstract case, conclude, "We think that confusion has from time to time been thrown on the subject by . . . , and (c) the assumption that a sufficient statistic contains all the information in only the technical sense of 'information' as measured by variance," (p. 241 of [8]). It is shown in this note that the information in a sample as defined herein, that is, in the Shannon-Wiener sense cannot be increased by any statistical operations and is invariant (not decreased) if and only if sufficient statistics are employed. For a similar property of Fisher's information see p. 717 of [6], Doob [19].

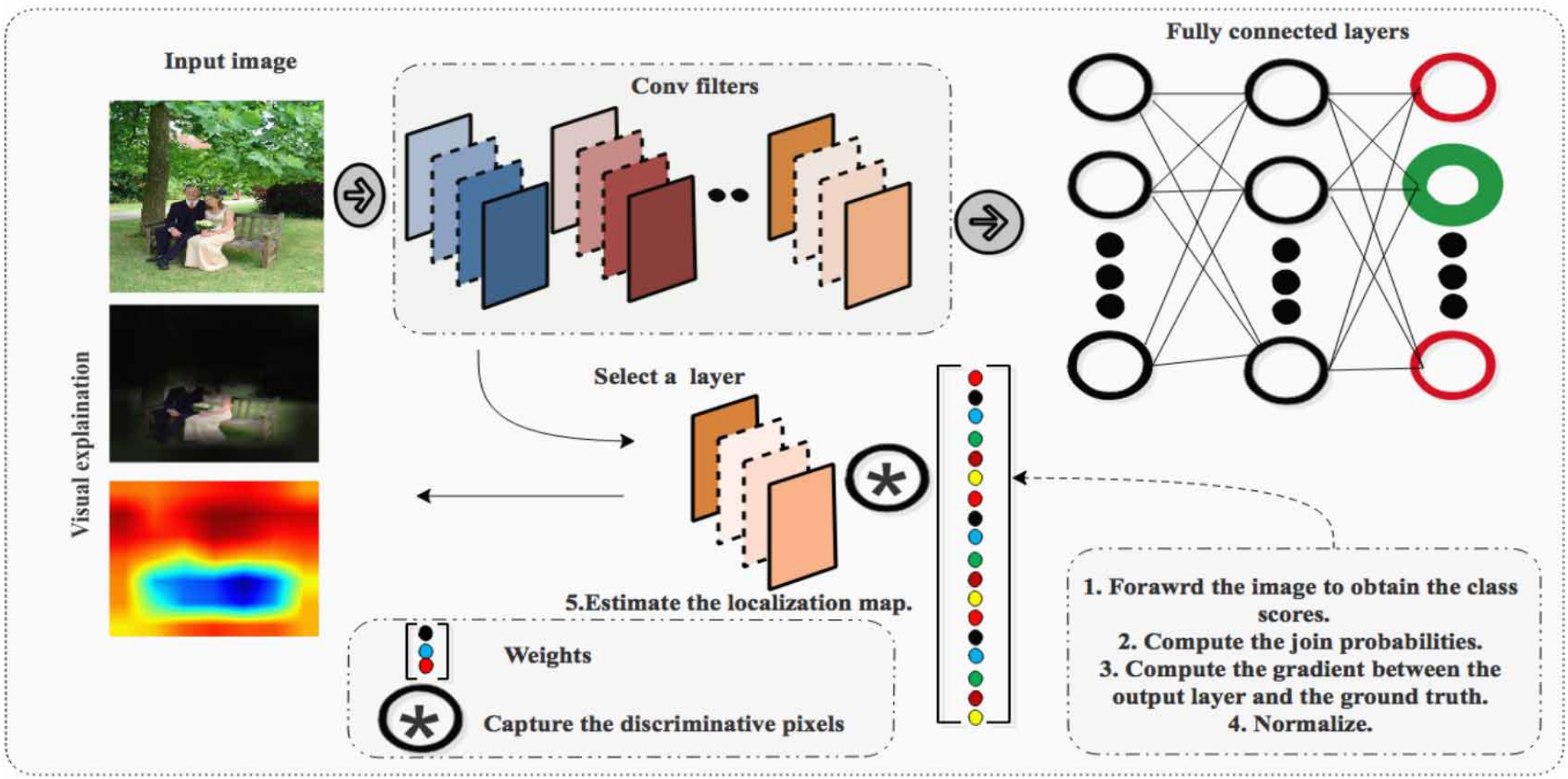
We are also concerned with the statistical problem of discrimination ([3], [17]), by considering a measure of the "distance" or "divergence" between statistical populations ([1], [2], [13]) in terms of our measure of information. For the statistician two populations differ more or less according as to how difficult it is to discriminate between them with the best test [14]. The particular measure of divergence we use has been considered by Jeffreys ([10], [11]) in another connection. He is primarily concerned with its use in providing an invariant density of *a priori* probability. A special case of this divergence is Mahalanobis' generalized distance [13].

Solomon Kullback
1907-1994

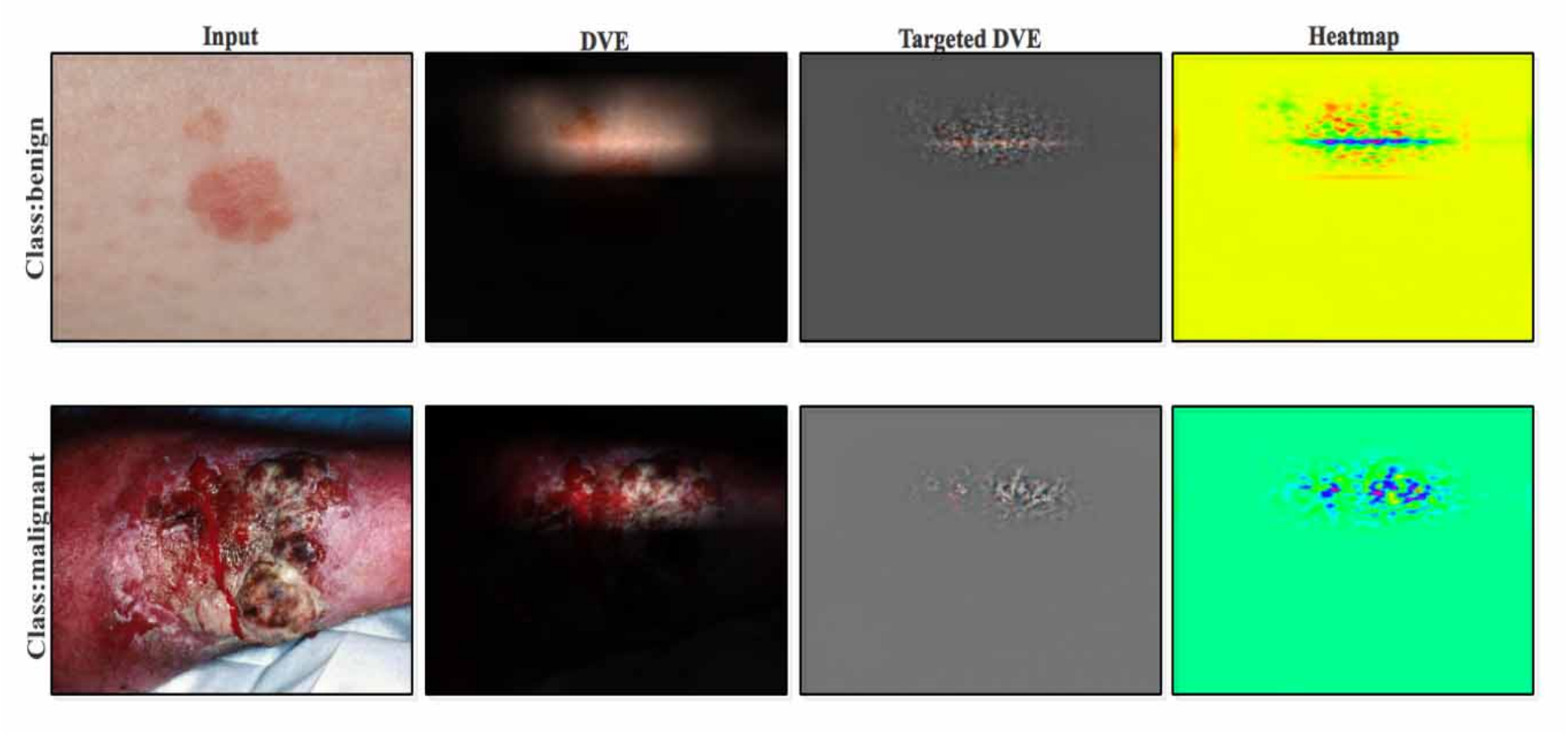
Richard Leibler
1914-2003

Kullback, S. & Leibler, R. A. 1951. On information and sufficiency. The annals of mathematical statistics, 22, (1), 79-86, www.jstor.org/stable/2236703

Deep Learning Explainability



Housam Khalifa Bashier Babiker & Randy Goebel 2017. Using KL-divergence to focus Deep Visual Explanation. arXiv preprint arXiv:1711.06431.



Housam Khalifa Bashier Babiker & Randy Goebel 2017. An Introduction to Deep Visual Explanation. arXiv preprint arXiv:1711.09482.

$$p_{ij} = \frac{(1 + ||k_i - k_j||^2)^{-1}}{\sum_{u \neq v}(1 + ||k_u - k_v||^2)^{-1}} \quad (1)$$

Here p_{ij} denotes the joint probabilities, k is the raw class scores before softmax , i indexes a neuron value and $\sum_{u \neq v}$ combines all the values. For the ground truth we estimate the pairwise affinities with perplexity. We then compute the KL-divergence gradient i.e. $\frac{\delta y'}{\delta y} \Rightarrow z$ derived here [6]. We also normalize the gradient to a zero mean and unit variance as follows:

$$\alpha = \frac{z - \mu}{\sigma z} \quad (2)$$

The obtained weights α capture the relevant information in the feature maps acquired by the network. These weights are applied to every feature map $x_i \in X$ as to identify the discriminative pixels which influence the final prediction output as follows:

$$E_{KL-divergence} = \sum_i \sum_j x_i * |\alpha_j| \quad (3)$$

Housam Khalifa Bashier Babiker & Randy Goebel 2017. Using KL-divergence to focus Deep Visual Explanation. arXiv preprint arXiv:1711.06431.

Algorithm 1 Proposed approach

Input: image, ground truth y
Output: Discriminative localization map $\Rightarrow E_{KL-divergence}$

Apply a single forward-pass to estimate $\Rightarrow y^{'}$
Compute the joint probabilities for both $y^{'}$ and y
Compute the gradient and normalize using (2) $\Rightarrow \alpha$
initialize $E_{KL-divergence}$ to zero
for $i = 1$ **to** $nFeatureMaps$ **do**
  Initialize temp to zero
  for $j = 1$ **to** $sizeof\alpha$ **do**
    $temp \leftarrow temp + (x_i * |\alpha_j|)$
end for
  $E_{KL-divergence} \leftarrow E_{KL-divergence} + temp$
end for

Housam Khalifa Bashier Babiker & Randy Goebel 2017. Using KL-divergence to focus Deep Visual Explanation. arXiv preprint arXiv:1711.06431.

Remember Shannon Entropy

$$\mathrm{H}[x] = -\sum_{x} p(x) \log_2 p(x)$$

Shannon, C. E. 1948. A Mathematical Theory of Communication. Bell System Technical Journal, 27, 379-423.

Important quantity in

- coding theory
- statistical physics
- machine learning

$$\mathrm{H}[\mathbf{y}|\mathbf{x}] = -\iint p(\mathbf{y},\mathbf{x}) \ln p(\mathbf{y}|\mathbf{x}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x}$$

$$\mathrm{H}[\mathbf{x},\mathbf{y}] = \mathrm{H}[\mathbf{y}|\mathbf{x}] + \mathrm{H}[\mathbf{x}]$$

The Kullback-Leibler Divergence

$$\mathrm{KL}(p\|q) = -\int p(\mathbf{x}) \ln q(\mathbf{x})\, \mathrm{d}\mathbf{x} - \left(-\int p(\mathbf{x}) \ln p(\mathbf{x})\, \mathrm{d}\mathbf{x}\right)$$

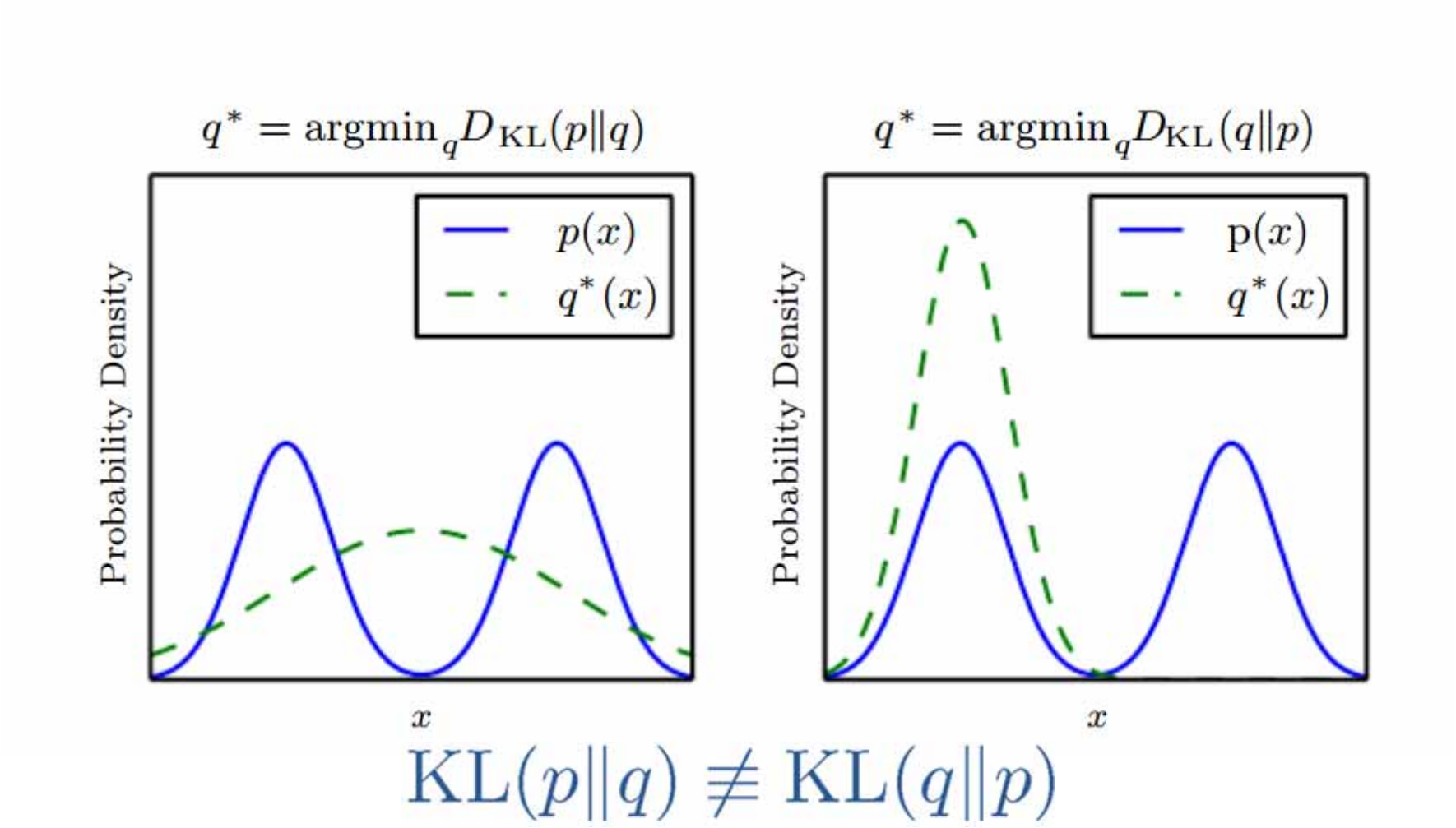
$$= -\int p(\mathbf{x}) \ln \left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\} \mathrm{d}\mathbf{x}$$

$$\mathrm{KL}(p\|q) \simeq \frac{1}{N} \sum_{n=1}^{N} \{-\ln q(\mathbf{x}_n|\boldsymbol{\theta}) + \ln p(\mathbf{x}_n)\}$$

$$\mathrm{KL}(p\|q) \geqslant 0$$

KL-divergence is often used to measure the distance between two distributions

Note: KL is not symmetric!



Goodfellow, I., Bengio, Y. & Courville, A. 2016. Deep Learning, Cambridge (MA), MIT Press.

- … are **robust** against noise;
- … can be applied to **complex time series** with good replication;
- … is **finite** for stochastic, noisy, composite processes;
- … the values correspond directly to irregularities – good for detecting **anomalies**

Mutual Information and Point Wise MI

$$\begin{aligned} \mathrm{I}[\mathbf{x},\mathbf{y}] &\equiv \mathrm{KL}(p(\mathbf{x},\mathbf{y})\|p(\mathbf{x})p(\mathbf{y})) \\ &= -\iint p(\mathbf{x},\mathbf{y}) \ln\left(\frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x},\mathbf{y})}\right) \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} \end{aligned}$$

$$\mathrm{I}[\mathbf{x},\mathbf{y}] = \mathrm{H}[\mathbf{x}] - \mathrm{H}[\mathbf{x}|\mathbf{y}] = \mathrm{H}[\mathbf{y}] - \mathrm{H}[\mathbf{y}|\mathbf{x}]$$

- Measures how much reduction in uncertainty of X given the information about Y
- Measures correlation between X and Y
- Related to the "channel capacity" in the original Shannon information theory

Bishop, C. M. 2007. *Pattern Recognition and Machine Learning,* Heidelberg, Springer.

Example: Disease-Disease Relationship

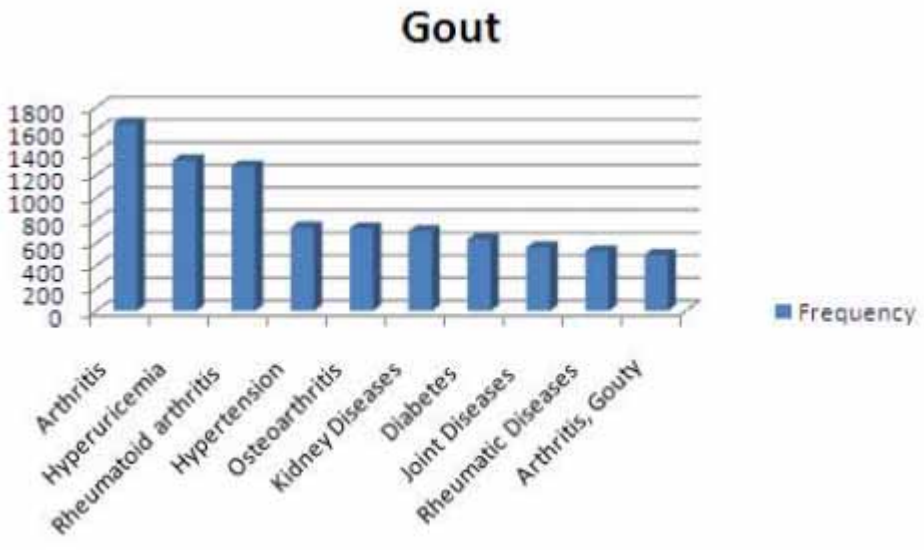
Let two words, w_i and w_j, have probabilities $P(w_i)$ and $P(w_j)$.
Then their mutual information $PMI\ (w_i, w_j)$ is defined as:

$$PMI(w_i, w_j) = \log\left(\frac{P(w_i, w_j)}{P(w_i)\,P(w_j)}\right)$$

For w_i denoting *rheumatoid arthritis* and w_j representing *diffuse scleritis* the following simple calculation yields:

$$P(w_i) = \frac{94{,}834}{20{,}033{,}079}, \quad P(w_j) = \frac{74}{20{,}033{,}079}$$

$$P(w_i, w_j) = \frac{13}{94{,}834}, \quad PMI(w_i, w_j) = 7{,}7.$$



Holzinger, A., Simonic, K. M. & Yildirim, P. Disease-Disease Relationships for Rheumatic Diseases: Web-Based Biomedical Textmining an Knowledge Discovery to Assist Medical Decision Making. 36th Annual IEEE Computer Software and Applications Conference (COMPSAC), 16-20 July 2012 2012 Izmir. IEEE, 573-580, doi:10.1109/COMPSAC.2012.77.

$$SCP(x,y) = p(x|y) \cdot p(y|x) = \frac{p(x,y)}{p(y)} \cdot \frac{p(x,y)}{p(x)} = \frac{p(x,y)^2}{p(x) \cdot p(y)}$$

Table 4 Comparison of FACTAs ranking of related concepts from the category Symptom for the query "rheumatoid arthritis" created by the methods co-occurrence frequency, PMI, and SCP

Frequency		PMI		SCP	
pain	5667	impaired body balance	7,8	swollen joints	0.002
Arthralgia	661	ASPIRIN INTOLERANCE	7,8	pain	0.001
fatigue	429	Epitrochlear lymphadenopathy	7,8	Arthralgia	0.001
diarrhea	301	swollen joints	7,4	fatigue	0.000
swollen joints	299	Joint tenderness	7	erythema	0.000
erythema	255	Occipital headache	6,2	splenomegaly	0.000
Back Pain	254	Neuromuscular excitation	6,2	Back Pain	0.000
headache	239	Restless sleep	5,8	polymyalgia	0.000
splenomegaly	228	joint crepitus	5,7	joint stiffness	0.000
Anesthesia	221	joint symptom	5,5	Joint tenderness	0.000
dyspnea	218	Painful feet	5,5	hip pain	0.000
weakness	210	feeling of malaise	5,5	metatarsalgia	0.000
nausea	199	Homan's sign	5,4	Skin Manifestations	0.000
Recovery of Function	193	Diffuse pain	5,2	neck pain	0.000
low back pain	167	Palmar erythema	5,2	Eye Manifestations	0.000
abdominal pain	141	Abnormal sensation	5,2	low back pain	0.000

Holzinger, A., Yildirim, P., Geier, M. & Simonic, K.-M. 2013. Quality-Based Knowledge Discovery from Medical Text on the Web. In: Pasi, G., Bordogna, G. & Jain, L. C. (eds.) Quality Issues in the Management of Web Information, Intelligent Systems Reference Library, ISRL 50. Berlin Heidelberg: Springer, pp. 145-158, doi:10.1007/978-3-642-37688-7_7.

- 1) Challenges include –omics data analysis, where KL divergence and related concepts could provide important **measures** for discovering biomarkers.
- 2) Hot topics are new entropy measures suitable for computations in the context of complex/uncertain data for ML algorithms.
- Inspiring is the abstract geometrical setting underlying ML main problems, e.g. Kernel functions can be completely understood in this perspective. Future work may include entropic concepts and geometrical settings.

- The case of higher order statistical structure in the data – nonlinear and hierarchical ?
- Outliers in the data – noise models?

- There are $\frac{D(D+1)}{2}$ parameters in a multi-variate Gaussian model – what happens if $D \gg$?

dimensionality reduction

Thank you!