Empirical Statistical Mechanics

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Example 1: Large Hamiltonian system

Large ($N \gg 1$) particles with position $x_j = q_j$ and momentum p_j ($j = 1, \cdots, N$).

- Least action principle

$$A = \int_{t_0}^{t} \mathcal{L}(x(s), \dot{x}(s), s)\, ds$$

- Lagrange equations of motion

$$\frac{\partial \mathcal{L}}{\partial x_j} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_j} = 0$$

- Hamiltonian

$$H = \sum_j p_j \dot{x}_j - \mathcal{L}, \quad p_j = \frac{\partial \mathcal{L}}{\partial \dot{x}_j}$$

- Hamiltonian system (common notation $q_j = x_j$)

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j}, \frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j},$$

- Conservation of the Hamiltonian H

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Example 2: Logistic map

$$T(x) = 4x(1-x), x \in [0,1]$$

Figure: Sensitive dependence

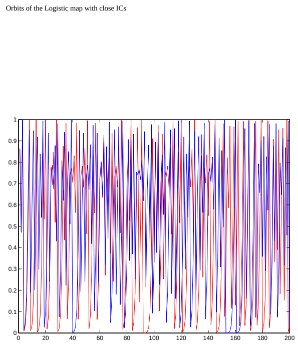
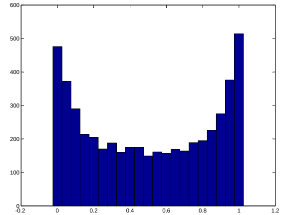


Figure: Statistical coherence



Example 3: Lorenz 96 model

Edward Norton Lorenz, 1917-2008

$$\textcolor{red}{Lorenz96}: \quad \frac{du_j}{dt} = (u_{j+1} - u_{j-2})u_{j-1} - u_j + F$$
$$j = 0, 1, \cdots, J; \qquad J = 5, F = -12$$

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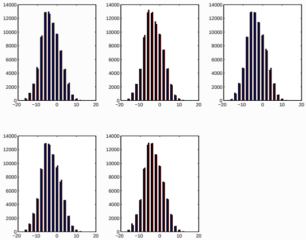

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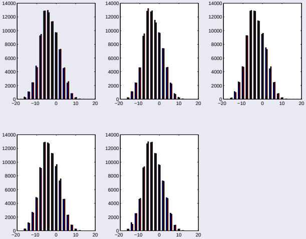

Example 4: Rayleigh-Bénard convection

$$\frac{1}{Pr}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) + \nabla p = \Delta \mathbf{u} + Ra\,\mathbf{k}\theta, \quad \nabla\cdot\mathbf{u} = 0, \quad \mathbf{u}|_{z=0,1} = 0,$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u}\cdot\nabla\theta - u_3 = \Delta\theta, \quad \theta|_{z=0,1} = 0. \quad (\theta = T - (1-z))$$

$$Pr = \frac{\nu}{\kappa},$$

$$Ra = \frac{g\alpha(T_{bottom} - T_{top})h^3}{\nu\kappa}$$

Figure: Lord Rayleigh (John William Strutt) 1842-1919

Figure: Henri Bénard (left), 1874-1939

RBC set-up and numerics

Figure: RBC set-up

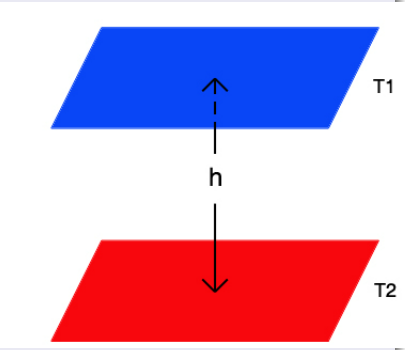

Figure: Numerical simulation

(∞ Pr. simulation)

Statistical Approaches

$$\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{u}), \quad \mathbf{u} \in H$$

$$S(t) : solutionsemigroup$$

- Long time average

$$< \Phi >= \lim_{T\to\infty} \frac{1}{T} \int_0^T \Phi(\mathbf{v}(t))\, dt$$

- Statistical coherence in terms of histogram implies independence on initial data.
- Spatial averages

$$< \Phi >_t = \int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v})$$

$\{\mu_t, t \geq 0\}$ statistical solutions

- Finite ensemble average $\mathbf{v}_j(t) = S(t)\mathbf{v}_{0j}, j = 1, \cdots, N$

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- Pull-back

$$\mu_0(S^{-1}(t)(E)) = \mu_t(E)$$

- Push-forward (Φ: suitable test functional)

$$\int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v}) = \int_H \Phi(S(t)\mathbf{v})\, d\mu_0(\mathbf{v})$$

- Finite ensemble example

$$\mu_0 = \sum_{j=1}^N p_j \delta_{\mathbf{v}_{0j}}(\mathbf{v}), \mu_t = \sum_{j=1}^N p_j \delta_{\mathbf{v}_j(t)}(\mathbf{v}), \mathbf{v}_j(t) = S(t)\mathbf{v}_{0j}$$

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Relative stability of statistical properties

- Finite ensemble

$$\frac{1}{N}\sum_{j=1}^{N}\Phi(\mathbf{u}_j(t))$$

- Total variation

$$|\mu_t(E) - \tilde{\mu}_t(E)| \leq |\mu_0(S^{-1}(t)E) - \tilde{\mu}_0(S^{-1}(t)E)|$$

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Liouville's equations

Figure: Joseph Liouville, 1809-1882

- Liouville type equation

$$\frac{d}{dt}\int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v}) = \int_H < \Phi'(\mathbf{v}), \mathbf{F}(\mathbf{v}) > \, d\mu_t(\mathbf{v})$$

Φ good test functionals e.g.

$$\Phi(\mathbf{v}) = \phi((\mathbf{v}, \mathbf{v}_1), \cdots, (\mathbf{v}, \mathbf{v}_N))$$

- Liouville equation (finite d)

$$\frac{\partial}{\partial t} p(\mathbf{v}, t) + \nabla \cdot (p(\mathbf{v}, t)\mathbf{F}(\mathbf{v})) = 0$$

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Figure: Eberhard Hopf, 1902-1983

Hopf's equation (special case of Liouville type)

$$\frac{d}{dt}\int_H e^{i(\mathbf{v},\mathbf{g})}\, d\mu_t(\mathbf{v})$$
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Invariant measures (IM)(Stationary Statistics Solutions)

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$$\mu(S^{-1}(t)(E) = \mu(E)$$

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Birkhoff's Ergodic Theorem

Figure: George David Birkhoff, 1884-1944

Definition

μ is ergodic if $\mu(E) = 0,$ or 1 for all invariant sets E.

Theorem (Birkhoff's Ergodic Theorem)

If μ is invariant and ergodic, the temporal and spatial averages are equivalent, i.e.

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \varphi(S(t)\mathbf{u})\, dt = \int_H \varphi(\mathbf{u})\, d\mu(\mathbf{u}),\ a$$

Examples of IM 1: dissipative

$$\frac{dr}{dt} = r(1 - r^2), \frac{d\theta}{dt} = 1.$$

$$\begin{aligned} \mu_1 &= \delta_0, \\ d\mu_2 &= \frac{1}{2\pi} d\theta, \quad \text{on } r = 1. \end{aligned}$$

- Non-uniqueness of invariant measure.
- Support of invariant measure may be singular.
- Question of physical relevance.

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Examples of IM 2: Hamiltonian

Hamiltonian system with energy $H(p,q)$ $(q = x)$

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$$d\mu(p,q) = Z^{-1}\exp(-\beta H(p,q))\,dpdq, Z = \int_H \exp(-\beta H(p,q))\,dpdq$$

  Z: partition function, β: inverse temperature

- Micro-canonical measure/distribution

$$d\mu = \chi^{-1}\exp(-\beta H(p,q))\delta(E - H(p,q))\,dpdq$$

$$\chi = \int \exp(-\beta H(p,q))\delta(E - H(p,q))\,dpdq = \exp(\frac{\mathcal{S}}{k})$$

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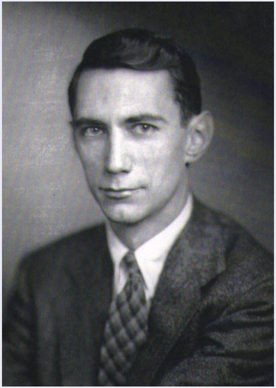
Shannon's entropy (measuring uncertainty)

Figure: Claude Shannon, 1916-2001



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$$\mathcal{S}(p) = \mathcal{S}(p_1, ..., p_n) = -\sum_{i=1}^{n} p_i \ln p_i.$$

$p \in \mathcal{PM}_n(\mathcal{A})$, probability measure on $\mathcal{A} = \{a_1, ..., a_n\}$

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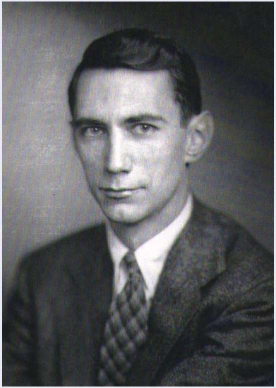

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Uniqueness of Shannon entropy

Figure: Edwin Thompson Jaynes, 1922-1998

Theorem (Jaynes)

- $H_n(p_1, ..., p_n)$: *continuous*
- $A(n) = H_n(1/n, ..., 1/n)$ *monotonic in n.*
- $\mathcal{A} = \{a_1, ..., a_n\} = \mathcal{A}_1 \bigcup \mathcal{A}_2$,
  $\mathcal{A}_1 = \{a_1, ..., a_k\}$,
  $\mathcal{A}_2 = \{a_{k+1}, ..., a_n\}$,
  $w_1 = p_1 + \cdots + p_k$,
  $w_2 = p_{k+1} + \cdots + p_n$,

$$H_n(p_1, ..., p_n) = H_2(w_1, w_2) + w_1 H_k(p_1/w_1, ..., p_k/w_1) + w_2 H_{n-k}(p_{k+1}/w_2, ..., p_n/w_2)$$

Then $\exists K > 0$, *s.t.* $H_n(p_1, ..., p_n) = K\mathcal{S}(p_1, ..., p_n) = -K \sum_{j=1}^{n} p_j \ln p_j$

Jaynes' maximum entropy principle

Given statistical measurements F_j of given functions f_j, $j = 1, ..., r \leq n - 1$,

$$F_j =< f_j >_p = \sum_{i=1}^{n} f_j(a_i) p_i, \quad j = 1, ..., r.$$

or continuous version

$$F_j =< f_j >_p = \int f_j(\mathbf{x}) p(\mathbf{x}) \, d\mathbf{x}.$$

Definition (Empirical maximum entropy principle)

Least biased / most probable pdf p^* is given by

$$max_{p \in \mathcal{C}} \mathcal{S}(p) = \mathcal{S}(p^*), \quad p^* \in \mathcal{C}$$

$$\mathcal{C} = \{p \in \mathcal{PM}(\mathcal{A}) \big| < f_j >_p = F_j, 1 \leq j \leq r\},$$

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Jaynes' maximum entropy principle

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Maximum relative entropy principle

- Relative entropy

$$\mathcal{S}(p, p^0) = -\sum_{j=1}^{N} p_j \ln \frac{p_j}{p_j^0} \quad = -P(p, p^0)$$

with prior distribution p^0

- Relative entropy as semi-distance

$$-\mathcal{S}(p, p^0) \geq 0, \forall p$$

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- No constraint. The one that maximizes the Shannon entropy on $\mathcal{A} = \{a_1, \cdots, a_N\}$ is the uniform distribution on $\mathcal{A}$.
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(application to PDE)

- $$\rho(\mathbf{x}, \lambda) \geq 0, \int \rho(\mathbf{x}, \lambda)\, d\lambda = 1.a.e.$$
- $$\int_{q-}^{q+} \rho(\mathbf{x}, \lambda)\, d\lambda = \text{Prob}\{q- \leq q(\mathbf{x}) < q+\}$$
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Maximum entropy principle remain the same

Barotropic quasi-geostrophic equation with topography

- Barotropic quasi-geostrophic equation

$$\frac{\partial q}{\partial t} + \nabla^{\perp}\psi \cdot \nabla q = 0, \quad q = \Delta\psi + h$$

q: potential vorticity, ψ: stream-function, h: bottom topography, $\Omega = (0, 2\pi) \times (0, 2\pi)$, per. b.c.

- Conserved quantities: kinetic energy E and total enstrophy $\mathcal{E}$

$$E = -\frac{1}{2|\Omega|}\int_{\Omega} \psi\Delta\psi \, d\mathbf{x},$$

$$\mathcal{E} = \frac{1}{2|\Omega|}\int_{\Omega} q^2 \, d\mathbf{x}$$

- There exist infinitely many conserved quantities.

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- Energy and total enstrophy as constraints

$$E(\rho) = -\frac{1}{2|\Omega|}\int_\Omega \bar{\psi}(\bar{q}-h), \quad \bar{q}(\mathbf{x}) = \int_{\mathcal{R}^1} \lambda\rho(\mathbf{x},\lambda)d\lambda, \bar{q} = \Delta\bar{\psi}+h,$$

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$$\frac{\delta\mathcal{S}}{\delta\rho} = -1-\ln\rho,$$

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Application of maximum entropy principle to barotropic QG, continued

- Most probable state ρ^*

$$-1 - \ln(\rho^*) = -\theta\lambda\bar{\psi}^* + \frac{\alpha}{2}\lambda^2 + \tilde{\gamma}(\mathbf{x})$$

$$\rho^*(\mathbf{x}, \lambda) = \frac{\sqrt{\alpha}}{\sqrt{2\pi}}\exp(-\frac{\alpha}{2}(\lambda - \frac{\theta}{\alpha}\bar{\psi}^*)^2)$$

  θ, α: Lagrange multipliers for energy and enstrophy, $\tilde{\gamma}(\mathbf{x})$: Lagrange multipliers for the pdf constraint.

- Mean field equation

$$\Delta\bar{\psi}^* + h = \frac{\theta}{\alpha}\bar{\psi}^* = \mu\bar{\psi}^*, \text{with } \mu = \frac{\theta}{\alpha}, \ \alpha > 0.$$

- Under generic topography, $\exists\mu = \mu(E) \in (-1, \infty)$, ψ_μ solves the mean field equation uniquely and is nonlinearly stable (Arnold-Kruskal stability).

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Energy circulation theory with a general prior

- BQG with bottom topography and channel geometry $\Omega = (0, 2\pi) \times (0, \pi)$

$$\psi = \psi' = \sum_{k \geq 1} \sum_{j \geq 0} (a_{jk} \cos(jx) + b_{jk} \sin(jx)) \sin(ky).$$

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$$E(\rho) = -\frac{1}{2|\Omega|} \int_\Omega \overline{\psi} \overline{\omega} d\mathbf{x}, \quad \Gamma(\rho) = \frac{1}{|\Omega|} \int_\Omega \int \lambda \rho(\mathbf{x}, \lambda) d\lambda d\mathbf{x}$$

- Most probable one-point statistics

$$\rho^*(\mathbf{x}, \lambda) = \frac{e^{(\theta\psi^* - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda)}{\int e^{(\theta\psi^* - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda) \, d\lambda}.$$

θ, γ Lagrange multipliers for energy and circulation respectively.

- Mean field equation

$$\Delta\psi^* + h = \frac{1}{\theta} \left(\frac{\partial}{\partial \psi} \ln \mathcal{Z}(\theta\psi, \mathbf{x}) \right) \Big|_{\psi = \psi^*}, \quad \mathcal{Z}(\psi, \mathbf{x}) = \int e^{(\psi - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda) \, d\lambda$$

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$$\rho^*(\mathbf{x}, \lambda) = \frac{e^{(\theta\psi^* - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda)}{\int e^{(\theta\psi^* - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda)\, d\lambda}.$$

θ, γ Lagrange multipliers for energy and circulation respectively.

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$$\Delta\psi^* + h = \frac{1}{\theta} \left(\frac{\partial}{\partial \psi} \ln \mathcal{Z}(\theta\psi, \mathbf{x}) \right) \bigg|_{\psi = \psi^*}, \quad \mathcal{Z}(\psi, \mathbf{x}) = \int e^{(\psi - \gamma)\lambda} \Pi_0(\mathbf{x}, \lambda)\, d\lambda$$

Energy circulation theory with a general prior

- BQG with bottom topography and channel geometry $\Omega = (0, 2\pi) \times (0, \pi)$

$$\psi = \psi' = \sum_{k\geq 1} \sum_{j \geq 0} (a_{jk} \cos(jx) + b_{jk} \sin(jx)) \sin(ky).$$

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Summary: empirical statistical mechanics

- Undamped/unforced setting customary
- Information theoretical approach: maximize Shannon entropy or relative entropy with prior and given measurements (conserved quantities)
- Conserved quantities become constraints on the one-point statistics ρ
- **Mean field equation**
$$\bar{q} = \mathcal{G}(\bar{\psi})$$
- Most of them (large scale structure) are stable under appropriate assumptions and hence physically relevant
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