Applications of large deviation theory

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Maties Machine Learning
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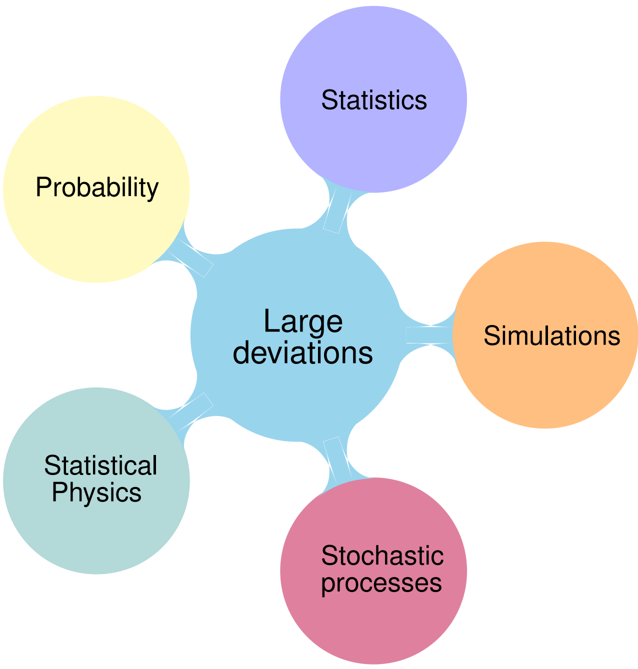
Overview



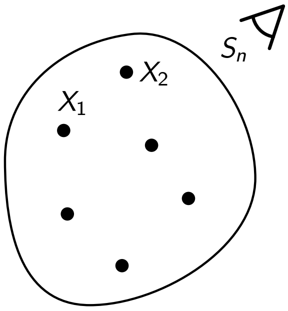
Goal

Explain how deterministic behavior arises from randomness

- Stochastic processes
- Many interacting components
- Rare events
- Typical or generic events
- Emergent determinism

Large deviation theory in one slide

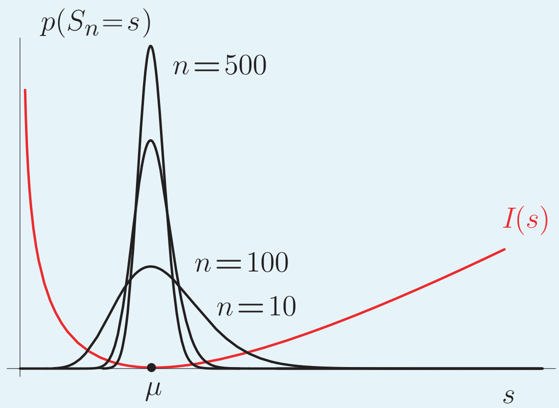
$S_n(\vec{X})$	Macro
$\vec{X} = (X_1, X_2, \ldots, X_n)$	Micro



Large deviation principle (LDP)

$$P(S_n = s) \approx e^{-nI(s)}$$

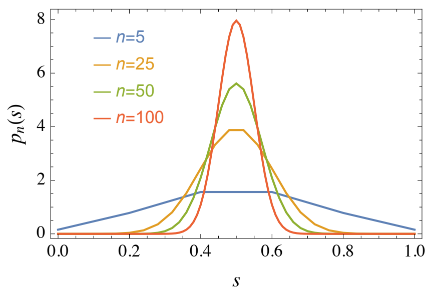
- $I(s)$ = rate function
- Exponentially rare events
- Typical value: $I(s^*) = 0$
- Concentration of probability



Coin tossing

H	T	T	H	T	$\cdots$
1	0	0	1	0	$\cdots$
X_1	X_2	X_3	X_4	X_5	$\cdots$

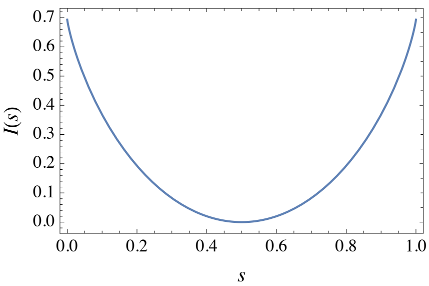
$$S_n = \frac{\#\text{ heads}}{n} = \frac{1}{n}\sum_{i=1}^{n} X_i$$



LDP

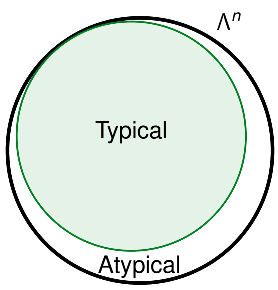
$$P(S_n = s) \approx e^{-nI(s)}$$

$$I(s) = s\log s + (1-s)\log(1-s) + \log 2$$



Typical sequences

$$\#\{\vec{X} : S_n = 0.5\} \approx 2^n$$



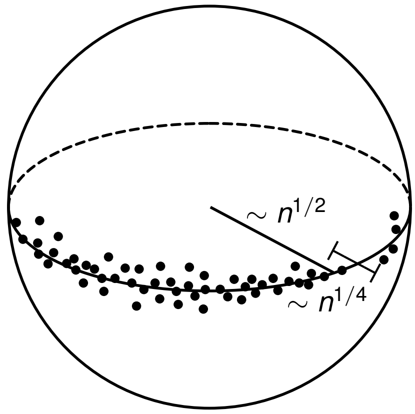
Gaussian vectors and hyperspheres

- Gaussian vector in n-dim:

$$\vec{X} = (X_1, X_2, \ldots, X_n)$$

- $X_i \sim \mathcal{N}(0,1)$ iid
- Rescaled "radius":

$$S_n = \frac{1}{n}\sum_{i=1}^{n} X_i^2$$



LDP

$$P(S_n = s) \approx e^{-nI(s)}$$

- Typical value: $S_n \to 1$
- Exponential concentration

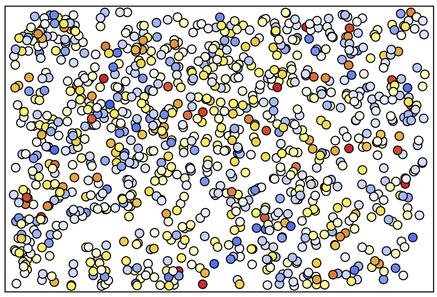
Typicality

- Most points lie on surface
- Asymptotically uniform
- Volume concentrated near surface as $n \to \infty$

Statistical physics

- Total energy:

$$U_N = \sum_{i=1}^{N} \frac{v_i^2}{2m}, \qquad N \sim 10^{23}$$



- Velocity distribution:

$$L_N(v) = \frac{\#\text{ particles } v_i \in [v, v+\Delta v]}{N\Delta v}$$

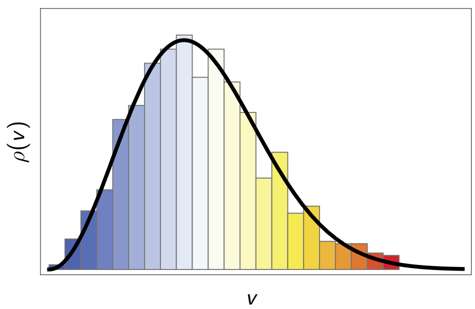
LDP

$$P(L_N = \rho) \approx e^{-NI(\rho)}$$

- Equilibrium distribution:

$$\rho^*(v) = c\, v^2 e^{-\frac{mv^2}{2k_B T}}$$

- Maxwell's distribution

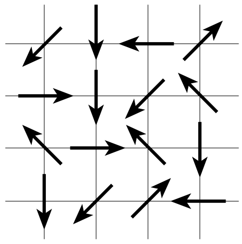


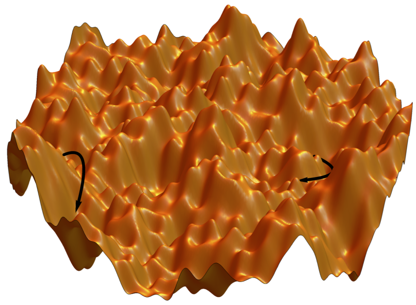
Spin glasses

- Energy:

$$H = -\sum_{ij} \underbrace{J_{ij}}_{\text{disorder}} \sigma_i \sigma_j + h \sum_i \sigma_i$$

- Find min energy (ground state)
- Count number $\Omega_N(u)$ local min with given energy





LDPs

$$\Omega_N(u) \approx e^{N\Sigma(u)}$$

- $\Sigma(u) =$ entropy

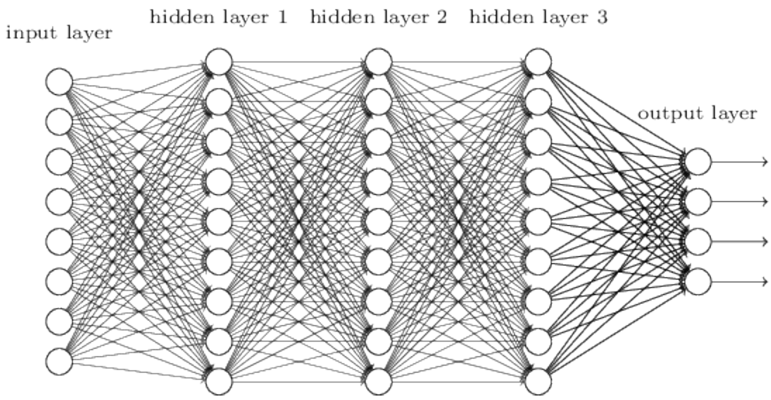
Typicality

- Exponentially many metastable states
- Most critical points are saddles in high dim

Problems from machine learning

- Neurons: $\{\sigma_i\}$
- Weights: $\{w_{ij}\}$
- Cost function:

$$\mathcal{C}(\text{input}, \text{output}, \{w_{ij}\})$$



Practical

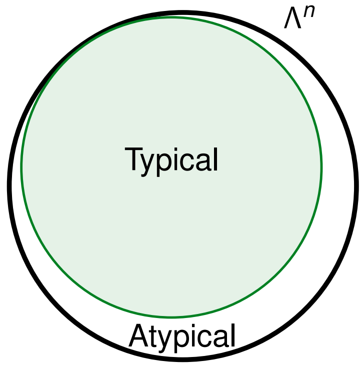
- Number of metastable states
- Typicality of data
- Overfitting fluctuations

Fundamental

- Why ML works at all?
- Generic attractors
- Represent typical features

Other applications

- Information theory
- Random graphs
- Markov process: X_t, $S_T[x]$
- Signal analysis
- Statistical physics
- Phase transitions
- Quantum systems
- ...



- Full space is huge
- Most states "look" the same

F. den Hollander, *Large Deviations*, AMS, 2000

H. Touchette, The large deviation approach to statistical mechanics, *Physics Reports* **478**, 2009

www.physics.sun.ac.za/~htouchette

Current research: LDs of Markov processes

- Process: $\{X_t\}_{t=0}^T$
- Observable: $A_T[x]$

LDP

$$P(A_T = a) \approx e^{-TI(a)}$$

Problems

- Predict how rare fluctuations happen
- Effective process describing fluctuations
- Related to non-Hermitian spectral problem