

# Workshop Information Theory as a Bridge Across the Geosciences and Modeling Sciences

Uwe Ehret (KIT)

Introduction to Information Theory

# Overview

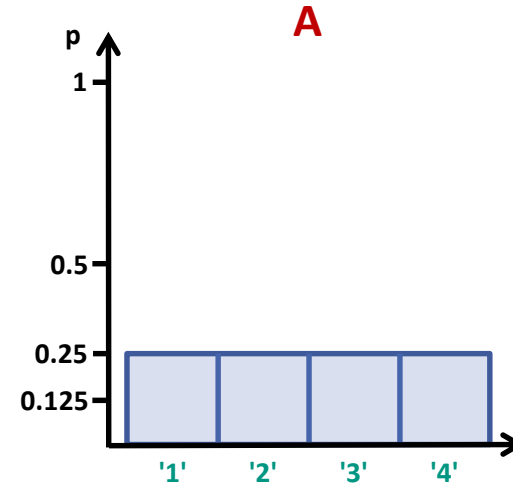
- Introduction
- Basics
- Limits
- Independence, Redundancy, Synergy
- Conservation, Dissipation, Innovation
- Applications
- Further reading

# Introduction

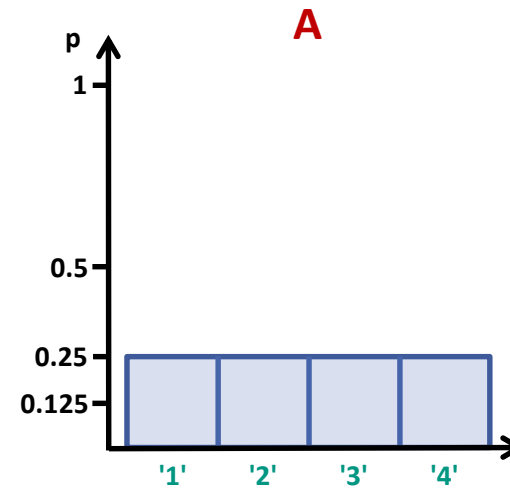
# Introduction

Data  $\neq$  Information

# Introduction



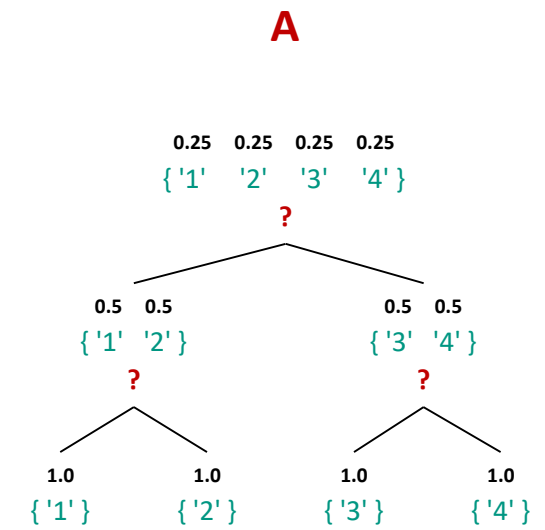
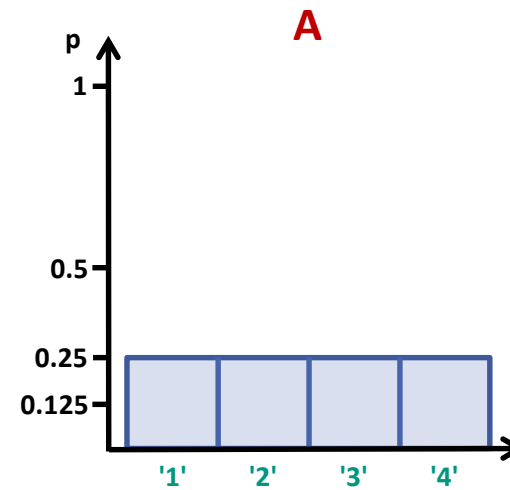
# Introduction



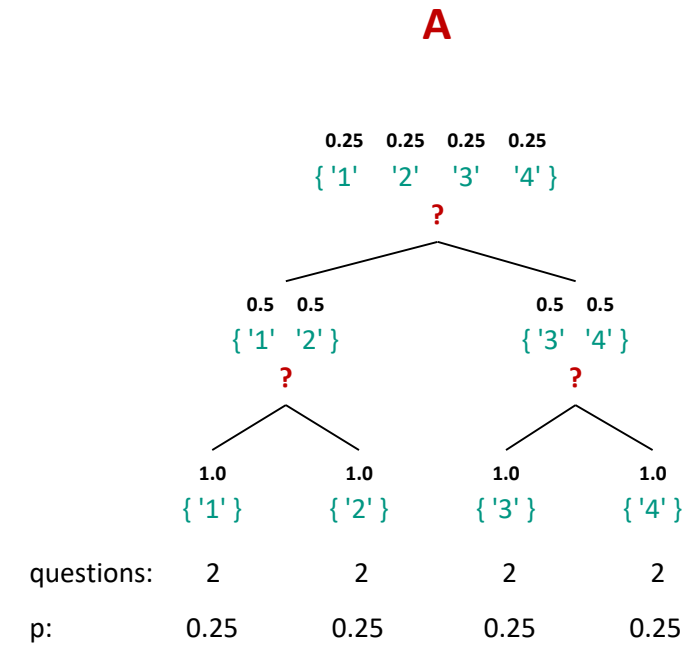
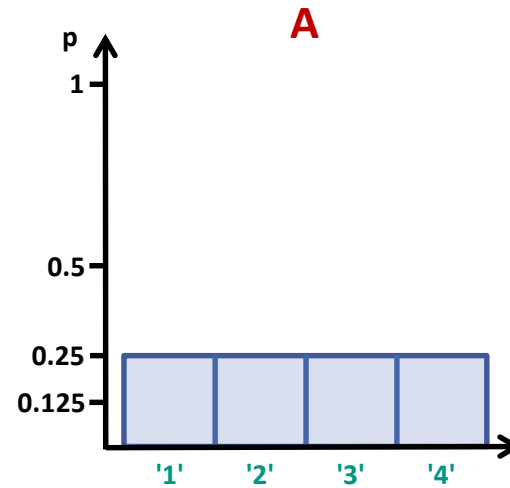
A

0.25 0.25 0.25 0.25  
{ '1' '2' '3' '4' }

# Introduction



# Introduction

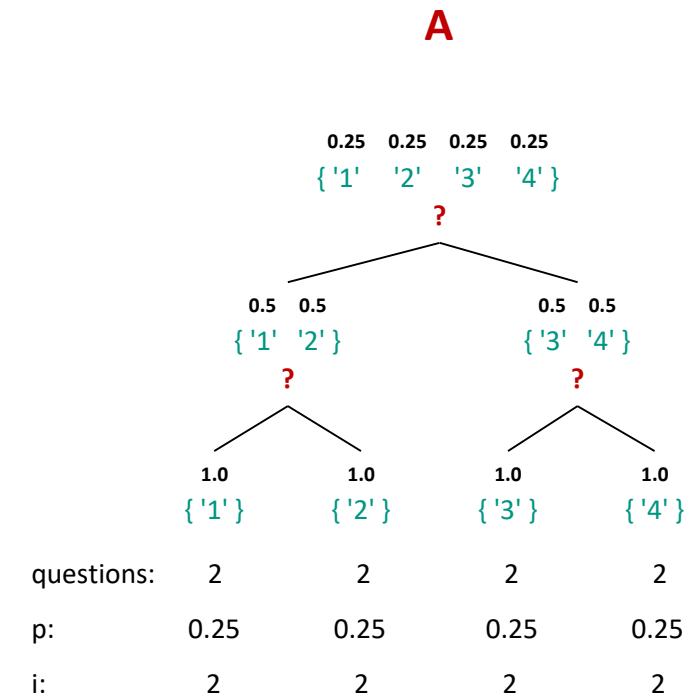
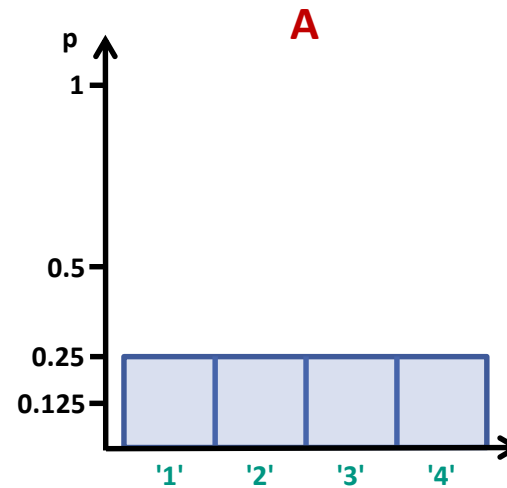




# Basics

## Information

$$i(x) = -\log_2(p(x))$$



# History

## ■ The "Big Bang" of Information Theory



$$i(x) = -\log_2(p(x))$$

### A Mathematical Theory of Communication

By C. E. SHANNON

#### INTRODUCTION

THE recent development of various methods of modulation such as PCM and PPM which exchange bandwidth for signal-to-noise ratio has intensified the interest in a general theory of communication. A basis for such a theory is contained in the important papers of Nyquist<sup>1</sup> and Hartley<sup>2</sup> on this subject. In the present paper we will extend the theory to include a number of new factors, in particular the effect of noise in the channel, and the savings possible due to the statistical structure of the original message and due to the nature of the final destination of the information.

The fundamental problem of communication is that of reproducing at one point either exactly or approximately a message selected at another point. Frequently the messages have *meaning*; that is they refer to or are correlated according to some system with certain physical or conceptual entities. These semantic aspects of communication are irrelevant to the engineering problem. The significant aspect is that the actual message is one *selected from a set* of possible messages. The system must be designed to operate for each possible selection, not just the one which will actually be chosen since this is unknown at the time of design.

If the number of messages in the set is finite then this number or any monotonic function of this number can be regarded as a measure of the information produced when one message is chosen from the set, all choices being equally likely. As was pointed out by Hartley the most natural choice is the logarithmic function. Although this definition must be generalized considerably when we consider the influence of the statistics of the message and when we have a continuous range of messages, we will in all cases use an essentially logarithmic measure.

The logarithmic measure is more convenient for various reasons:

1. It is practically more useful. Parameters of engineering importance

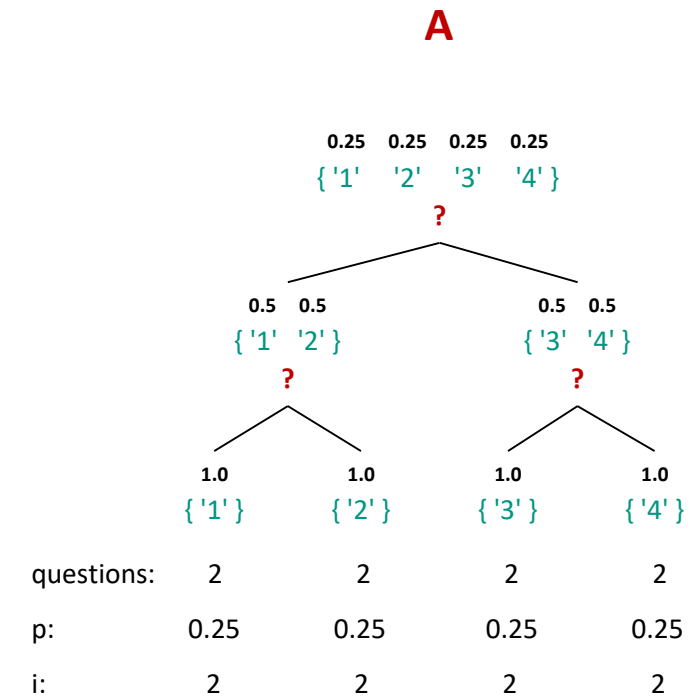
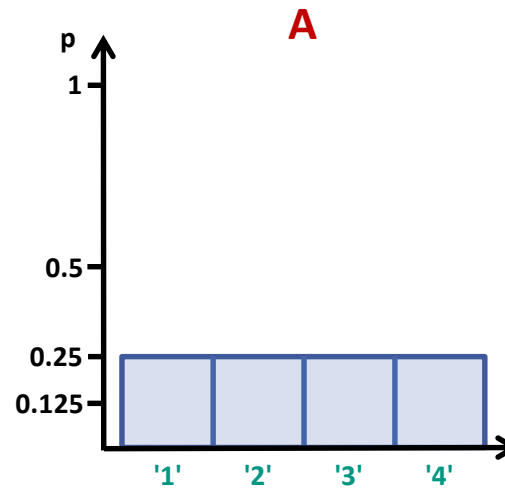
<sup>1</sup> Nyquist, H., "Certain Factors Affecting Telegraph Speed," *Bell System Technical Journal*, April 1924, p. 324; "Certain Topics in Telegraph Transmission Theory," *A. I. E. E. Trans.*, v. 47, April 1928, p. 617.

<sup>2</sup> Hartley, R. V. L., "Transmission of Information," *Bell System Technical Journal*, July 1928, p. 535.

# Basics

## Information

$$i(x) = -\log_2(p(x))$$

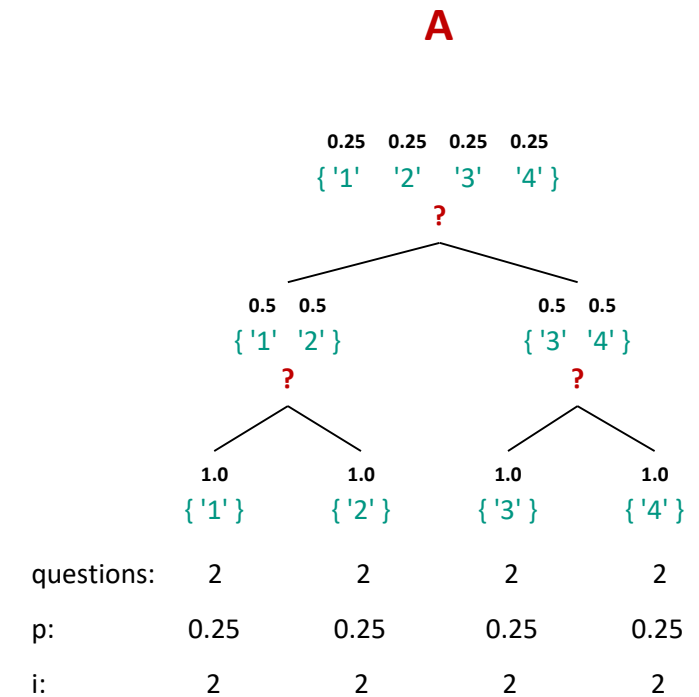
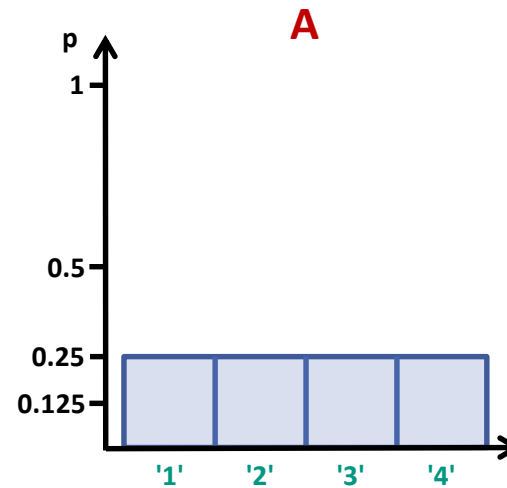


Information = # of optimal binary questions between prior and posterior state of uncertainty  
 1 question = 1 bit

# Basics

## Information

$$i(x) = -\log_2(p(x))$$

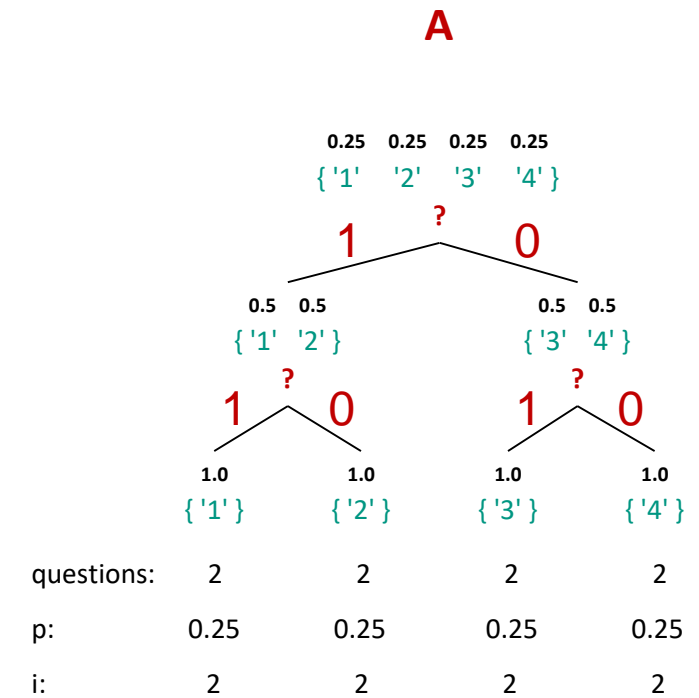
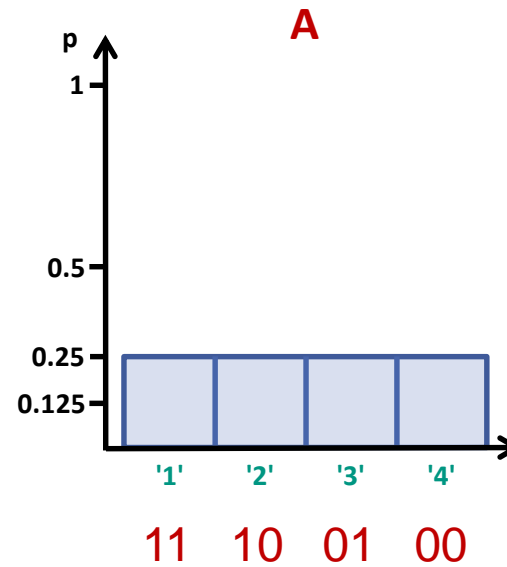


Uncertainty = missing information

# Basics

## Information

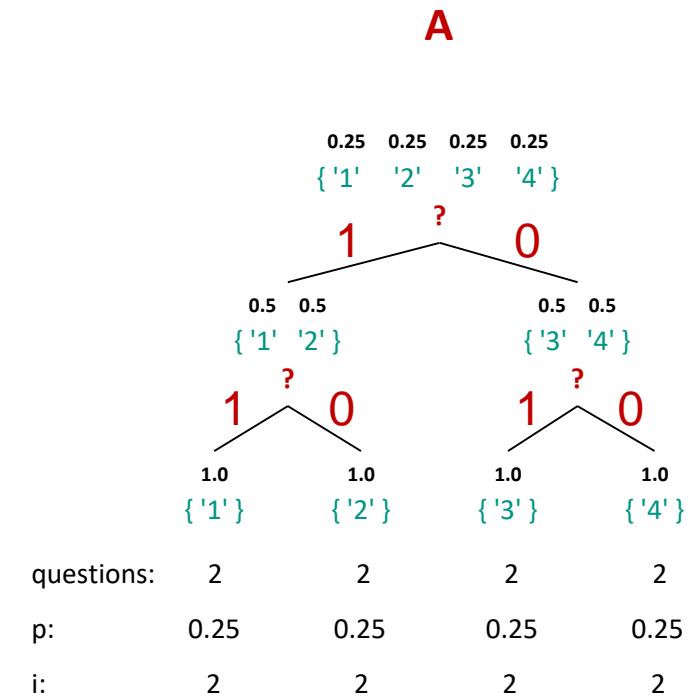
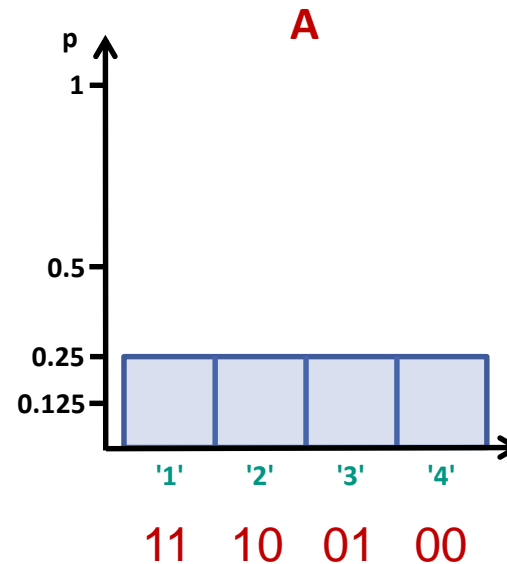
$$i(x) = -\log_2(p(x))$$



# Basics

## Information

$$i(x) = -\log_2(p(x))$$

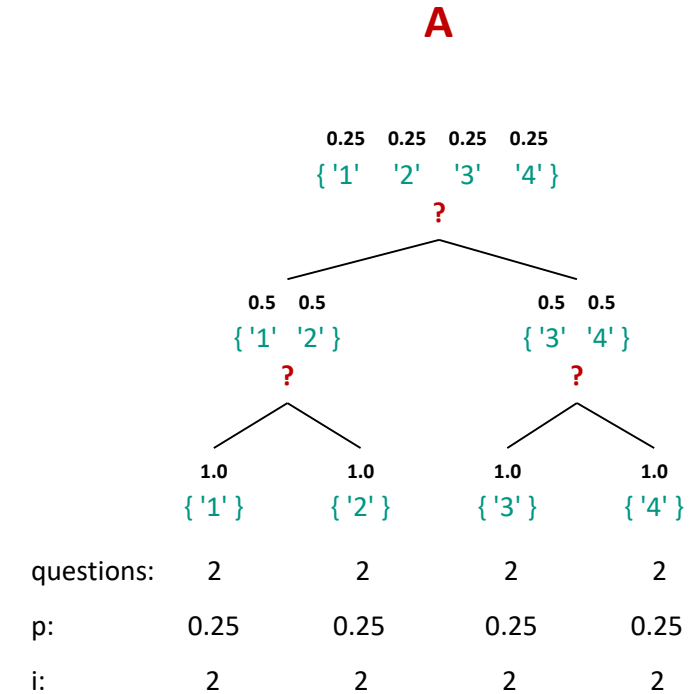
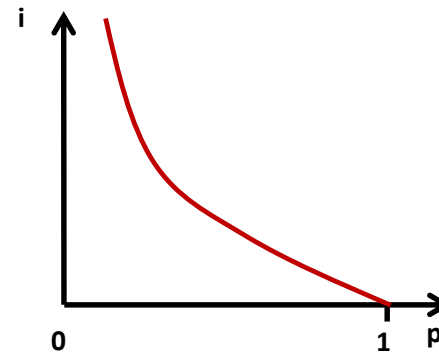


Any set of symbols can be expressed in a 1/0 alphabet ...  
 ... and can be interpreted as a sequence of answers on Yes/No questions  
 $H_2O = 1001000\ 110010\ 1001111$

# Basics

## Information

$$i(x) = -\log_2(p(x))$$

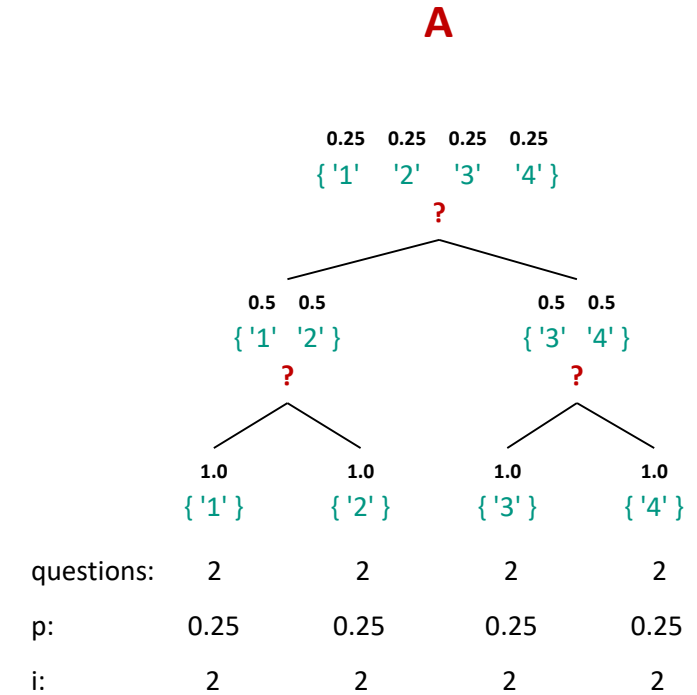


The smaller the probability of a signal, the more informative it is  
 Information is additive (probabilities are multiplicative)

# Basics

## ■ Entropy

$$i(x) = -\log_2(p(x))$$



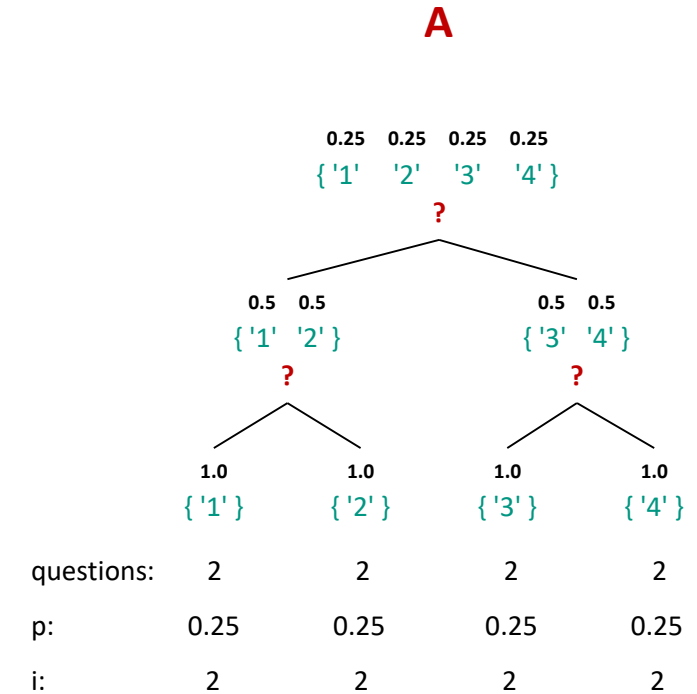


# Basics

## ■ Entropy

$$i(x) = -\log_2(p(x))$$

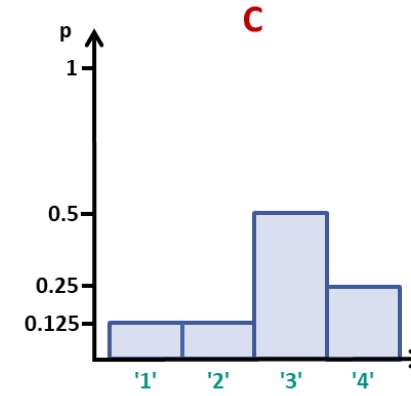
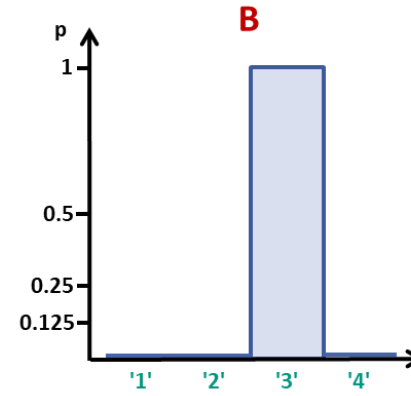
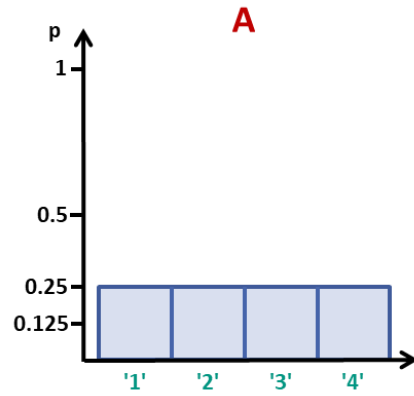
$$H(X) = E(i(X)) = \sum_{j=1}^n i_j * p(x_j)$$



Entropy = Average # of questions

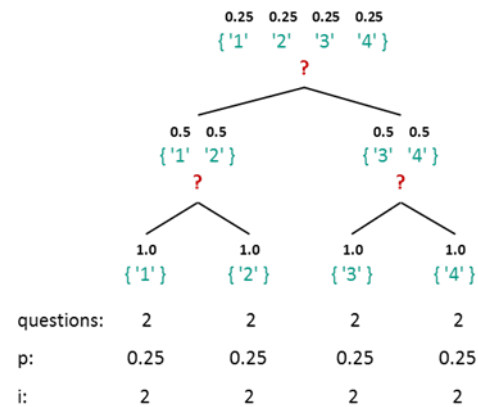
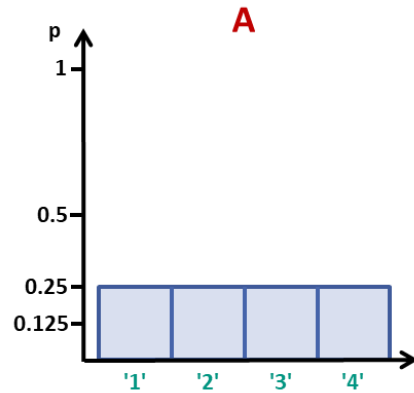
# Basics

## ■ Entropy

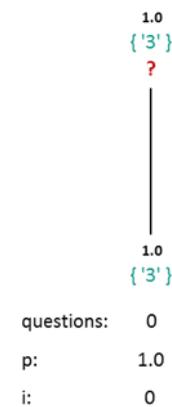
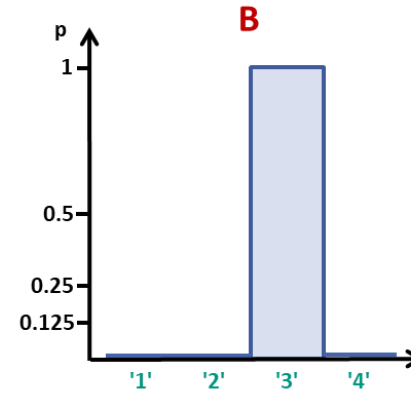


# Basics

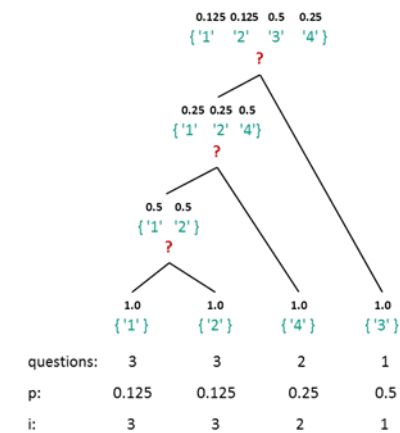
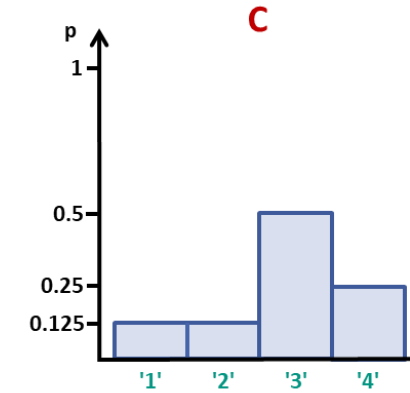
## Entropy



$$H(A) = 2 \text{ bit}$$



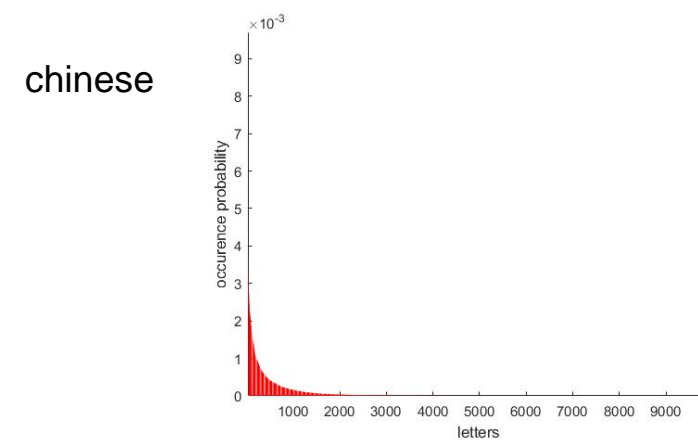
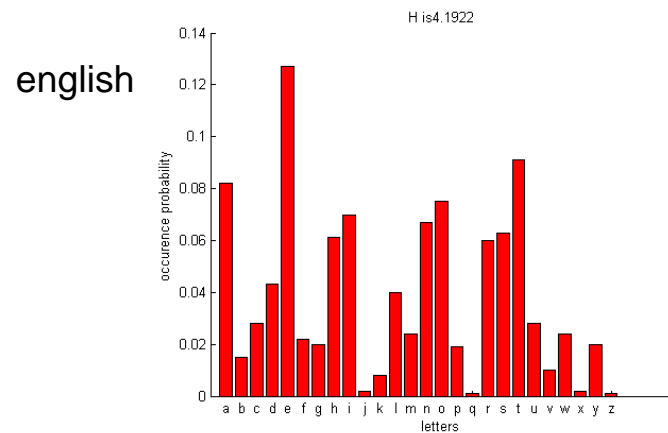
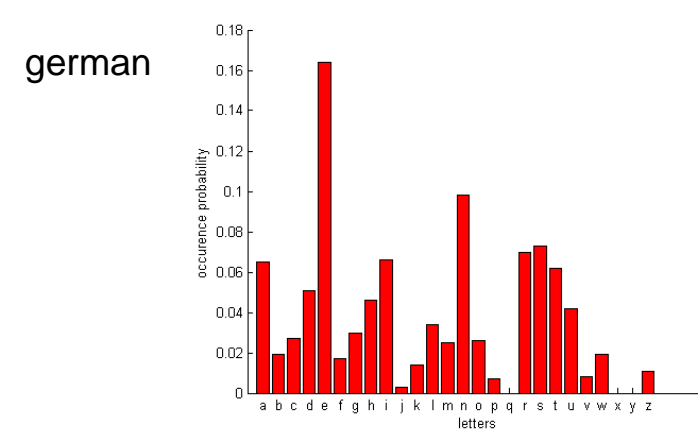
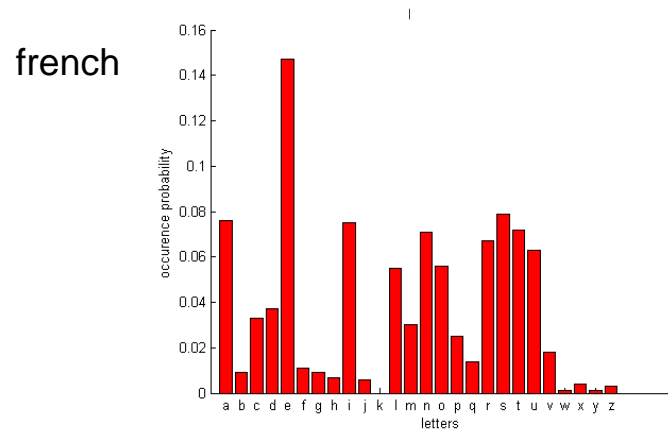
$$H(B) = 0 \text{ bit}$$



$$H(C) = 1.75 \text{ bit}$$

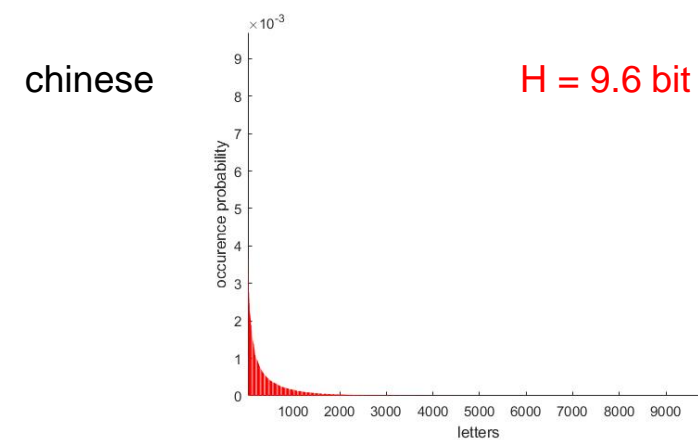
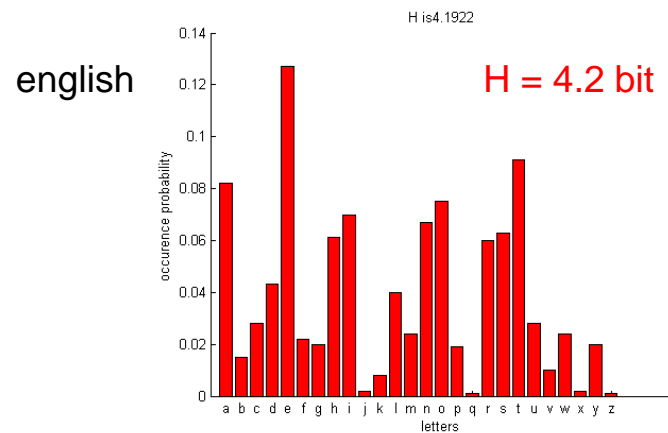
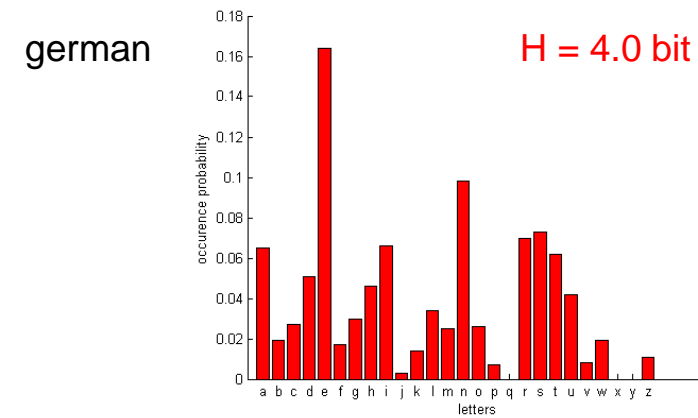
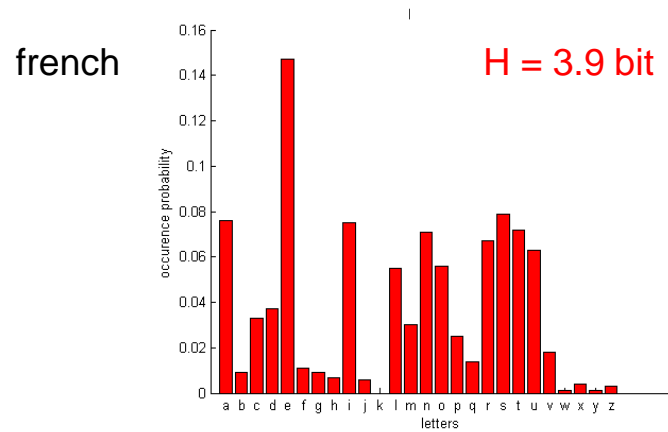
# Basics

- How much information can we transmit with different alphabets?



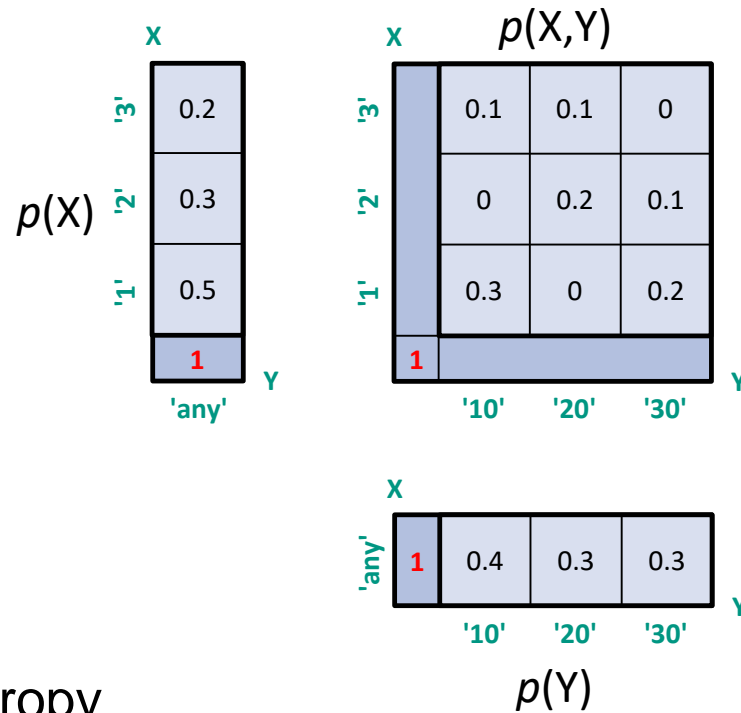
# Basics

- How much information can we transmit with different alphabets?



# Basics

- What happens if the probability distribution is more than 1-d?



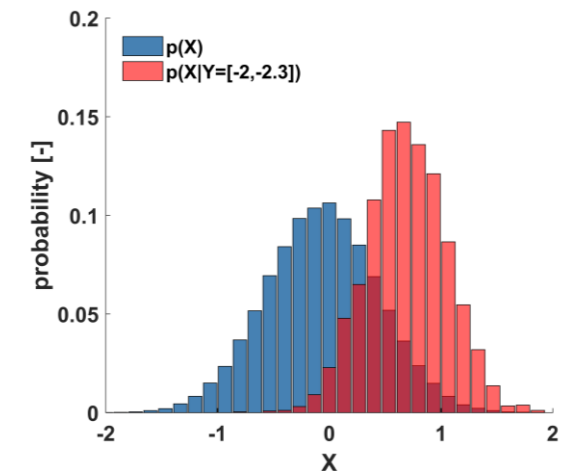
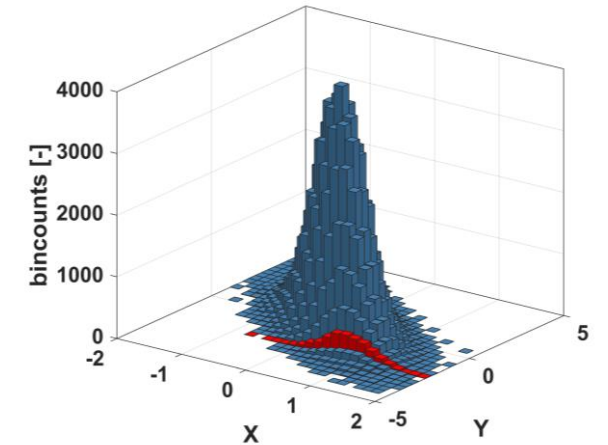
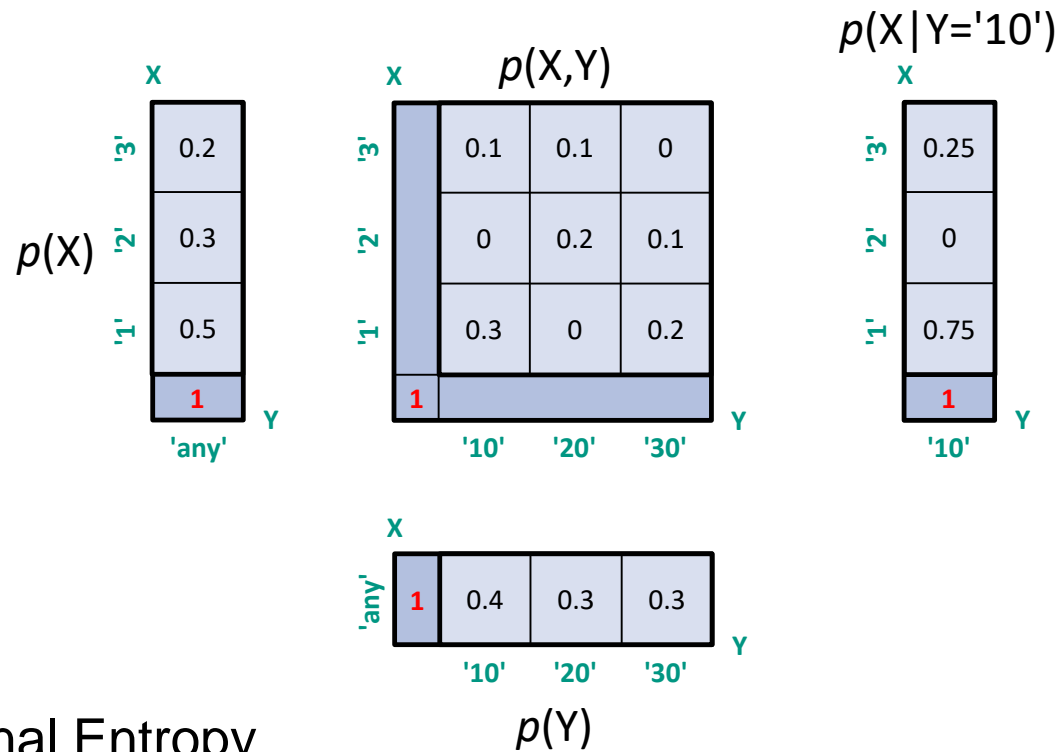
- Joint entropy is the entropy of a joint distribution
- Can be calculated for an any-dimensional distribution
- Can be interpreted as the average number of binary questions required to guess a paired signal  $(x,y)$

- Joint Entropy

$$H(X, Y) = \sum_{i=1}^m \sum_{j=1}^n p(x_i, y_j) \cdot -\log_2(p(x_i, y_j))$$

# Basics

- What happens if we have prior knowledge of  $y$  when guessing  $x$  from  $(x,y)$ ?



- Conditional Entropy

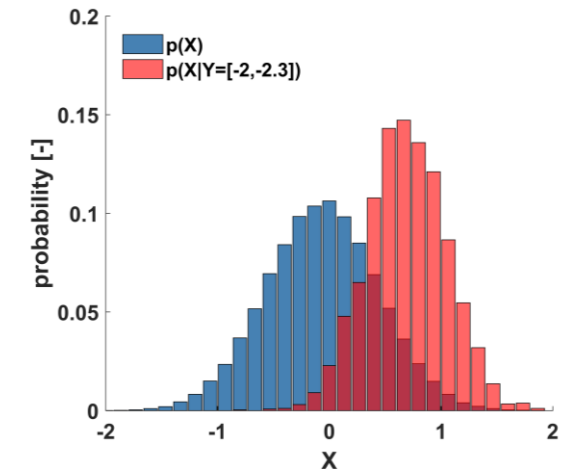
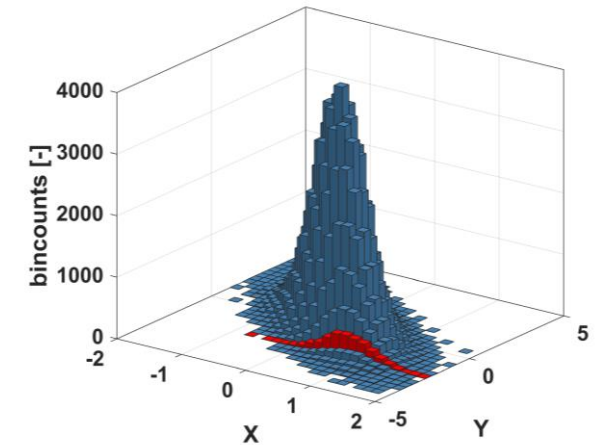
$$H(X|Y) = \sum_{j=1}^n p(y_j) \cdot H(X|Y = y_j)$$

# Basics

- Information inequality
  - Compared to entropy  $H(X)$  of the target, conditional entropy is the reduced uncertainty thanks to having advance knowledge of  $y$  when guessing  $x$  of a pair  $(x,y)$
  - While for a particular  $y_j$ ,  $H(X|Y=y_j)$  can be  $>$ ,  $<$ , or  $= H(X)$ , **on average** it holds

$$H(X) \geq H(X|Y)$$

Information can't hurt! (but there is a catch)





# Basics

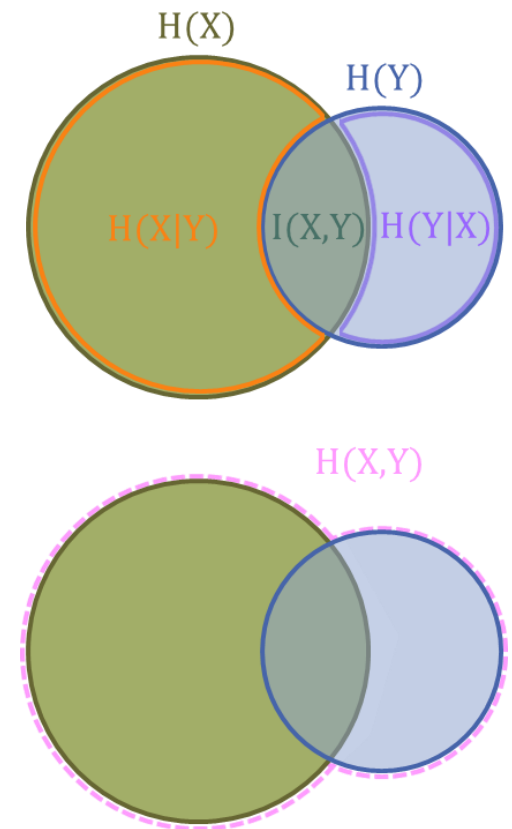
- The relation between Joint Entropy, Entropy, and Conditional Entropy

$$\begin{aligned}
 H(X, Y) &= H(X) + H(Y|X) \\
 &= H(Y) + H(X|Y)
 \end{aligned}$$

- Mutual information

$$\begin{aligned}
 I(X, Y) &= H(X) - H(X|Y) \\
 &= H(Y) - H(Y|X)
 \end{aligned}$$

- X knows in absolute terms as much about Y as Y knows about X!
- In relative terms it may differ

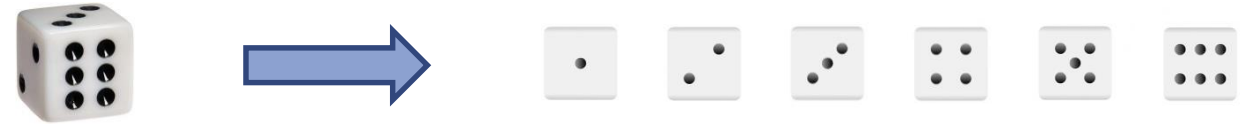


# Basics

- Sources of uncertainty

# Basics

- Sources of uncertainty
  - Variability (system)



# Basics

- Sources of uncertainty

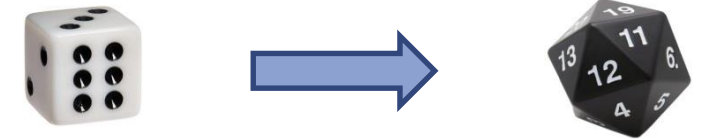
- Variability (system)

- Representativity (sample size)



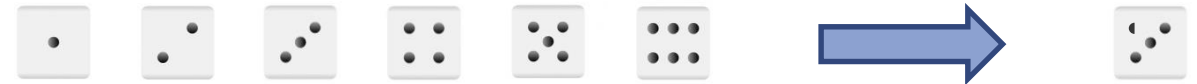
# Basics

- Sources of uncertainty
  - Variability (system)
  - Representativity (sample size)
  - Consistency (application)



# Basics

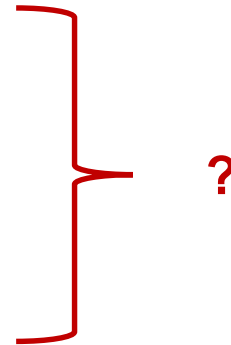
- Sources of uncertainty
  - Variability (system)
  - Representativity (sample size)
  - Consistency (application)
  - Compression (memory)



# Basics

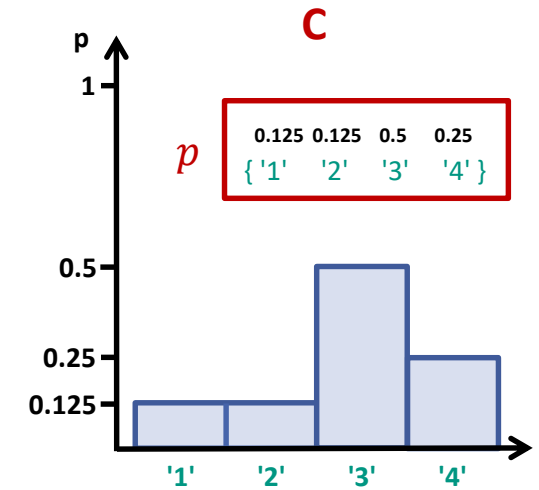
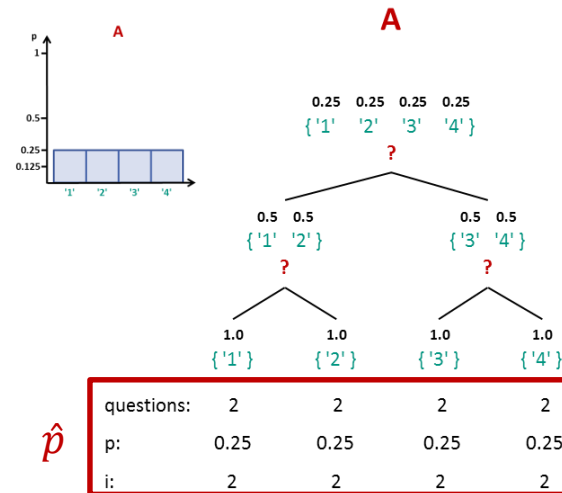
- Sources of uncertainty
  - Variability (system)
  - Representativity (sample size)
  - Consistency (application)
  - Compression (memory)

(Conditional) Entropy



# Basics

## ■ Crossentropy



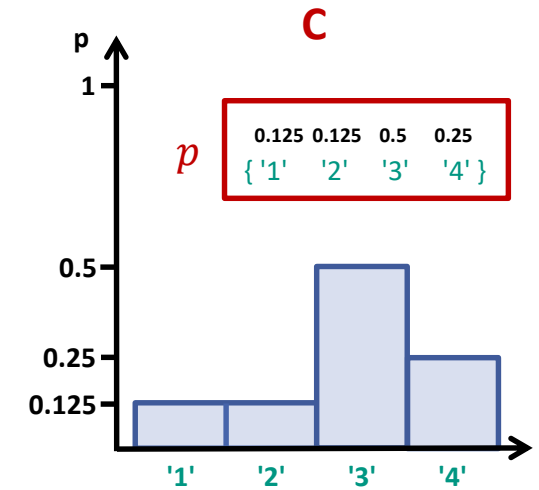
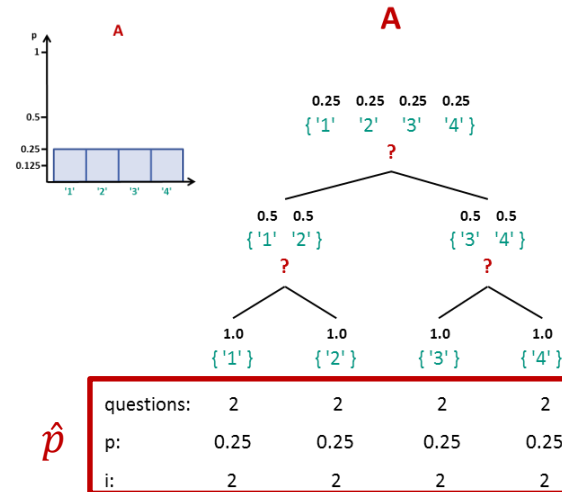
$$H(C) = 1.75 \text{ bit}$$



# Basics

## ■ Crossentropy

$$H_{cross}(X||\hat{X}) = \sum_{j=1}^n p(x_j) \cdot -\log_2(\hat{p}(x_j))$$



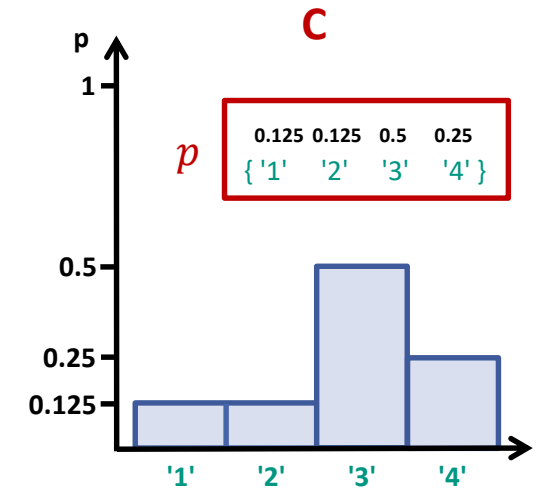
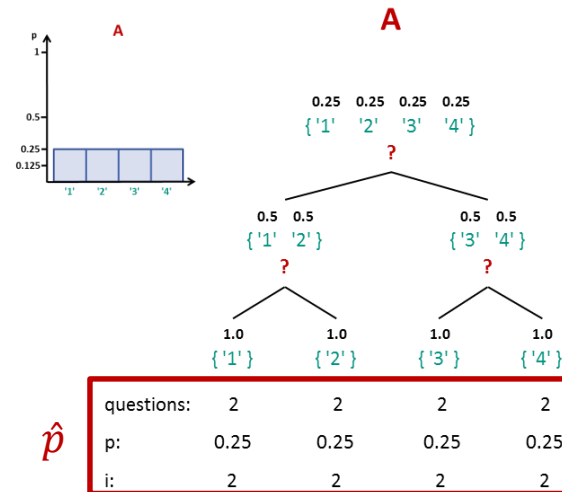
$$H(C) = 1.75 \text{ bit}$$

$$H(C||A) = 2 \text{ bit}$$

# Basics

## ■ Crossentropy

$$H_{cross}(X||\hat{X}) = \sum_{j=1}^n p(x_j) \cdot -\log_2(\hat{p}(x_j))$$



$$H(C) = 1.75 \text{ bit}$$

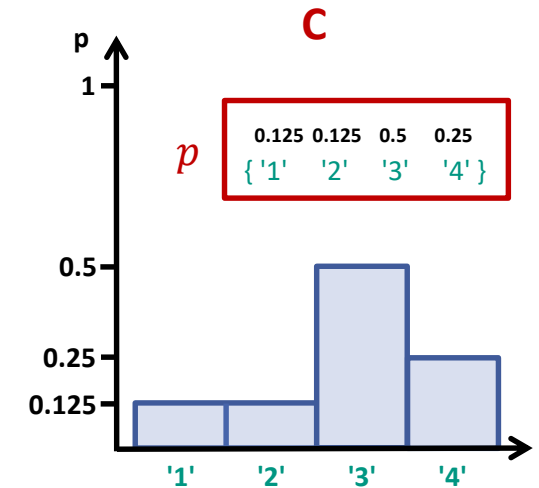
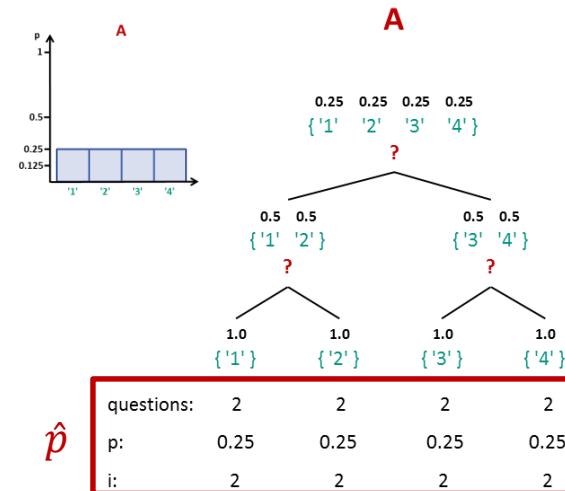
$$H(C||A) = 2 \text{ bit}$$

Crossentropy measures total uncertainty from  
 Variability (data-uncertainty)  
 Representativity, Consistency, Compression (model-uncertainty)

# Basics

## ■ Kullback-Leibler divergence

$$D_{KL}(X||\hat{X}) = H_{cross}(X||\hat{X}) - H(X)$$



$$H(C) = 1.75 \text{ bit}$$

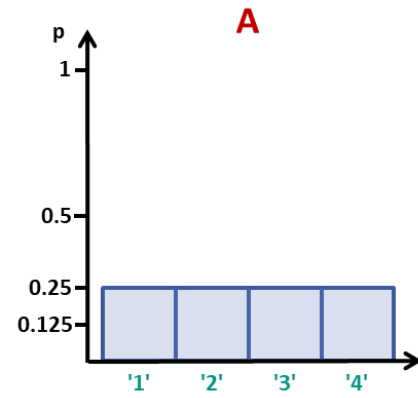
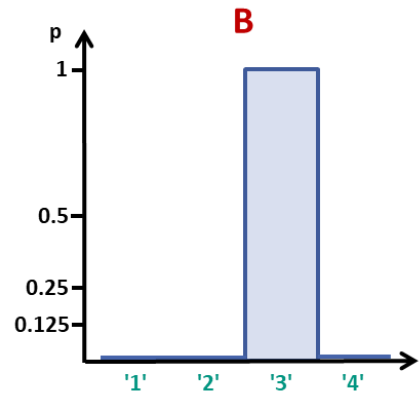
$$H(C||A) = 2 \text{ bit}$$

$$D_{KL}(C||A) = 0.25 \text{ bit}$$

Kullback-Leibler divergence measures model-uncertainty

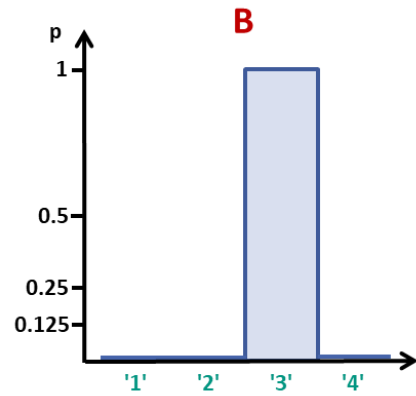
# Limits

## ■ Entropy limits

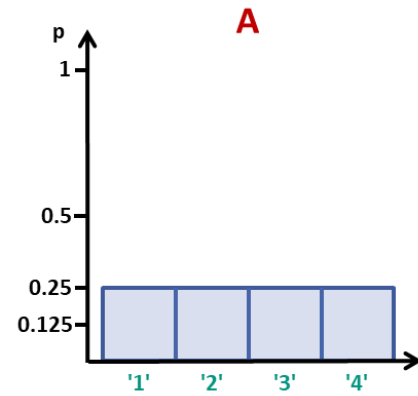


# Limits

## ■ Entropy limits



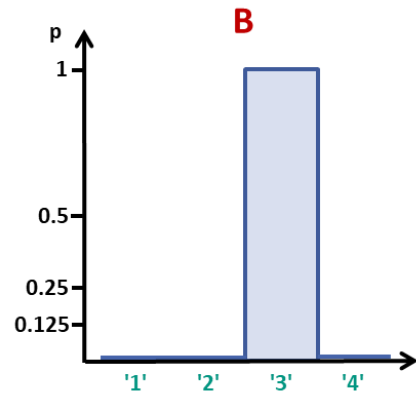
$$H(B) = 0 \text{ bit}$$



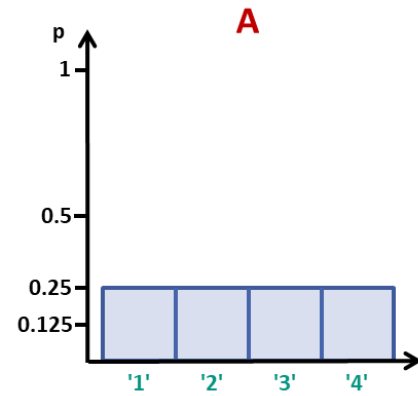
$$H(A) = 2 \text{ bit} = \log_2(\# \text{ of bins})$$

# Limits

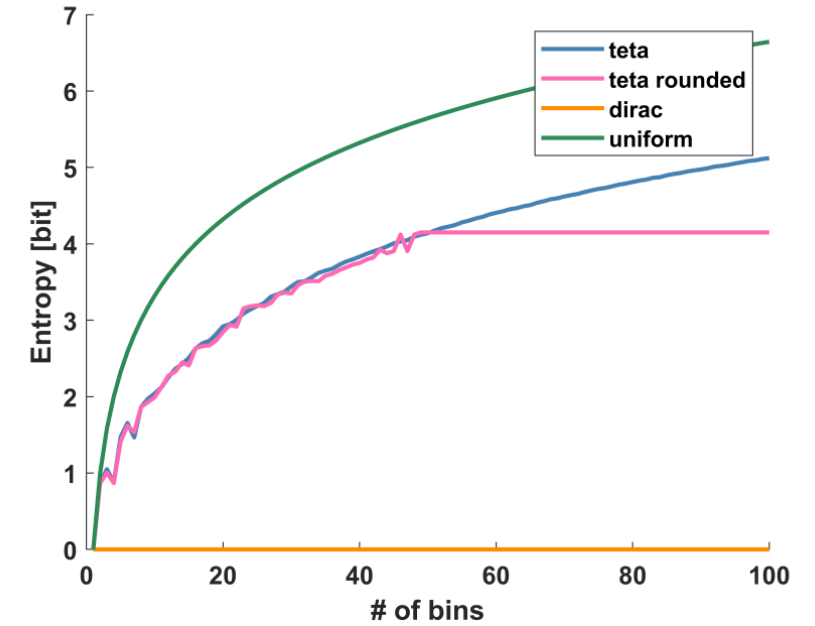
## Entropy limits



$$H(B) = 0 \text{ bit}$$

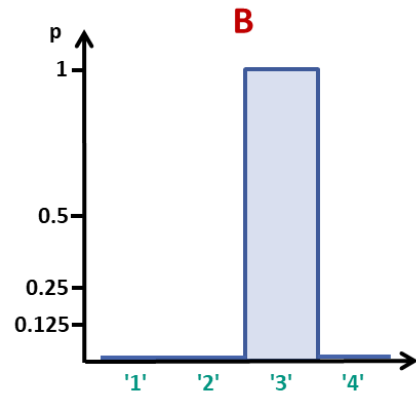


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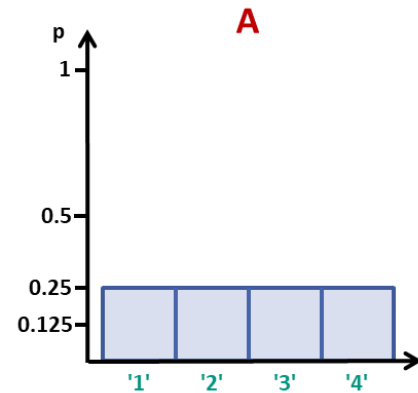


# Limits

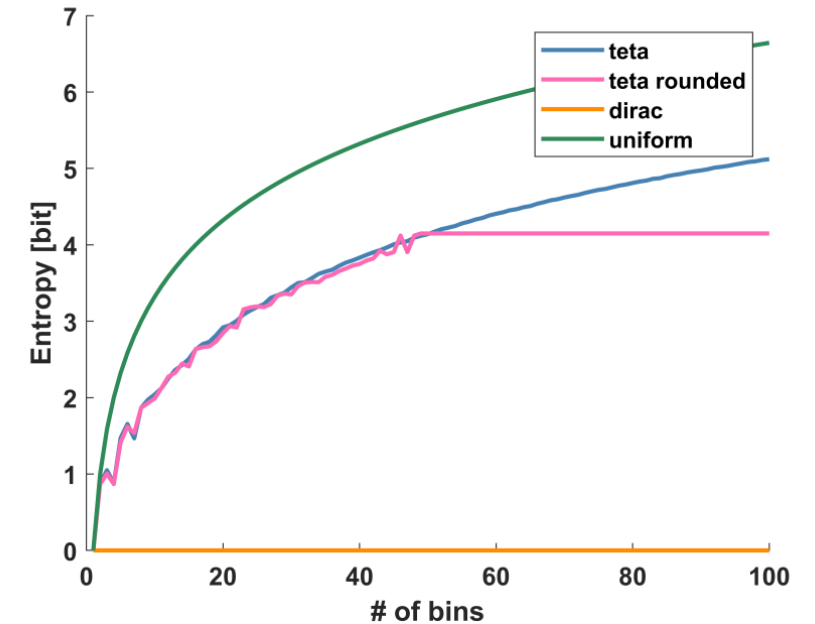
## ■ Entropy limits



$$H(B) = 0 \text{ bit}$$



$$H(A) = 2 \text{ bit} = \log_2(\# \text{ of bins})$$



## ■ Maximum Entropy principle for inference

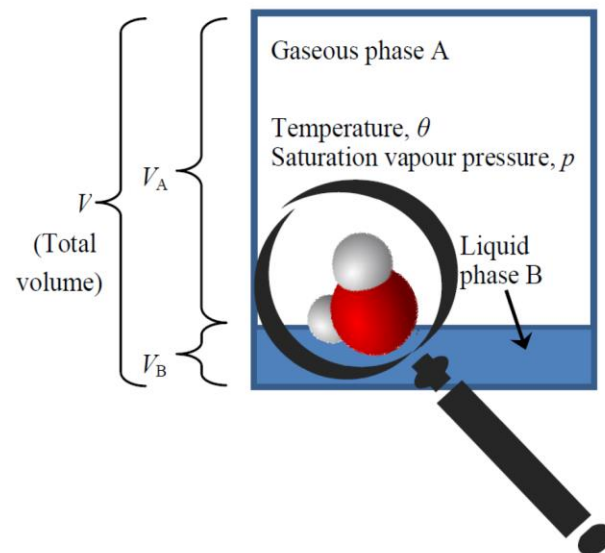
- Jaynes (1957, 2003): "given all known constraints, all remaining unknowns should be represented by maximum entropy estimates"

# Limits

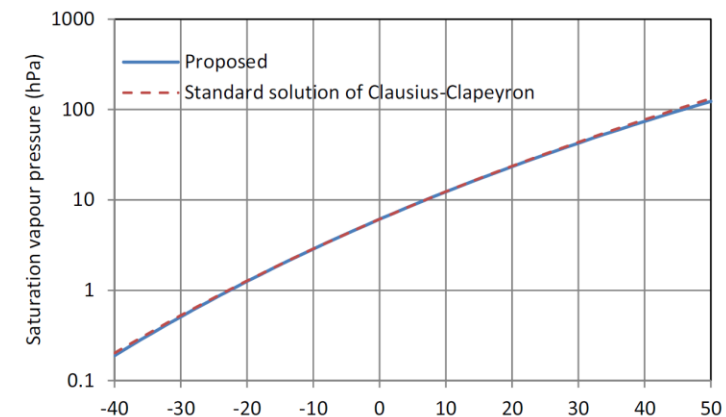
## ■ Koutsoyiannis (2014)

- Uses elementary physical constraints and the Maximum Entropy Principle to derive ideal gas law, Clausius-Clapeyron relation, and others

**Figure 2.** Explanatory sketch indicating basic quantities involved in the equilibrium of the water vapour with liquid water, with zoom on a single molecule which “tries to hide itself” by maximizing the combined uncertainty related to its phase (being either gaseous or liquid with probabilities  $\pi_A$  and  $\pi_B$ , respectively), position and kinetic state.



**Figure 3. (upper)** Comparison of saturation vapour pressure obtained by the proposed Equation (40) and by the standard but inconsistent Equation (41). **(lower)** Comparison of relative differences of the saturation vapour pressure obtained by the proposed Equation (40), as well as by Equation (41), with accurate measurement data of different origins, as indicated in the legend (for details on data see [34]).



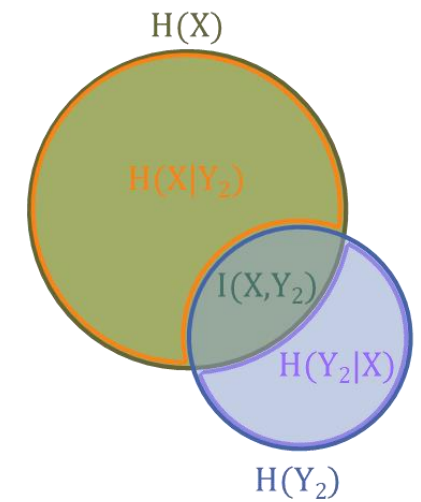
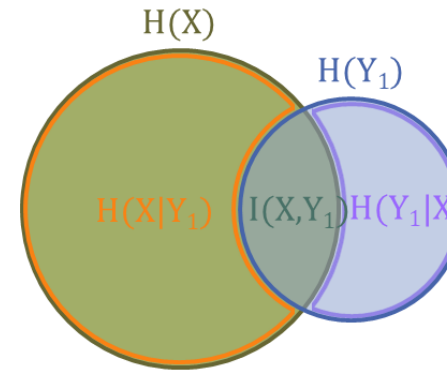


# Independence, Redundancy, Synergy

- What happens to mutual information if more than one predictor exists?

- Remember mutual information

$$I(X, Y) = H(X) - H(X|Y)$$



# Independence, Redundancy, Synergy

- What happens to mutual information if more than one predictor exists?

- Remember mutual information

$$I(X, Y) = H(X) - H(X|Y)$$

- Independence

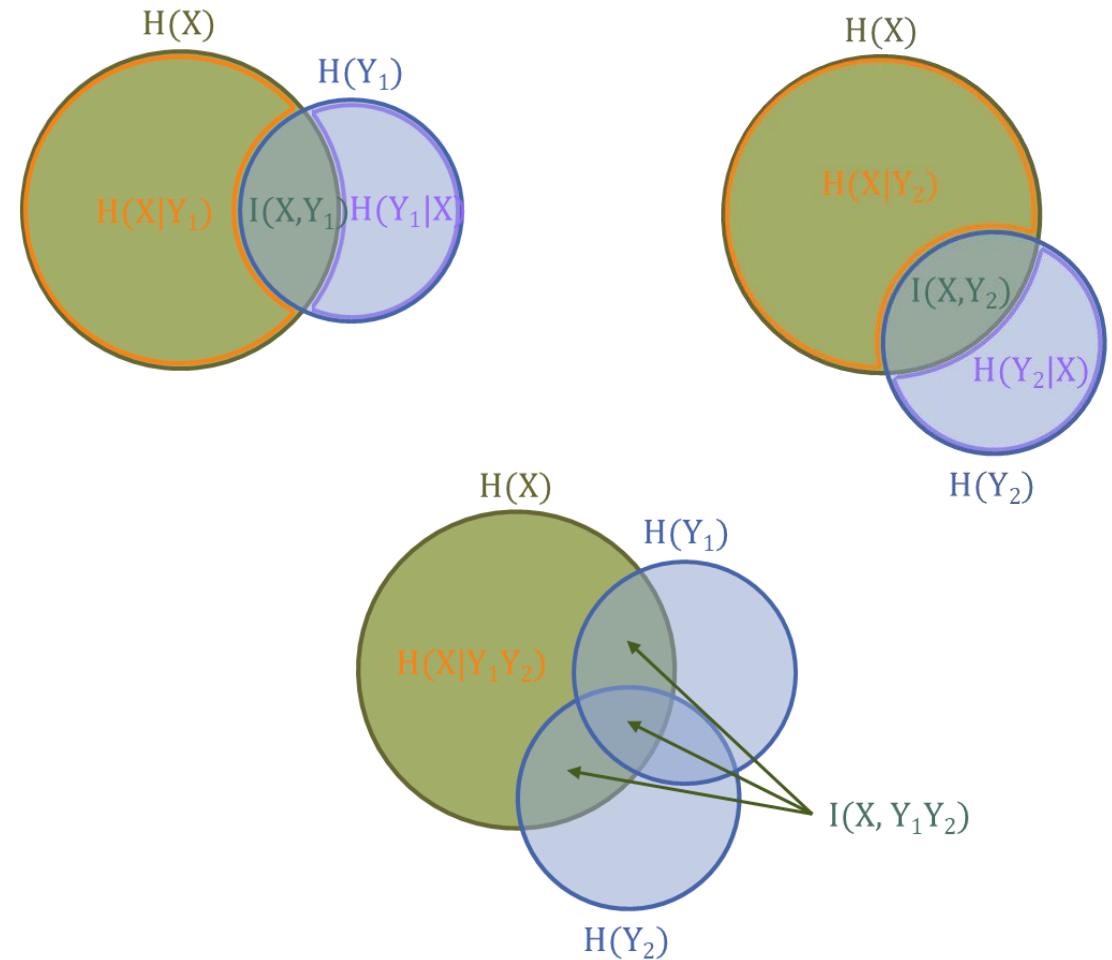
$$I(X, Y_1 Y_2) = I(X, Y_1) + I(X, Y_2)$$

- Redundancy

$$I(X, Y_1 Y_2) < I(X, Y_1) + I(X, Y_2)$$

- Synergy

$$I(X, Y_1 Y_2) > I(X, Y_1) + I(X, Y_2)$$



# Independence, Redundancy, Synergy

Some data

Y1	Y2	X
1	1	1
1	2	1
2	1	2
2	2	2
1	1	3
2	1	3
1	2	4
2	2	4

$$H(X) = 2$$

$$I(X, Y_1) = 0.5$$

$$I(X, Y_2) = 0.5$$

$$I(X, Y_1 Y_2) = 1$$

$$1 = 0.5 + 0.5$$

→ independence

# Independence, Redundancy, Synergy

Some data

Y1	Y2	X
1	1	1
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 $I(X, Y_1) = 0.5$   
 $I(X, Y_2) = 0.5$   
 $I(X, Y_1 Y_2) = 1$   
 $1 = 0.5 + 0.5$   
 → independence

CopyPaste

Y1	Y2	X
0	0	0
0	0	0
1	1	0
1	1	1

$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
 $I(X, Y_2) = 0.31$   
 $I(X, Y_1 Y_2) = 0.31$   
 $0.31 < 0.31 + 0.31$   
 → redundancy

# Independence, Redundancy, Synergy

Some data

Y1	Y2	X
1	1	1
1	2	1
2	1	2
2	2	2
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 $1 = 0.5 + 0.5$   
 → independence

CopyPaste

Y1	Y2	X
0	0	0
0	0	0
1	1	0
1	1	1

$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
 $I(X, Y_2) = 0.31$   
 $I(X, Y_1 Y_2) = 0.31$   
 $0.31 < 0.31 + 0.31$   
 → redundancy

OR

Y1	Y2	X
0	0	0
0	1	1
1	0	1
1	1	1

$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
 $I(X, Y_2) = 0.31$   
 $I(X, Y_1 Y_2) = 0.81$   
 $0.81 > 0.31 + 0.31$   
 → synergy

# Independence, Redundancy, Synergy

Some data

Y1	Y2	X
1	1	1
1	2	1
2	1	2
2	2	2
1	1	3
2	1	3
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 → independence

CopyPaste

Y1	Y2	X
0	0	0
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$H(X) = 0.81$   
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 $I(X, Y_2) = 0.31$   
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 $0.31 < 0.31 + 0.31$   
 → redundancy

OR

Y1	Y2	X
0	0	0
0	1	1
1	0	1
1	1	1

$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
 $I(X, Y_2) = 0.31$   
 $I(X, Y_1 Y_2) = 0.81$   
 $0.81 > 0.31 + 0.31$   
 → synergy

XOR

Y1	Y2	X
0	0	0
0	1	1
1	0	1
1	1	0

$H(X) = 1$   
 $I(X, Y_1) = 0$   
 $I(X, Y_2) = 0$   
 $I(X, Y_1 Y_2) = 1$   
 $1 > 0 + 0$   
 → synergy

# Independence, Redundancy, Synergy

Some data

Y1	Y2	X
1	1	1
1	2	1
2	1	2
2	2	2
1	1	3
2	1	3
1	2	4
2	2	4

$H(X) = 2$   
 $I(X, Y_1) = 0.5$   
 $I(X, Y_2) = 0.5$   
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 $1 = 0.5 + 0.5$   
 → independence

CopyPaste

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$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
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 $I(X, Y_1 Y_2) = 0.31$   
 $0.31 < 0.31 + 0.31$   
 → redundancy

OR

Y1	Y2	X
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1	0	1
1	1	1

$H(X) = 0.81$   
 $I(X, Y_1) = 0.31$   
 $I(X, Y_2) = 0.31$   
 $I(X, Y_1 Y_2) = 0.81$   
 $0.81 > 0.31 + 0.31$   
 → synergy

XOR

Y1	Y2	X
0	0	0
0	1	1
1	0	1
1	1	0

$H(X) = 1$   
 $I(X, Y_1) = 0$   
 $I(X, Y_2) = 0$   
 $I(X, Y_1 Y_2) = 1$   
 $1 > 0 + 0$   
 → synergy

I, R, S can jointly occur in the same data set and compensate

# Conservation, Dissipation, Innovation

- Data processing inequality
  - "...no processing of Y, deterministic or random, can increase the information that Y contains about X."  
(Cover and Thomas, 2006)

$$H(X|Y) \leq H(X|f(Y))$$




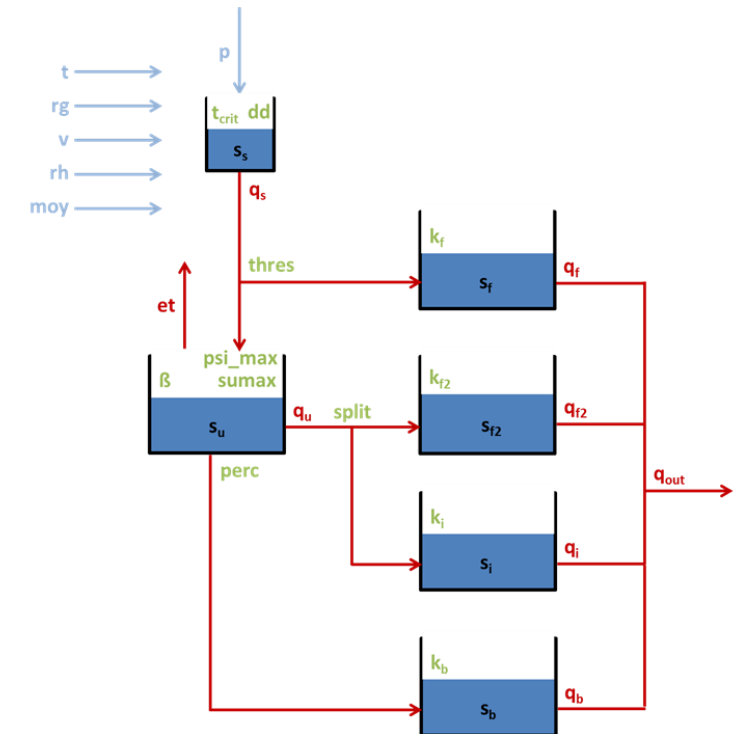
# Conservation, Dissipation, Innovation

## ■ Data processing inequality

- "...no processing of Y, deterministic or random, can increase the information that Y contains about X."  
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$$H(X|Y) \leq H(X|f(Y))$$

$$q_{out} = f(q_i) \quad q_i = f(q_u) \quad q_u = f(q_s) \quad q_s = f(p)$$





# Conservation, Dissipation, Innovation

## ■ Data processing inequality

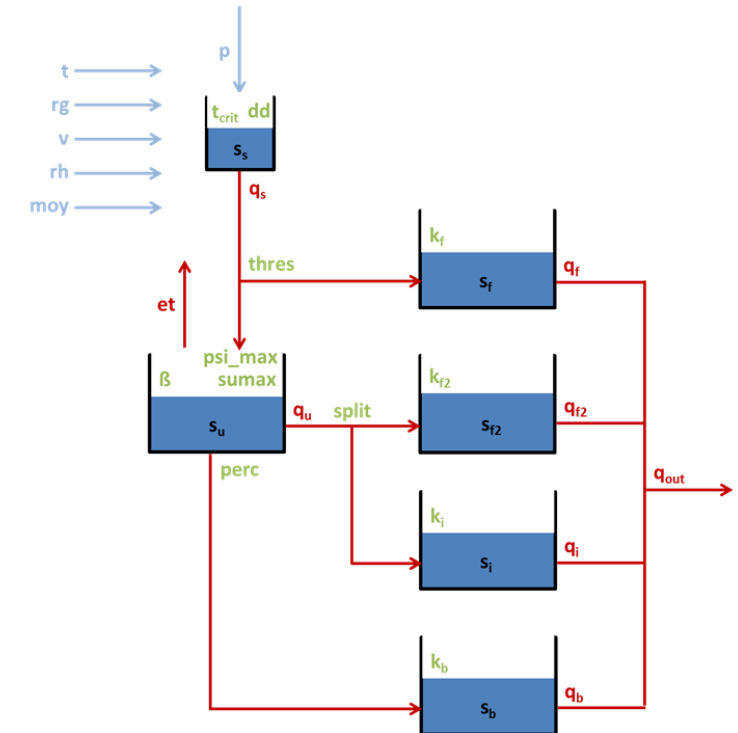
- "...no processing of Y, deterministic or random, can increase the information that Y contains about X."  
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$$H(X|Y) \leq H(X|f(Y))$$

$$q_{out} = f(q_i) \quad q_i = f(q_u) \quad q_u = f(q_s) \quad q_s = f(p)$$


Why building models as series of data transformations, if no information is gained?

$$q_{out} = f(q_i) \quad q_i = f(q_u) \quad q_u = f(q_s) \quad q_s = f(p)$$

# Conservation, Dissipation, Innovation

- Variability and Innovation

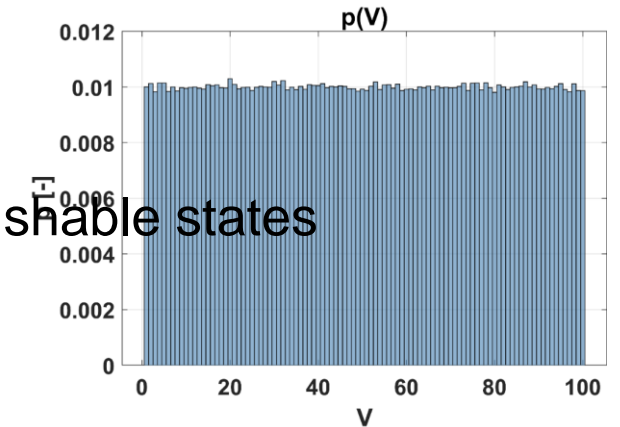
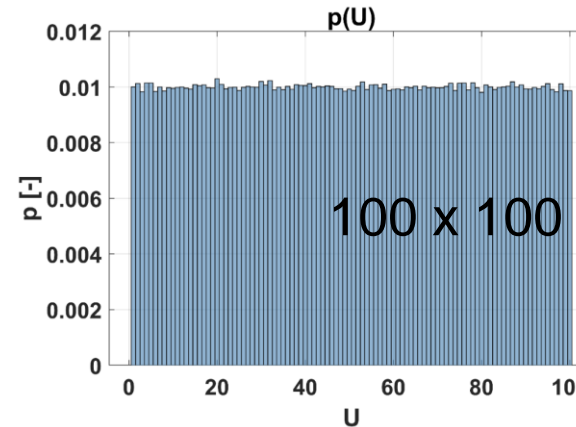
# Conservation, Dissipation, Innovation

## Variability and Innovation

$$X = U + V$$

## Variability and Innovation

- $H(U,V) = 13.28$  bit



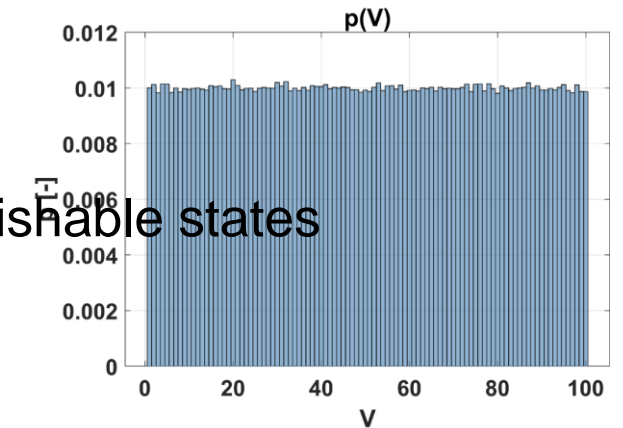
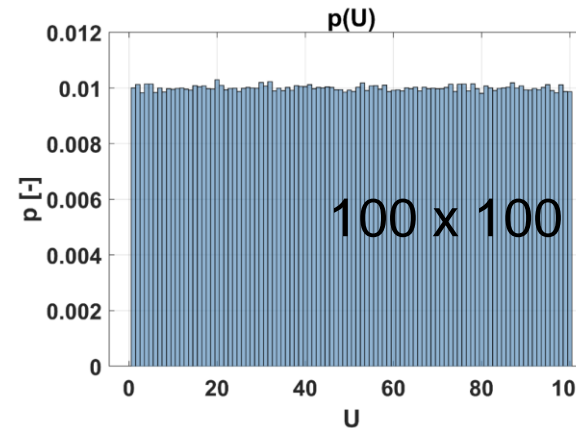
100 x 100 distinguishable states

# Conservation, Dissipation, Innovation

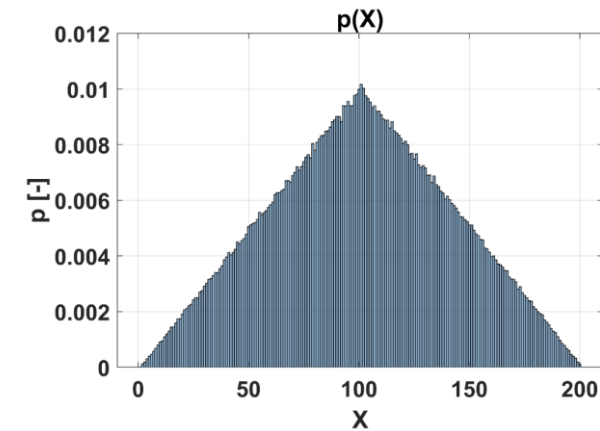
## Variability and Innovation

$$X = U + V$$

- $H(U, V) = 13.28$  bit
- $H(X|U, V) = 0$  bit



100 x 100 distinguishable states

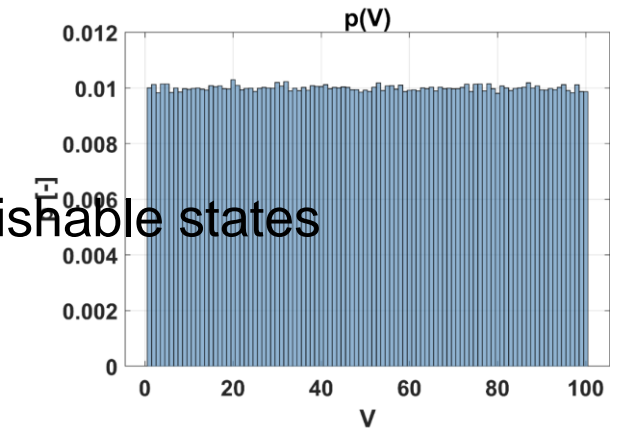
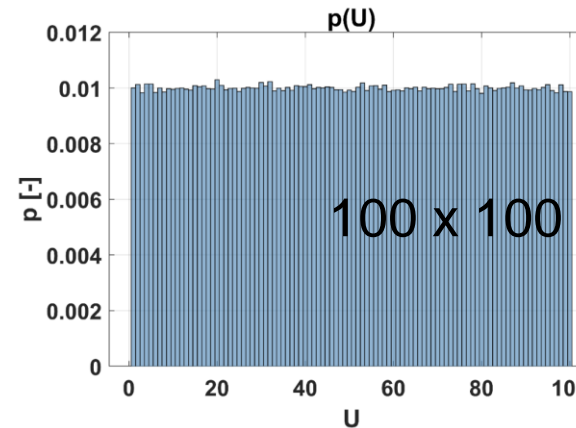


# Conservation, Dissipation, Innovation

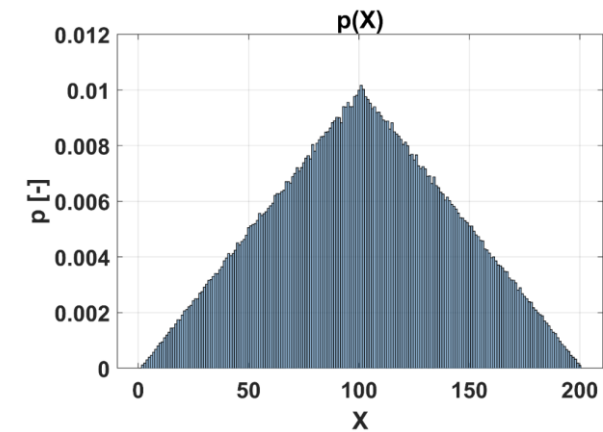
## Variability and Innovation

$$X = U + V$$

- $H(U, V) = 13.28$  bit
- $H(X|U, V) = 0$  bit



100 x 100 distinguishable states



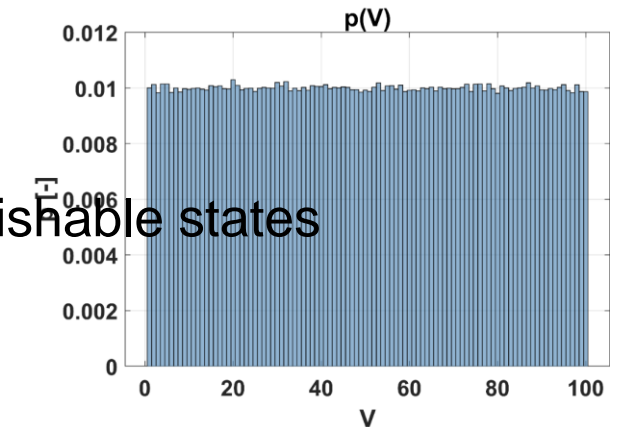
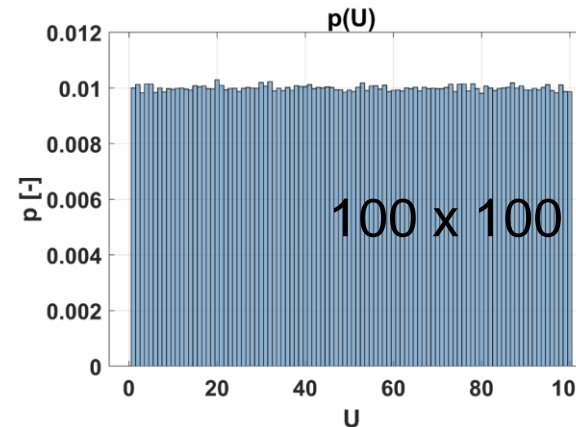
200 distinguishable states

# Conservation, Dissipation, Innovation

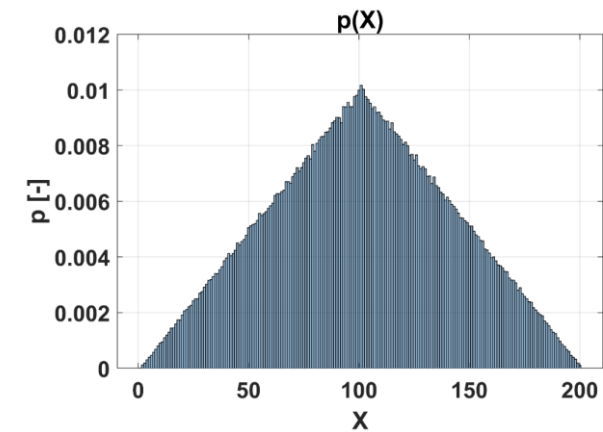
## Variability and Innovation

$$X = U + V$$

- $H(U,V) = 13.28$  bit
- $H(X|U,V) = 0$  bit
- $H(X) = 7.36$  bit < 13.28 bit!



100 x 100 distinguishable states



200 distinguishable states

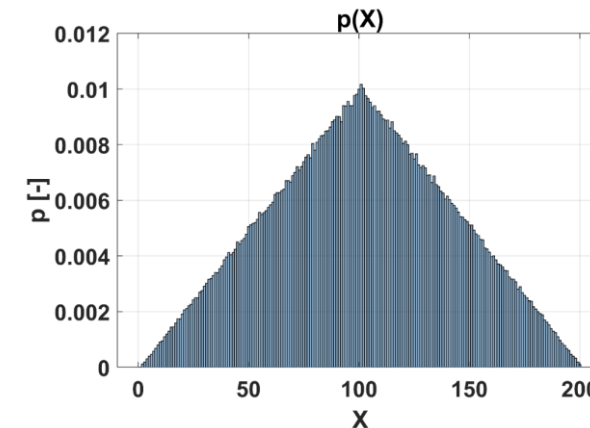
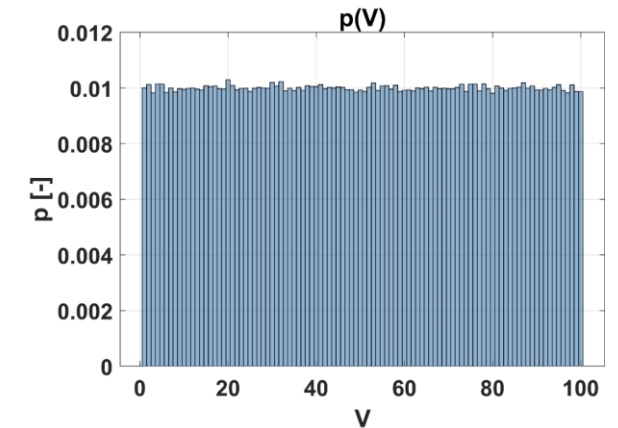
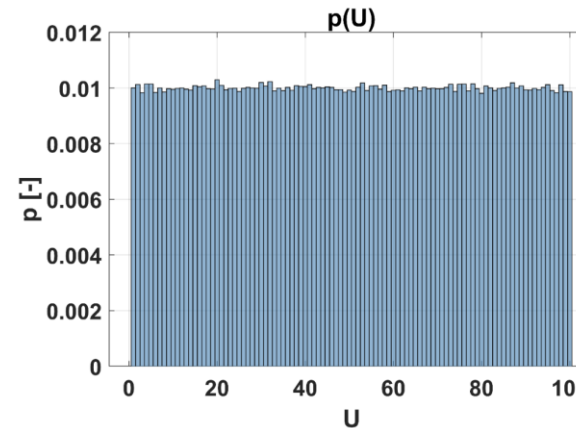
# Conservation, Dissipation, Innovation

## Variability and Innovation

$$X = U + V$$

- $H(U, V) = 13.28$  bit
- $H(X|U, V) = 0$  bit
- $H(X) = 7.36$  bit < 13.28 bit!

$$H(X = f(U, V)) \leq H(U, V)$$



Are things getting ever more boring?

How then does a random-number generator work?



# Conservation, Dissipation, Innovation

Why building models if no information is gained?

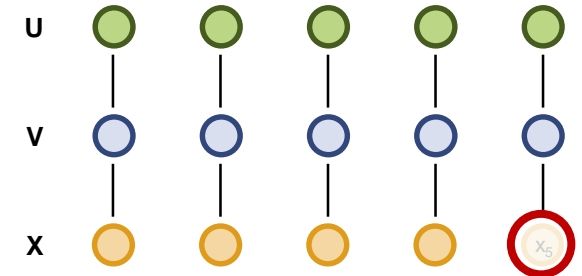
Are things getting ever more boring?

How then does a random-number generator work?

# Conservation, Dissipation, Innovation

- Independent events

$$X = f(U, V)$$



Why building models if no information is gained?

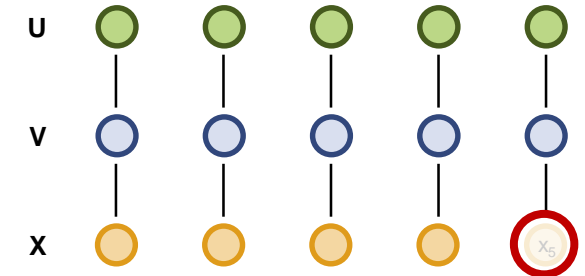
Are things getting ever more boring?

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# Conservation, Dissipation, Innovation

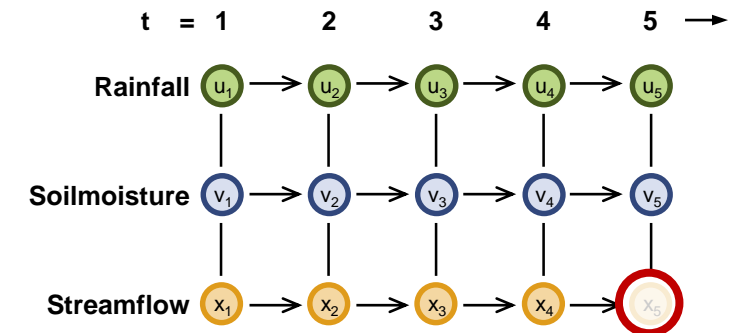
- Independent events

$$X = f(U, V)$$



- Order & memory does the trick!

$$X_t = f(U, V, X_{t-1})$$

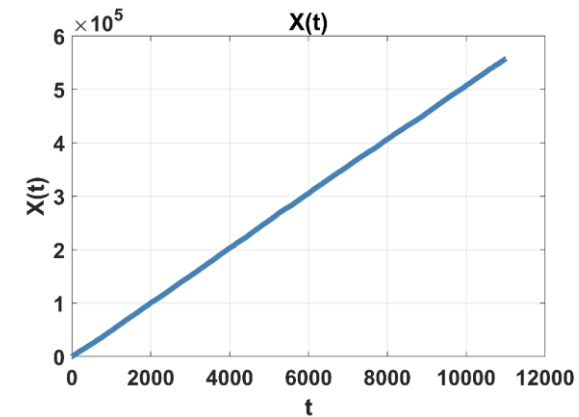
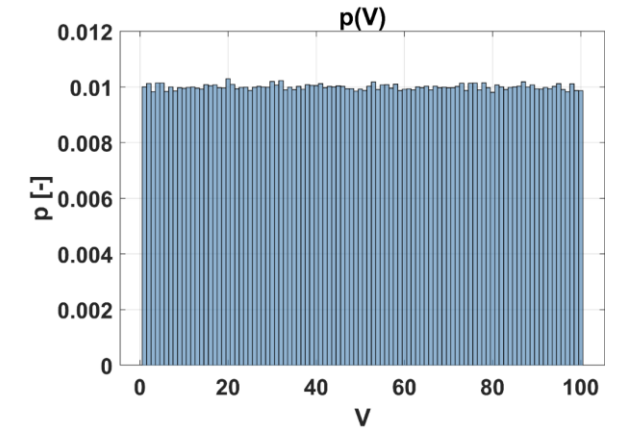
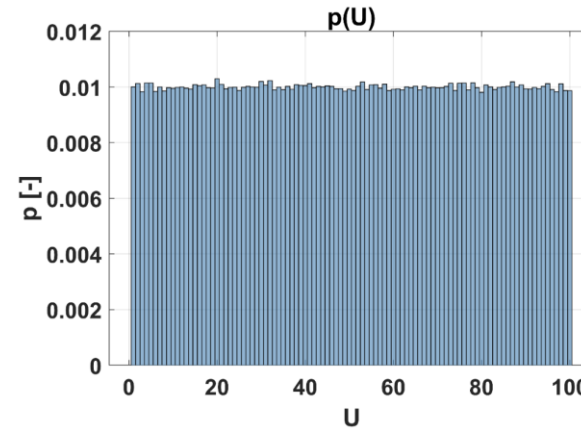


# Conservation, Dissipation, Innovation

- Order & Memory!

$$X_t = U + V + X_{t-1}$$

- $H(U,V) = 13.28$  bit



# Conservation, Dissipation, Innovation

- Order & Memory!

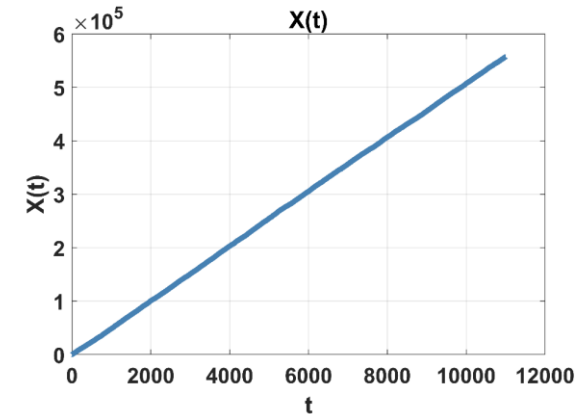
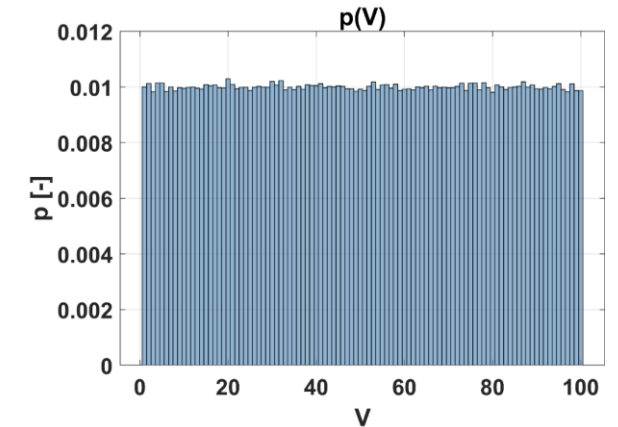
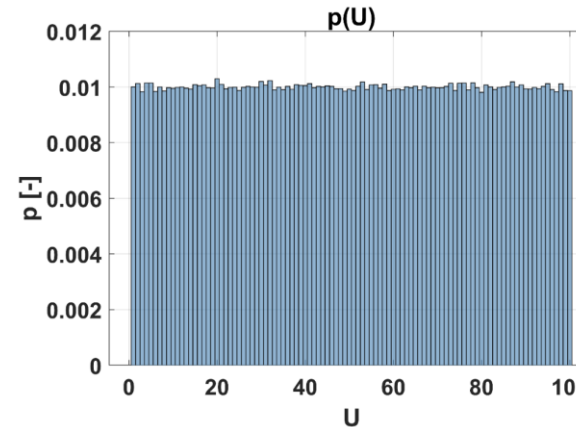
$$X_t = U + V + X_{t-1}$$

- $H(U,V) = 13.28$  bit

after 11000 timesteps

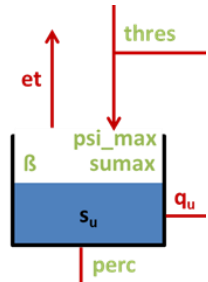
- $H(X) = 13.42$  bit  $>$  13.28 bit!

$$H(X_t = f(U, V, X_{t-1})) > H(U, V) \quad \text{is possible!}$$

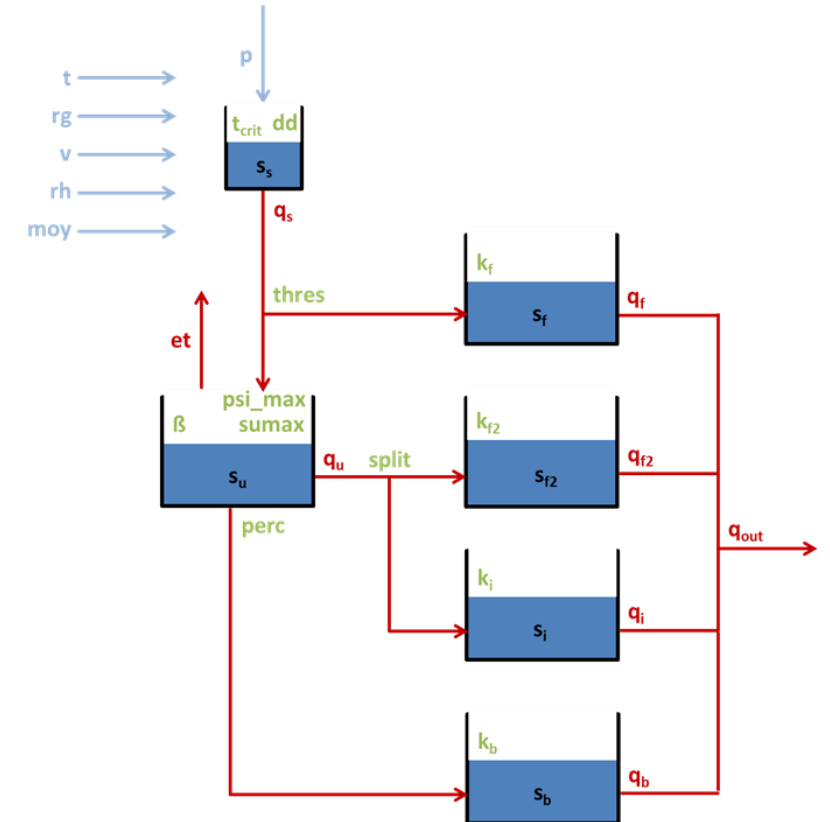


# Conservation, Dissipation, Innovation

- Equation-based models
  - Recursion/Memory terms!



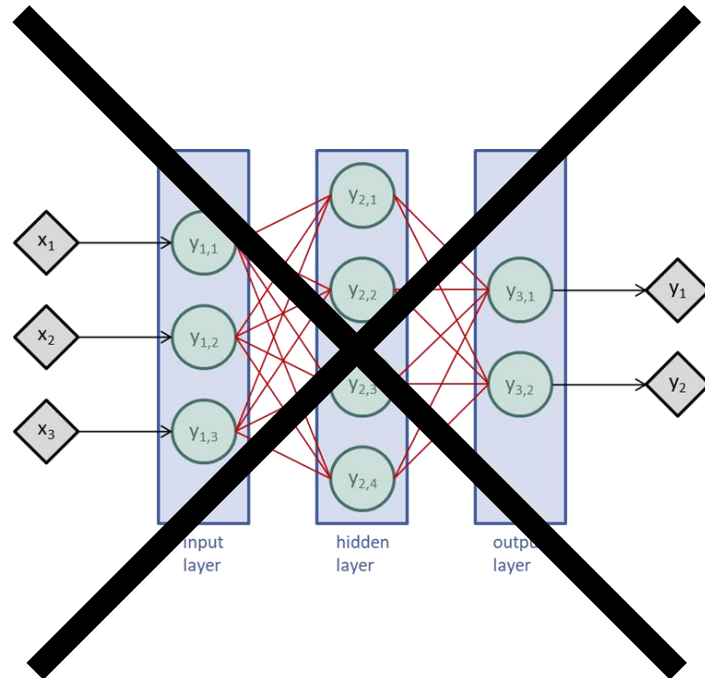
$$s_{u,t} = s_{u,t-1} + q_{s,t} - et - q_u - q_{perc}$$



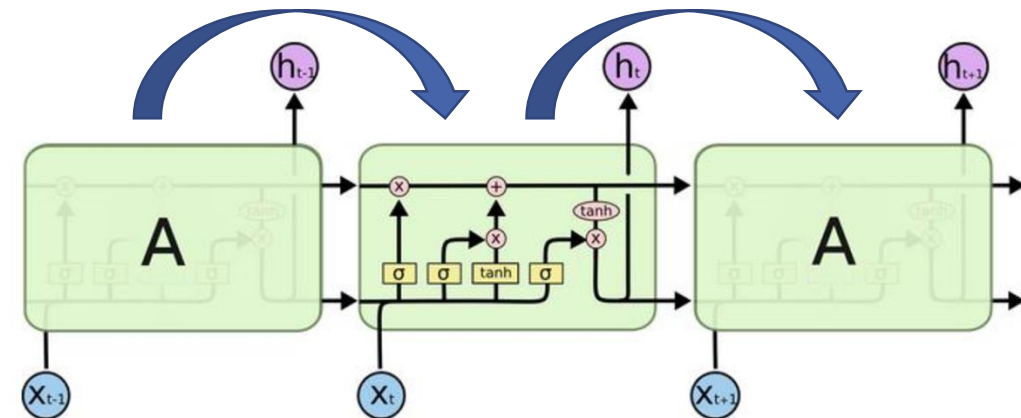
# Conservation, Dissipation, Innovation

- Data-based models

Neural Network




Long Short-Term **Memory** (LSTM) Network



# Conservation, Dissipation, Innovation

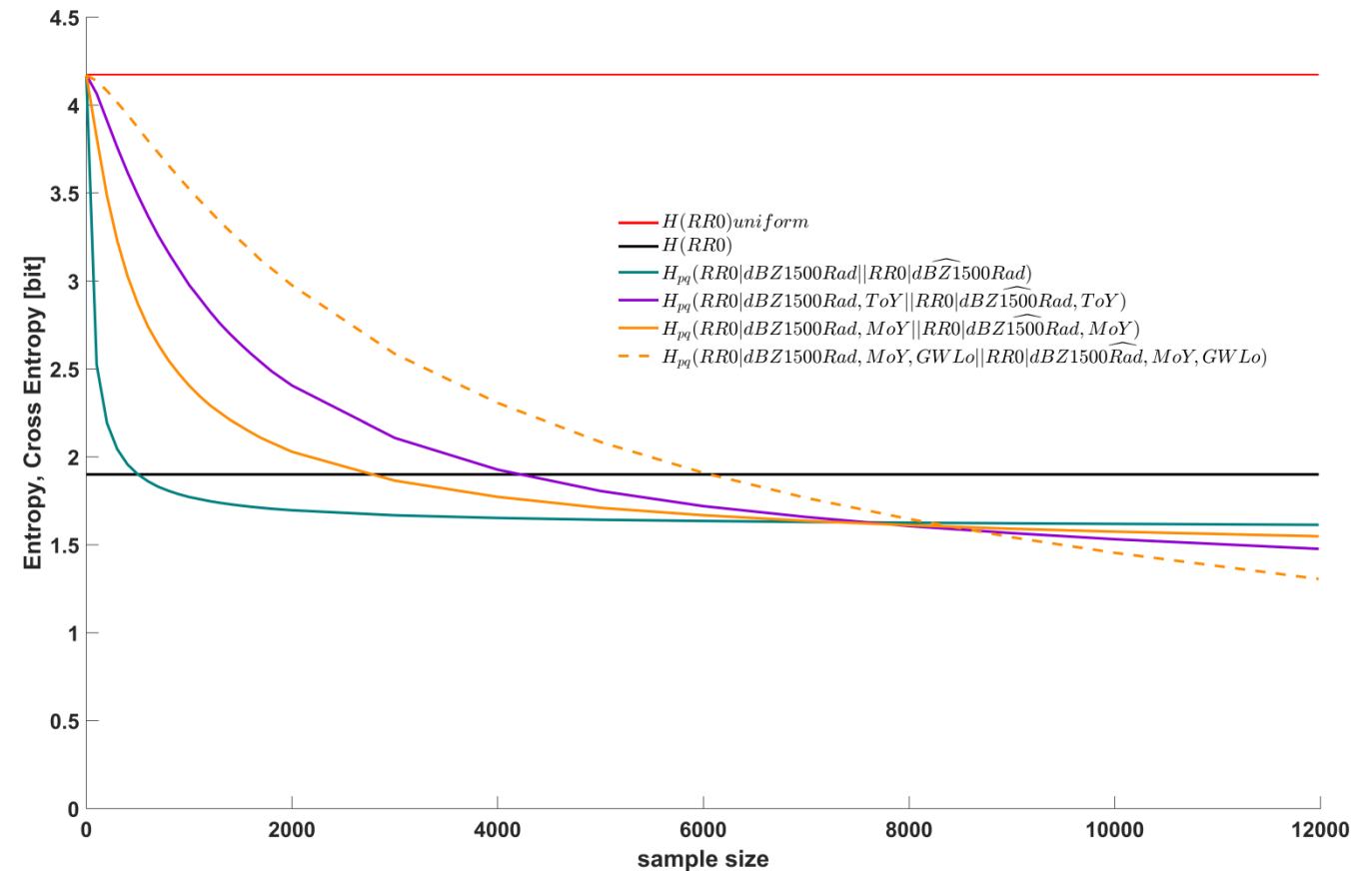
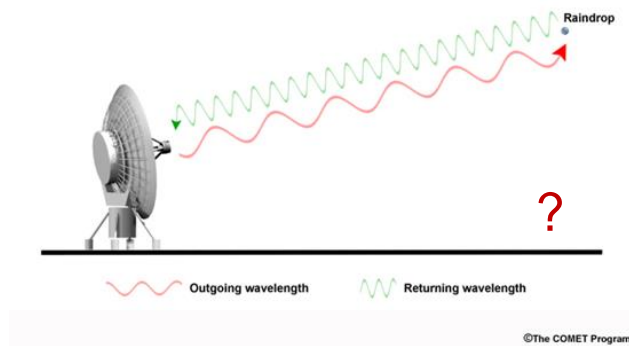
- Random-number generator
  - Linear congruential generator

$$x_t = (a \cdot x_{t-1} + b) \bmod m$$




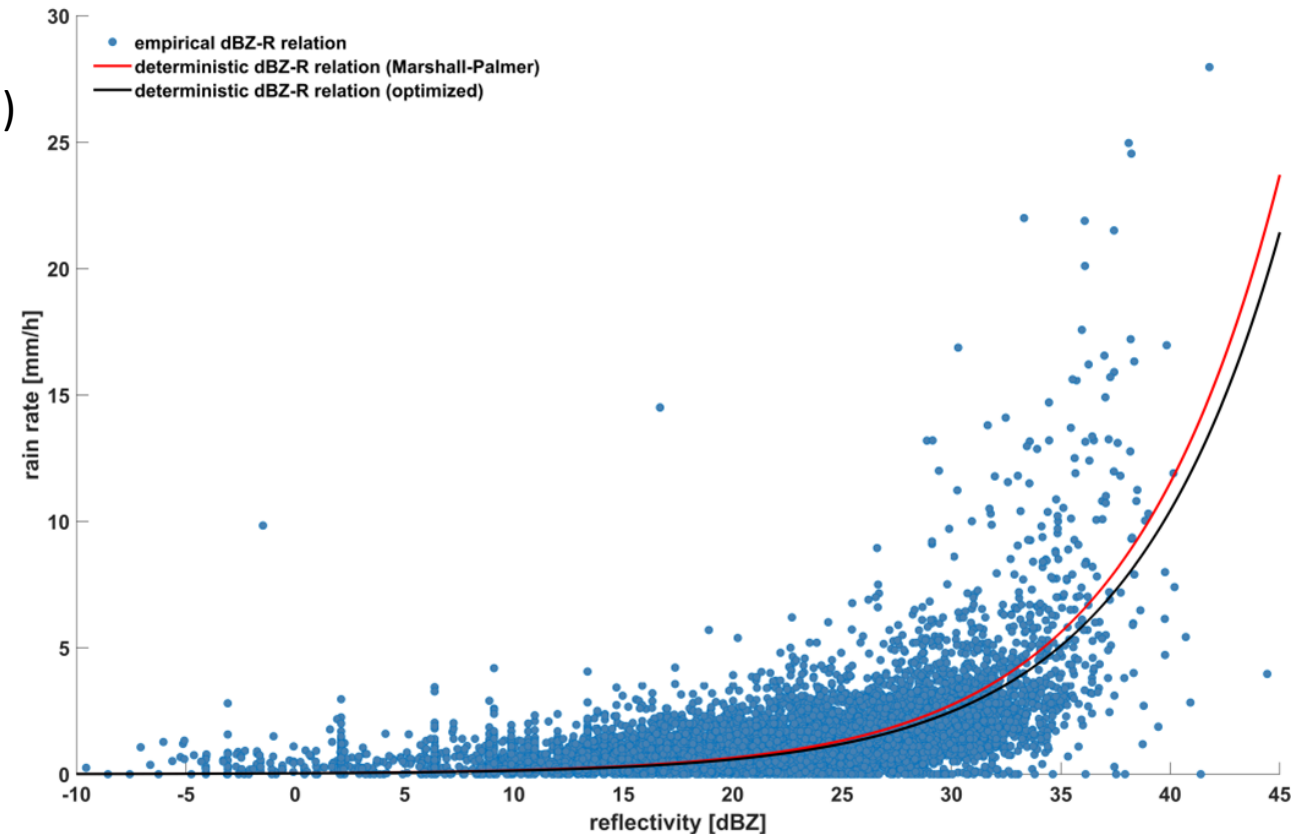
# Applications

- Neuper and Ehret (2019)
  - Quantify the information effect of limited sample size and number of predictors



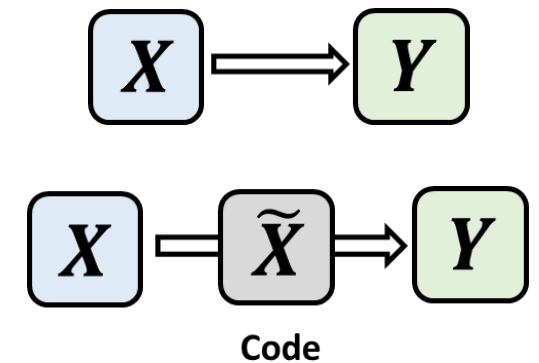
# Applications

- Neuper and Ehret (2019)
  - Quantify the information effect of deterministic compression
    - $H(RR) = 1.90$  bit
    - $H(RR | dBZ) = 1.61$  bit
    - $H_{\text{cross}}(RR | dBZ | \text{Marshall-Palmer}) = \mathbf{5.04 \text{ bit (!)}}$



# Applications

- Tishby et al. (2000)
  - Propose an information-based mechanism for feature extraction in ML
  
- We want to use  $X$  to predict  $Y$
- We only need the part in  $X$  that is informative about  $Y$
- We can squeeze  $X$  through a bottleneck formed by a limited set of codewords  $\tilde{X}$ , which preserves information about  $Y$
- There is a tradeoff between compressing the representation and preserving meaningful information



$$\min_{p(\tilde{x}|\mathbf{x})} \mathcal{L}[p(\tilde{x}|\mathbf{x})] = I(\mathbf{X}; \tilde{\mathbf{X}}) - \beta \cdot I(\tilde{\mathbf{X}}; \mathbf{Y})$$

Minimize Mutual Information between  $\mathbf{X}$  and  $\tilde{\mathbf{X}}$  to achieve a minimal representation

Lagrange multiplier  $\beta > 0$  balances the constraints

Maximize Mutual Information between  $\tilde{\mathbf{X}}$  and  $\mathbf{Y}$  to achieve a good prediction



# Further reading

## ■ Papers

- Shannon, C. E. (1948): A mathematical theory of communication, Bell system technical journal, 27, 623-656, [citeulike-article-id:1584479](#). [The big bang paper](#)
- Kullback, S., and Leibler, R. A. (1951): On Information and Sufficiency, Ann. Math. Statist., 22, 79-86, [10.1214/aoms/1177729694](#). [Another classic](#)
- Weijs, S. (2011): Information Theory for Risk-based Water System Operation, PhD thesis, Faculty of Civil Engineering & Geosciences, section Water Resources Management, TU Delft, The Netherlands, Delft, 210 pp. [Very accessible and applied](#)
- Pechlivanidis, I.G.; Jackson, B.; McMillan, H.; Gupta, H.V. (2016): Robust informational entropy-based descriptors of flow in catchment hydrology. Hydrol. Sci. J. , 61, 1–18. [Robust binning](#)
- Knuth, K. H. (2019): Optimal data-based binning for histograms and histogram-based probability density models, Digital Signal Processing, 95, 102581. [Optimal binning](#)
- Kumar, P., and Ruddell, B. L. (2010): Information Driven Ecohydrologic Self-Organization, Entropy, 12, 2085-2096, [10.3390/e12102085](#). [Application to Ecohydrological context](#)

# Further reading

## ■ Textbooks

- Cover, T., and Thomas, J. A. (2006): Elements of Information Theory, Wiley Series in Telecommunications and Signal Processing, Wiley-Interscience. [Rigorous, comprehensive, the must-have](#)
- Singh, V. P. (213): Entropy Theory and its Application in Environmental and Water Engineering, John Wiley & Sons, Ltd. [Various application examples](#)

## ■ Journals

- Entropy (MDPI) <https://www.mdpi.com/journal/entropy>. [All kinds of disciplines and applications](#)

## ■ Tutorials

- Nicholas Timme and Christopher Lapish: A Tutorial for Information Theory in Neuroscience. <https://www.eneuro.org/content/5/3/ENEURO.0052-18.2018>. [Great tutorial for newcomers](#)



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