Théorie des grandes déviations:
Des mathématiques à la physique

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Plan

Themes
• Typical states
• Fluctuations around typicality
• Many components

Outline
• A bit of history
• Basics of large deviations
• Equilibrium systems
• Nonequilibrium systems

Lewis (80s)
Graham (80s)

Lanford (1973)

Onsager (1953)

Einstein (1910)

Boltzmann (1877)

Ellis (1984)

Gärtner (1977)

Freidlin-Wentzell (70s)

Donsker-Varadhan (70s)

Sanov (1957)

Cramér (1938)
Boltzmann (1877)

- Energy levels: $j = 1, 2, 3, 4, \ldots, N$
- Particles: $i = 1, 2, 3, 4, \ldots, N$

- Energy distribution:
  \[ w_j = \# \text{ particles in level } j \]

- Multinomial distribution:
  \[
  \ln \frac{N!}{\prod_j w_j!} \approx -N \sum_j w_j \ln w_j = Ns(w)
  \]

- Probability:
  \[ P(w) \approx e^{Ns(w)} \]

Einstein (1910)

- Generalize Boltzmann
- Macrostate: $M_N$
- Density of states (complexion):
  \[ W(m) = \# \text{ microstates with } M_N = m \]

Einstein’s postulate

\[ W(m) = e^{Ns(m)} \]

- Probability:
  \[ P(m) = e^{N[s(m) - s(m^*)]} \]

- Equilibrium: $s(m^*)$ is max
Cramér (1938)

- Sample mean:
  $$S_n = \frac{1}{n} \sum_{i=1}^{n} X_i, \quad X_i \sim p(x) \text{ IID}$$

- Cumulant:
  $$\lambda(k) = \ln E[e^{kX}] = \int p(x) e^{kx} \, dx$$

- Probability density:
  $$P(S_n = s) = e^{-nI(s)} \frac{1}{\sqrt{n}} \left( b_0 + \frac{b_1}{n} + \cdots \right)$$

- Rate function:
  $$I(s) = \max_{k \in \mathbb{R}} \{ ks - \lambda(k) \}$$

Sanov (1957)

- Sequence of IID RVs:
  $$X_1, X_2, \ldots, X_n \quad X_i \sim p(x)$$

- Empirical distribution:
  $$L_n(x) = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i, x}$$

- Empirical distribution:
  $$P(L_n = \rho) \approx e^{-nD(\rho||p)}$$

- Relative entropy:
  $$D(\rho||p) = \int dx \rho(x) \ln \frac{\rho(x)}{p(x)}$$

- Law of Large Numbers: $$L_n \to \rho$$
Large deviation theory

- Random variable: \( A_n \)
- Probability density: \( P(A_n = a) \)

Large deviation principle (LDP)

\[
P(A_n = a) \approx e^{-n I(a)}
\]

- Meaning of \( \approx \):
  \[
  \ln P(a) = -n I(a) + o(n)
  \]
  \[
  \lim_{n \to \infty} \frac{1}{n} \ln P(a) = I(a)
  \]

- Rate function: \( I(a) \geq 0 \)

Goals of large deviation theory

1. Prove that a large deviation principle exists
2. Calculate the rate function

Varadhan’s Theorem

- LDP:
  \[
P(A_n = a) \approx e^{-n I(a)}
  \]

- Exponential expectation:
  \[
  E[e^{nf(A_n)}] = \int e^{nf(a)} P(A_n = a) \, da
  \]

- Limit functional:
  \[
  \lambda(f) = \lim_{n \to \infty} \frac{1}{n} \ln E[e^{nf(A_n)}]
  \]

**Theorem:** Varadhan (1966)

\[
\lambda(f) = \max_a \{f(a) - I(a)\}
\]

Special case: \( f(a) = ka \)

\[
\lambda(k) = \max_a \{ka - I(a)\}
\]
Gärtner-Ellis Theorem

Scaled cumulant generating function (SCGF)

\[ \lambda(k) = \lim_{n \to \infty} \frac{1}{n} \ln E[e^{nkA_n}], \quad k \in \mathbb{R} \]

**Theorem:** Gärtner (1977), Ellis (1984)

If \( \lambda(k) \) is differentiable, then

1. **LDP:**
   \[ P(A_n = a) \approx e^{-nI(a)} \]
2. **Rate function:**
   \[ I(a) = \max_k \{ ka - \lambda(k) \} \]

- \( I(a) \) is the Legendre transform of \( \lambda(k) \)

Cramer’s Theorem

- **Sample mean:**
  \[ S_n = \frac{1}{n} \sum_{i=1}^{n} X_i, \quad X_i \sim p(x), \text{ IID} \]
- **SCGF:**
  \[ \lambda(k) = \lim_{n \to \infty} \frac{1}{n} \ln E[e^{nkS_n}] = \ln E[e^{kX}] \]

**Gaussian**

\[ \lambda(k) = \mu k + \frac{\sigma^2}{2} k^2, \quad k \in \mathbb{R} \]
\[ I(s) = \frac{1}{2\sigma^2} (s - \mu)^2, \quad s \in \mathbb{R} \]

**Exponential**

\[ \lambda(k) = -\ln(1 - \mu k), \quad k < \frac{1}{\mu} \]
\[ I(s) = \frac{s}{\mu} - 1 - \ln \frac{s}{\mu}, \quad s > 0 \]
Sanov’s Theorem

- \( n \) IID random variables:
  \[
  \omega = \omega_1, \omega_2, \ldots, \omega_n, \quad P(\omega_i = j) = p_j
  \]

- Empirical frequencies:
  \[
  L_{n,j} = \frac{1}{n} \sum_{i=1}^{n} \delta_{\omega_i,j} = \frac{\#(\omega_i = j)}{n}, \quad L_n = (L_{n,1}, L_{n,2}, \ldots)
  \]

Gärtner-Ellis

- SCGF:
  \[
  \lambda(k) = \lim_{n \to \infty} \frac{1}{n} \ln E[e^{nk \cdot L_n}] = \ln \sum_{j=1}^{q} p_j e^{k_j}
  \]

- Rate function:
  \[
  D(\mu) = \inf_k \{k \cdot \mu - \lambda(k)\} = \sum_{j=1}^{q} \mu_j \ln \frac{\mu_j}{p_j}
  \]

Beyond IID

Markov processes

- \( \{X_t\}_{t=0}^{T} \)
- \( A_T = \frac{1}{T} \int_{0}^{T} f(X_t) \, dt \)
- \( P(A_T = a) \approx e^{-Tf(a)} \)
- Long time limit
- Donsker & Varadhan (1975)

SDEs

- \( \dot{x}(t) = f(x(t)) + \sqrt{\epsilon} \xi(t) \)
- \( P[x] \approx e^{-f[x]/\epsilon} \)
- Low noise limit
- Freidlin & Wentzell (1970s)
- Onsager & Machlup (1953)

Applications

- Noisy dynamical systems
- Interacting SDEs
- Stochastic PDEs
- Interacting particle systems
- RWs random environments
- Queueing theory
- Statistics, estimation
- Information theory
Summary

\[ P(A_n = a) \approx e^{-nI(a)} \]

- Law of Large Numbers
  - Typical value = zeros of \( I(a) \)
- Central Limit Theorem
  - Quadratic minima = Gaussian fluctuations
  - Small deviations
- Large deviations
  - Fluctuations away from typical value

General theory of typical states and fluctuations

Equilibrium systems

- \( N \) particles
- Microstate: \( \omega = \omega_1, \omega_2, \ldots, \omega_N \)
- Statistical ensemble: \( P(\omega) \)
- Macrostate: \( M_N(\omega) \)
- Macrostate distribution:

\[ P(M_N = m) = \sum_{\omega : M_N(\omega) = m} P(\omega) \]

Problems

- Calculate \( P(M_N = m) \)
- Find most probable values of \( M_N \) (= equilibrium states)
- Study fluctuations around most probable values
- Thermodynamic limit \( N \to \infty \)
Equilibrium large deviations

**Microcanonical**

Einstein (1910)

\[ P_u(M_N = m) = e^{S(u,m)/k_B} \]

- Extensivity: \( S \sim N \)
- LDP:
  \[ P_u(M_N = m) \approx e^{-NI_u(m)} \]

**Canonical**

Landau (1937)

\[ P_\beta(M_N = m) = e^{-F(\beta,m)} \]

- Extensivity: \( F \sim N \)
- LDP:
  \[ P_\beta(M_N = m) \approx e^{-NI_\beta(m)} \]

- Exponential concentration of probability
- Equilibrium states = minima and zeros of \( I \)

Maxwell distribution

- Velocity distribution:
  \[ L_N(v) = \frac{\# \text{ particles with } v_i \in [v, v + \Delta v]}{N\Delta v} \]

Sanov’s Theorem

\[ P_u(L_N = \rho) \approx e^{-NI_u(\rho)} \]

- Equilibrium distribution:
  \[ \rho^*(v) = c v^2 e^{-\frac{mv^2}{2k_B T}} \]
Entropy and free energy

- Density of states:
  \[ \Omega(u) = \# \omega \text{ with } U/N = u \]

- Large deviation form: \( \Omega(u) \approx e^{Ns(u)} \)

Gärtner-Ellis Theorem

\[ s(u) = \min_{\beta} \{ \beta u - \varphi(\beta) \} \]

- Free energy:
  \[ \varphi(\beta) = \lim_{N \to \infty} -\frac{1}{N} \ln Z(\beta), \quad Z(\beta) = \int d\omega \, e^{-\beta U(\omega)} \]

- \( Z(\beta) = \) partition function = generating function
- \( \varphi(\beta) = \) free energy = SCGF
- Basis of Legendre transform in thermodynamics

Sources and applications

- Finite-range systems
  Lanford (1973)
- Spin systems
  Ellis (1980s)
- Bose condensation
  Lewis (1980s)
- 2D turbulence
- Long-range systems
- Quantum systems
  Lenci, Lebowitz (2000)
- Spin glasses

- Large deviation structure
- Typical states and fluctuations
Nonequilibrium systems

- Process: \( X_t \)
  - One or many particles
  - Markov process
  - External forces
  - Boundary reservoirs
- Trajectory: \( \{x_t\}_{t=0}^T \)
- Path distribution: \( P[x] \)
- Observable: \( A_N, T[x] \)

Problems

- Calculate \( P(A_N, T = a) \)
- Find most probable values of \( A_N, T \) (= stationary states)
- Study fluctuations around typical values
- Scaling limits:
  \[
  N \to \infty \quad T \to \infty \quad \text{noise} \to 0
  \]

Example: Pulled Brownian particle

- Glass bead in water
- Laser tweezers
- Langevin dynamics:
  \[
  m \ddot{x}(t) = -\alpha \dot{x} - k [x(t) - vt] + \xi(t)
  \]
- Fluctuating work:
  \[
  W_T = \Delta U + Q_T
  \]

LDP

\[
P(W_T = w) \approx e^{-TI(w)}
\]

Fluctuation relation

\[
\frac{P(W_T = w)}{P(W_T = -w)} = e^{Tcw}
\]
Applications

- Driven nonequilibrium systems
- Interacting particle models
  - Current, density fluctuations
  - Macroscopic, hydrodynamic limit
- Thermal activation
  - Kramers escape problem
- Disordered systems
- Multifractals
- Chaotic systems
- Quantum systems

- Exponentially rare fluctuations
- Exponential concentration of typical states
- Same theory for equilibrium and nonequilibrium systems

Summary

- Random variables — ensembles — stochastic systems
- Most probable values — equilibrium states — typical states
- Fluctuations — rare events
- Rate function = entropy
- Cumulant function = free energy
- Scaling limit: \( N \to \infty, T \to \infty, \epsilon \to 0 \)
- Unified language for statistical mechanics

H. Touchette
The large deviation approach to statistical mechanics
Physics Reports 478, 1-69, 2009

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

Prochain exposé

- Markov processes conditioned on large deviations
- When a fluctuation happens, how does it happen?