Agenda: Information, Probability, Statistical Entropy

1

- Information and probability
  - simple combinatorics.
  - Probability distributions, joint probabilities.
  - stochastic variables, correlations.
  - Statistical entropy
  - Monte Carlo simulations
- Partition of probability
- Phase space evolution (Eta Theorem)
- Partition functions for different degrees of freedom
- Gibbs stability criteria, equilibrium

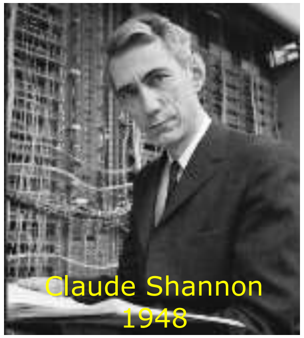
Reading Assignments
Weeks 4 & 5
LN III.1- III.6:

Kondepudi Ch. 20
Additional Material

McQuarrie & Simon
Ch. 3 & 4

Math Chapters
MC B, E

Aspects of Information Theory



In the absence of information, probability replaces certainty.

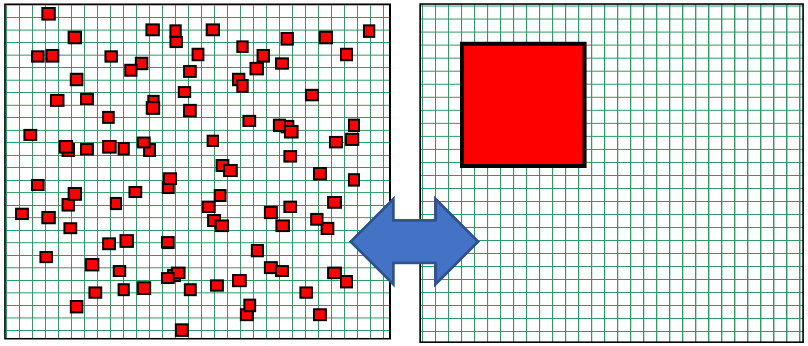
Information theory provides probability as an objective link be-tween randomness and certainty.

$$H=-\sum p(x)\log p(x)$$

Important theorist
Claude Shannon, "Father of Information Theory"

2

"If a situation (event) is very likely to occur (high probability) → information provided with its occurrence is low." And vice versa.



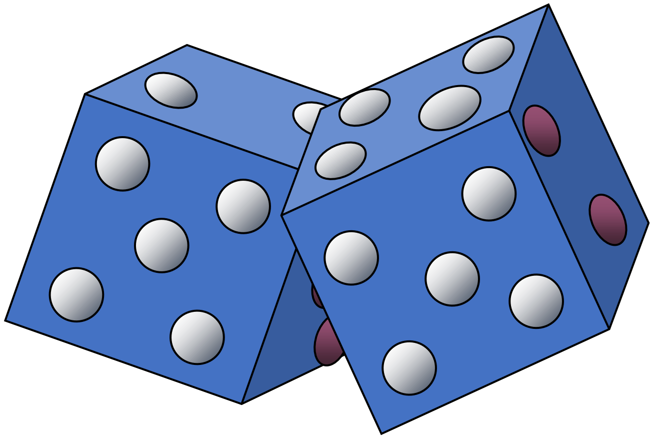
Random positions = first guess if nothing known about particles

Particles cluster in a corner → deduce mutual attraction → significant info

Illustration:
Two possible 2-dim micro-states for a system of 100 particles distributed differently over the available phase space.

Simple Probability Concepts

W. Udo Schröder 2023



Probability: understood as being relative to set of many uncertain events, experiments, measurements, outcomes, …

If instances of a type of event x_n occur in random selection, without hidden preference (bias), one can estimate

Probability ←→ combinatorics

Conduct experiment/measurement → probability for event type ***x***

$N(x_k) = \textit{frequency of events } x_k$

Probability ***a posteriori***

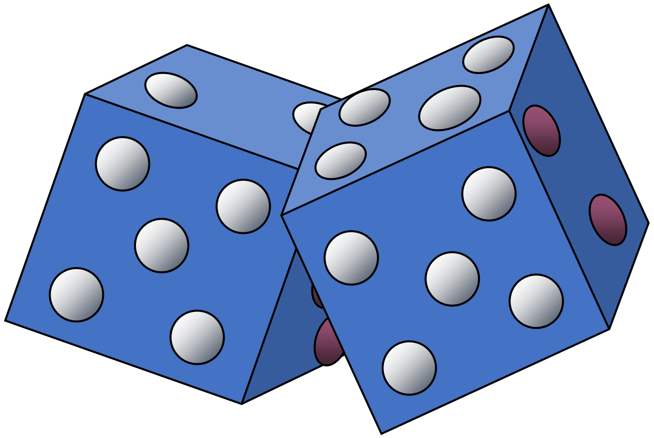
$$P(x_n) = \lim_{N\to\infty} \frac{N(x_n)}{\sum_k N(x_k)}$$

Example: experiment (unbiased) rolling *1* dice 1000x →

Expect (***a priori***) face with "6" $P(6) = 1/6 = 0.1667$ → $N(6) = 166\ (167)$

observe (***a posteriori***) face with "6" : $N(6) = 173$ → $P(6) = 0.173 \approx 1/6$

Probability Distributions

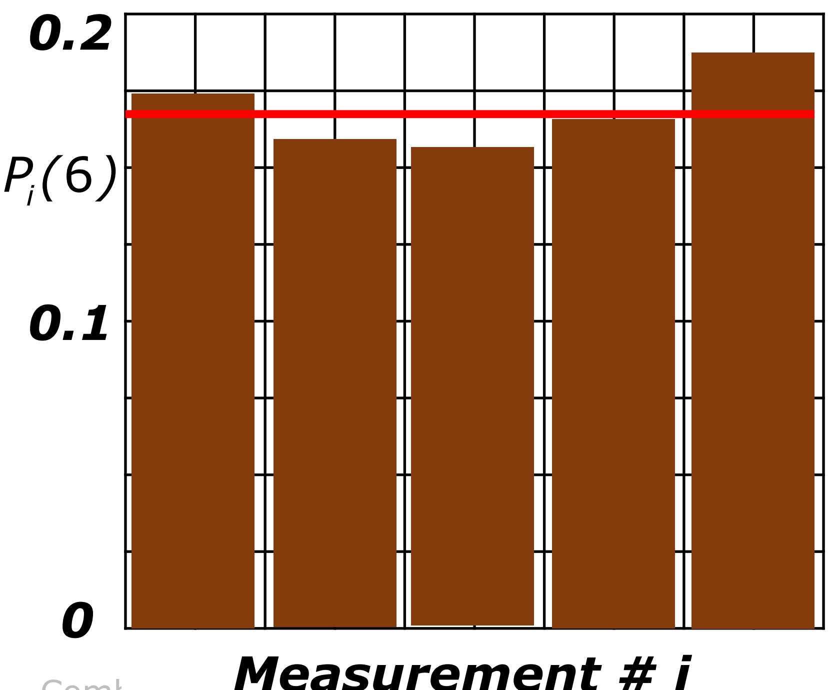


Conduct many *(M=5)* measurements of 1000 rolls of one die → *M-5* different probabilities for event type ***x* =“6”**
→ ***a posteriori*** probability

$N(x_k) = \textit{frequency of events } x_k$

$\{N(6)\} = \{175, 160, 155, 167, 182\}$

$$P_i(6) = \lim_{N\to\infty} \frac{N_i(6)}{\sum_k^{1\cdots6} N_i(k)}; \quad i = 1,..,M$$



Mean/average probability

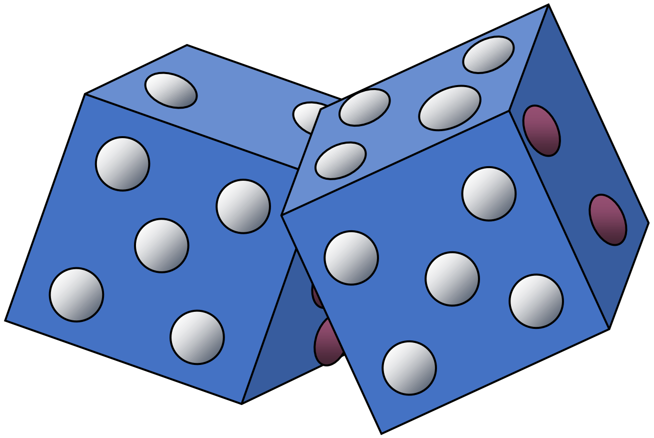
$$\langle P(6)\rangle_i := \sum_{i=1}^{M} w_i \cdot P(6)_i = \sum_{i=1}^{M} \frac{1}{M} \cdot P(6)_i$$

Measurements of equal quality

$\rightarrow$ *Equal weights* $w_i = 1/M$

$\rightarrow \langle P(6)\rangle_i = 0.168$

Probability Distributions



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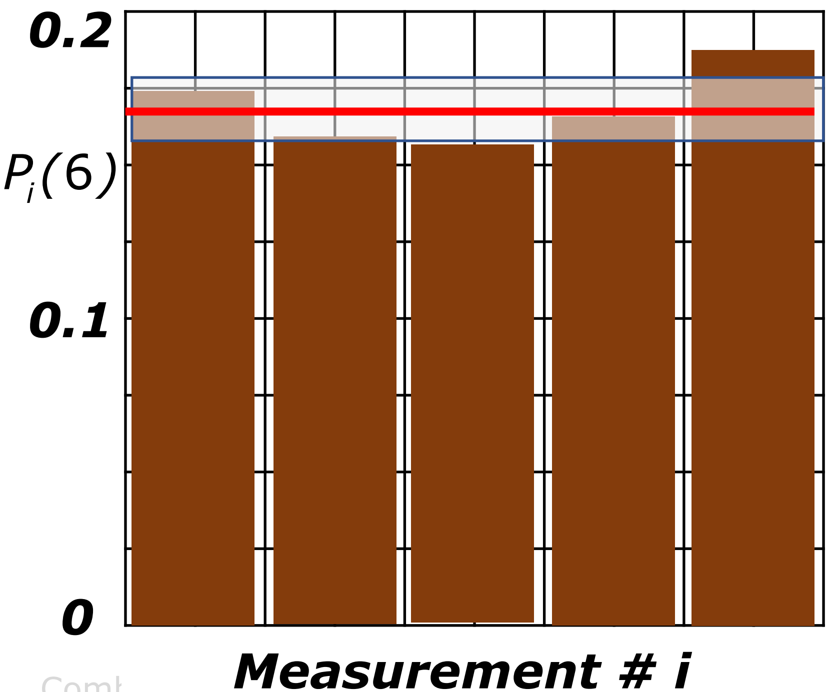


Variance/Standard Deviation

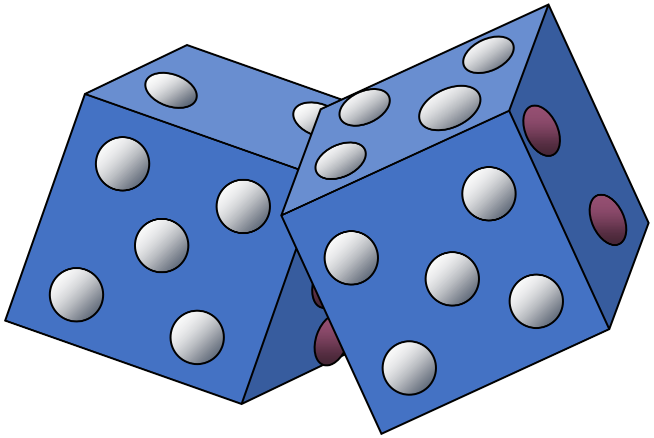
$$\sigma_P^2(6) := \frac{1}{M(M-1)} \sum_{i=1}^{M} \left(P(6)_i - \langle P \rangle\right)^2$$

$$\sigma_P^2(6) = 2.4 \cdot 10^{-5} \rightarrow \sigma_P(6) = 0.005$$

$$\langle P(6) \rangle_i = (0.168 \pm 0.005)$$

$$a\ priori: P(6) = 1/6 = 0.167$$

Probability Combinations



Additive, inclusive or exclusive, cumulative, multiplicative, conditional probabilities.

Sum & product rules for disjoint (independent) probabilities

Outcome of one trial (→Event E1) has no effect on the result of the next trial (→Event E2). The corresponding probabilities are independent of one another and add

A priori probability to get a face "*6*" in either of two trials, the first or the second throw of a dice, equals the sum of both

$$P_{1\vee 2}(6) = P_1(6) + P_2(6) = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$$

OR inclusive

Simultaneous (***joint***) ***a priori*** probability to get a face "*6*" ***in both*** trials, the first ***and*** the second throw of a dice, equals the ***product*** of both

$$P_{1\wedge 2}(6\,|\,6) = P_1(6)\cdot P_2(6) = \frac{1}{6}\cdot\frac{1}{6} = \frac{1}{36}$$

AND

Properties of ***a priori*** Probabilities

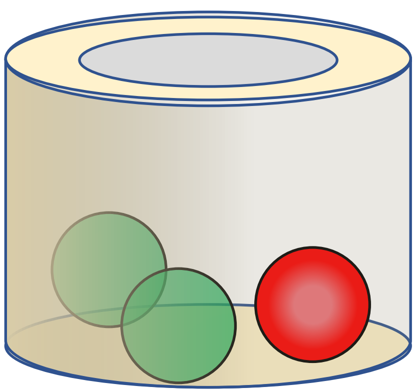
- The probability for an event is $0 \le P \le 1$
- The probability of an impossible event is zero, $P = 0$.
- The probability for one of the possible outcomes to occur is $P = \sum_i P_i = 1$
- If two events (E1 and E2) are independent (disjoint, mutually exclusive), the probability of the sum ("OR") event is the sum of the probabilities, $P_{1 \vee 2} = P_1 + P_2$
- If two events are not mutually exclusive, $P_{1 \vee 2} = P_1 + P_2 - P_{1 \wedge 2}$
- If two events (E1 and E2) are independent (not mutually exclusive), the probability for simultaneous occurrence is the product $P_{1 \wedge 2} = P_1 \cdot P_2$
- Additional considerations for conditional ***(marginal)*** probabilities, example $P\{E_1 \mid E_2\} := Probability\{E_1\}, \; given \; E_2$

Conditional Probabilities

Constraints on a set of events → conditional probability **$P\{E|\text{condition}\}$**.

Example drawing from 3 balls *(R, G, G)* hidden in a box. What are *a priori* probabilities for a sequence *1*. draw, *2*. draw,…. e.g. G_2,R_1…

Depends on 1. draw returned or not! If returned, uncorrelated draws →



$$P(G_2R_1) = P(G_2)\cdot P(R_1) = \frac{2}{3}\cdot\frac{1}{3} = \frac{2}{9}$$

If ball is not returned, correlated=conditional draws →

Given that *Red* was drawn first

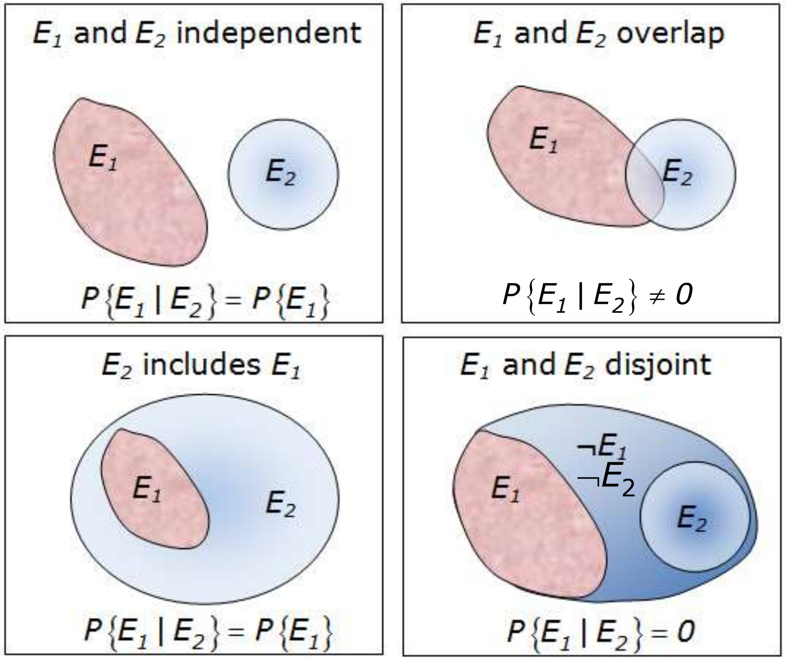
$$P(G_2R_1) \to P\{G_2 \mid R_1\}\cdot P(R_1) = 1\cdot\frac{1}{3} = \frac{1}{3}$$

3. draw

$$P(G_3G_2R_1) = P\{G_3 \mid G_2R_1\}\cdot P(G_2R_1) = 1\cdot\frac{1}{3} = \frac{1}{3}$$

Statistical Event Domains

Possible relations are illustrated between hypothetical domains of probable events



$P\{E_1\}$, $P\{E_2\}$, and $P\{\neg E_1 \vee \neg E_2\}$

Independent events E_1 and E_2 or if $E_1 \subset E_2 \rightarrow E_2$ has no influence on the probability for $E_1 \rightarrow$ Conditional

$$P\{E_1 | E_2\}(given\ E_2 = T) = P\{E_1\}$$

If two events are mutually exclusive,

$$P\{E_1 \wedge E_2\} = 0 = P\{E_1 | E_2\}$$

If E_1, E_2 not disjoint :

$$P\{E_1 \wedge E_2\} = P\{E_1 | E_2\} \cdot P(E_2)$$
$$= P\{E_2 | E_1\} \cdot P(E_1)$$

Bayes' Theorem

$$P\{E_1 | E_2\} = P(E_1) \cdot \frac{P\{E_2 | E_1\}}{P(E_2)}$$

Fractional probability for

$E_2 = T(if\ E_1 = T) / Total\ P(E_2)$

Prior probability $P(E_1) = suspicion,\ guess$

Bayes' Theorem: Rain or Sun ?

$P\{E_2 = rain\} = 0.25$

Datum

$P\{E_1 \mid given\ E_2 = rain\} = 0.8$

$E_2 = partly\ cloudy$

$P\{E_2\} = 0.42$

Event E_1 = people carry umbrellas

$P\{E_1\} = 0.20$

E_2 = other reasons

$P\{E_1 \mid E_2\} = 0.1$

$P\{E_2 = sun\} = 0.33$

Datum

$P\{E_1 \mid given\ E_2 = sun\} = 0.1$

Prob for $E_2 = rain$ when observing umbrellas

$$P\{E_2 = rain \mid E_1 - umbr.\} = P(E_2 = r)\cdot\frac{P\{E_1 = u \mid E_2 = r\}}{P(E_1 = u)} = 0.25\cdot\frac{0.8}{0.2} = 1$$

Discrete Multivariate Probability Distributions

Bias Test*:* Randomly draw colored dies ($i=1\text{-}5$) out of bag. Roll each die many times and record face frequencies ($j=1,\ldots,6$). Normalize to total # rolls.

→dim{$\boldsymbol{p_{ij}}$} domain =5x6=30 →Data must fulfill independent constraints:

$$\text{Color } u_i = \sum_{j=1}^{6} p_{ij} \rightarrow \sum_{i=1}^{5} u_i = 1 \qquad \text{Face } \upsilon_j = \sum_{j=1}^{5} p_{ij} \rightarrow \sum_{j=1}^{6} \upsilon_j = 1$$

Color i ↓ / Face j →	1	2	3	4	5	6	$u_i = \sum_{j=1}^{6} p_{ij}$
red							$u_1 = 0.10$
blue				p_{24}			$u_2 = 0.30$
green							$u_3 = 0.20$
white							$u_4 = 0.25$
black							$u_5 = 0.15$
$v_j = \sum_{i=1}^{5} p_{ij}$	v_1 0.131	v_2 0.148	v_3 0.163	v_4 0.162	v_5 0.200	v_6 0.196	← ↑ Data

After Dill & Bromberg

Discrete Multivariate Probabilities

Compare a priori with posteriori probabilities to find bias. Example: blue die with face "4" from overlap (simultaneous) probability domains.

A priori : $P(blue, any\,\#) = 1/5; \quad P(any, 4) = 1/6 \rightarrow P(blue) \wedge P(4) = 1/30 = 0.033$

A posteriori : $P(blue) \wedge P(4) = u_2 \cdot v_4 = 0.3 \cdot 0.162 = 0.049$

But $0.049/0.033 \approx 1.5 = u_2/0.2$

i	j = 1	2	3	4	5	6	$u_i = \sum_{j=1}^{6} p_{ij}$
red	0.016	0.018	0.018	0.017	0.015	0.016	u_1 = 0.10
blue	0.025	0.035	0.045	0.055	0.065	0.075	u_2 = 0.30
green	0.030	0.028	0.032	0.030	0.050	0.030	u_3 = 0.20
white	0.040	0.042	0.038	0.040	0.040	0.050	u_4 = 0.25
black	0.020	0.025	0.030	0.020	0.030	0.025	u_5 = 0.15
$v_j = \sum_{i=1}^{5} p_{ij}$	v_1 0.131	v_2 0.148	v_3 0.163	v_4 0.162	v_5 0.200	v_6 0.196	

Data from Dill & Bromberg

End

Probability & Combinatorics