From normal to anomalous deterministic diffusion
Part 1: Normal deterministic diffusion

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Setting the scene

nonequilibrium conditions →

		equilibrium	nonequilibrium steady states	nonequilibrium non-steady states
microscopic	**dynamical systems**	ergodic hypothesis	**microscopic chaos** strong	weak
↓	**statistical mechanics**	Gibbs ensembles	**complexity** fractal SRB measures	infinite measures
macroscopic	**thermodynamics**	thermodynamic properties	**deterministic transport** normal	anomalous

⇒ theory of nonequilibrium statistical physics starting from microscopic chaos?

approach should be particularly useful for

small nonlinear systems

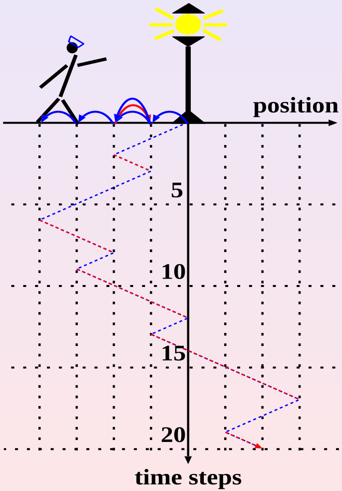
Outline

three parts:

1. **Normal deterministic diffusion:**
   some basics of dynamical systems theory for maps and escape rate theory of deterministic diffusion
2. **From normal to anomalous deterministic diffusion:**
   normal diffusion in particle billiards and anomalous diffusion in intermittent maps
3. **Anomalous (deterministic) diffusion:**
   generalized diffusion and Langevin equations, fluctuation relations and biological cell migration

The drunken sailor at a lamppost

random walk in one dimension (K. Pearson, 1905):



- steps of length s with probability $p(\pm s) = 1/2$ to the left/right
- single steps *uncorrelated*: Markov process (coin tossing)
- define diffusion coefficient as

$$D := \lim_{n\to\infty} \frac{1}{2n} < (x_n - x_0)^2 >$$

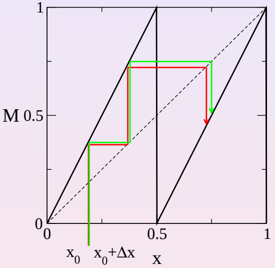
with discrete time step $n \in \mathbb{N}$ and average over the initial density $< \ldots > := \int dx \ \varrho(x) \ldots$ of positions $x = x_0 \ , \ x \in \mathbb{R}$

- for *sailor:* $D = s^2/2$

Bernoulli shift and dynamical instability

idea: study **diffusion** on the basis of **deterministic chaos**

Bernoulli shift $M(x) = 2x \bmod 1$ with $x_{n+1} = M(x_n)$:



apply small perturbation $\Delta x_0 := \tilde{x}_0 - x_0 \ll 1$ and iterate:

$$\Delta x_n = 2\Delta x_{n-1} = 2^n \Delta x_0 = e^{n \ln 2} \Delta x_0$$

$\Rightarrow$ exponential dynamical instability with Ljapunov exponent $\lambda := \ln 2 > 0$: **Ljapunov chaos**

Ljapunov exponent

local definition for one-dimensional maps via *time average*:

$$\lambda(x) := \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln \left|M'(x_i)\right| \ , \ x = x_0$$

if map is ergodic: time average = ensemble average,

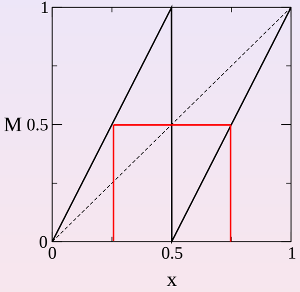
$$\lambda = \langle \ln |M'(x)| \rangle$$ **Birkhoff's theorem**

with average over an invariant probability density $\varrho(x)$ that is related to the map's SRB measure via $\mu(x) = \int_0^x dy\, \varrho(y)$

Bernoulli shift is *expanding*: $\forall x \, |M'(x)| > 1$, hence 'hyperbolic'

normalizable pdf exists, here simply $\varrho(x) = 1 \Rightarrow \lambda = \ln 2$

Kolmogorov-Sinai entropy



- define a partition $\{W_i^n\}$ of the phase space and *refine* it by iterating the critical point n times backwards
- let $\mu(w)$ be the SRB measure of a partition element $w \in \{W_i^n\}$
- define $H_n := -\sum_{w \in \{W_i^n\}} \mu(w) \ln \mu(w)$,

  where n denotes the level of refinement
- the limit $h_{ks} := \lim_{n\to\infty} \frac{1}{n} H_n$ defines the Kolmogorov-Sinai (metric) entropy (if the partition is generating)

for Bernoulli shift with uniform measure refinement yields $H_n = n \ln 2$, hence $h_{ks} = \ln 2 > 0$: **measure-theoretic chaos**

Pesin theorem

note: for Bernoulli shift $\lambda = \ln 2$ and $h_{ks} = \ln 2$

Theorem

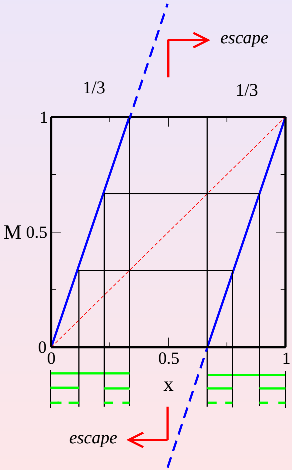
For closed C^2 Anosov systems the KS-entropy is equal to the sum of positive Lyapunov exponents.
Pesin (1976), Ledrappier, Young (1984)

believed to hold for a wider class of systems

for one-dimensional hyperbolic maps: $\boxed{h_{ks} = \lambda}$

Escape from a fractal repeller

piecewise linear map, slope $a = 3$, with **escape**:



- take a uniform ensemble of N_0 points; calculate the number N_n of points that survive after n iterations: $N_n = (2/3)N_{n-1} = N_0 e^{-n \ln(3/2)} =: N_0 e^{-\gamma n}$
- for hyperbolic maps N_n decreases exponentially with escape rate γ; repeller forms a **fractal** Cantor set

Escape rate formula

note: for open systems λ , h_{ks} must be computed with respect to the invariant measure on the fractal repeller $\mathcal{R}$

for our example:

$$\lambda(\mathcal{R}) = \ln 3 \, , \; h_{ks}(\mathcal{R}) = \ln 2 \text{ (as before)} \, , \; \gamma = \ln(3/2)$$

$$\Rightarrow \boxed{\gamma = \lambda(\mathcal{R}) - h_{ks}(\mathcal{R})}$$

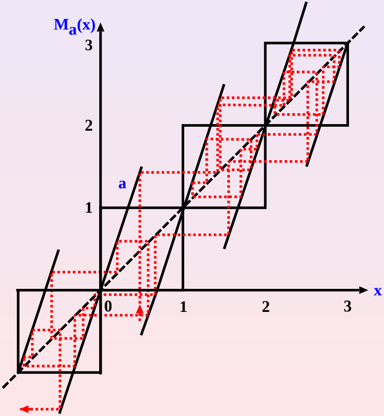
no coincidence: this is the **escape rate formula** of Kantz, Grassberger (1985)

• proven for Anosov diffeomorphisms with 'holes' by Chernov, Markarian (1997)
• $\exists$ position dependence of escape rates, cf. Bunimovich, Yurchenko (2008) and ff

A simple deterministic diffusive map

continue the previous map on the unit interval by a *lift of degree one*, $M_a(x+1) = M_a(x) + 1$, where a denotes the slope:

Grossmann/Geisel/Kapral et al. (1982)



three questions:

- Does this map exhibit diffusion?
- If so, can one calculate the diffusion coefficient?
- And if so, is there any relation between this coefficient and dynamical systems quantities?

Escape rate formalism, Step 1: diffusion equation

solve the ordinary one-dimensional **diffusion equation**

$$\frac{\partial n}{\partial t} = D\,\frac{\partial^2 n}{\partial x^2}$$

with $n = n(x,t)$ distribution function at point x and time t; D defines the diffusion coefficient

solution for absorbing boundaries, $n(0,t) = n(L,t) = 0$:

$$n(x,t) = \sum_{m=1}^{\infty} \exp\left(-\left(\frac{\pi m}{L}\right)^2 Dt\right) a_m \sin\left(\frac{\pi m}{L}x\right)$$

with a_m determined by the initial density $n(x,0)$

Q: do we get the same for our deterministic chaotic model?

Escape rate formalism, Step 2: FP equation

solve the **Frobenius-Perron** (Liouville) **equation**

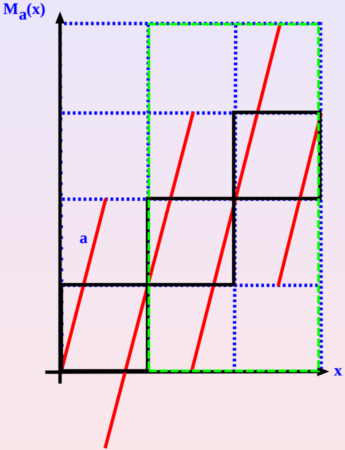
$$\varrho_{n+1}(y) = \int dx\ \varrho_n(x)\,\delta(y - M_a(x))$$

for the probability density $\varrho_n(x)$ of $M_a(x)$

• basic idea: construct FP-operator as transition matrix $T(a)$ applied to column vector $\underline{\varrho}_n$ of the probability density $\varrho_n(x)$:

$$\underline{\varrho}_{n+1} = \frac{1}{a}\,T(a)\,\underline{\varrho}_n$$

example: construction of T for $a = 4$



Markov partition

$$T(4) = \begin{pmatrix} & \vdots & \vdots & \\ \cdots & 1 & 0 & \cdots \\ & 2 & 1 & \\ & 1 & 2 & \\ \cdots & 0 & 1 & \cdots \\ & \vdots & \vdots & \end{pmatrix}$$

topological transition matrix

• solve the FP-equation: let $T(4)\,|\phi_m(x)>=\chi_m(4)\,|\phi_m(x)>$ be the eigenvalue problem of $T(4)$ with eigenvalues $\chi_m(4)$ and eigenvectors $|\phi_m(x)>$

$|\rho_{n+1}(x)>=\underline{\varrho}_{n+1}$ by spectral decomposition:

$$
\begin{aligned}
|\rho_{n+1}(x)> &= \frac{1}{4}\sum_{m=1}^{L}\chi_m(4)\,|\phi_m(x)><\phi_m(x)|\rho_n(x)> \\
&= \sum_{m=1}^{L}\exp\left(-n\ln\frac{4}{\chi_m(4)}\right)|\phi_m(x)><\phi_m(x)|\rho_0(x)>
\end{aligned}
$$

for initial probability density vector $|\rho_0(x)>$

• solve the eigenvalue problem for absorbing boundaries, $\varrho_n(0)=\varrho_n(L)$: analytical solution only available in special cases, as for $a=4$

Escape rate formalism, Step 3: match the solutions

match the largest eigenmodes in the limit of chain length $L \to \infty$ and time $n \to \infty$

- **diffusion equation:** $n(x,t) \simeq \exp\left(-\left(\frac{\pi}{L}\right)^2 Dt\right) A \sin\left(\frac{\pi}{L}x\right)$
- **FP-equation:** $\rho_{n+1}(x) \simeq \exp(-\gamma(4)n)\tilde{A}\sin\left(\frac{\pi}{L+1}k\right)$
  $k = 1,\ldots,L \quad , \quad k-1 < x \leq k \;,$

where $\gamma(4) = \ln\frac{4}{\chi_{max}(4)}$ is the escape rate with $\chi_{max}(4) = 2 + 2\cos\frac{\pi}{L+1}$ as the largest eigenvalue of $T(4)$

- **match:** $$D(4) = \left(\frac{L}{\pi}\right)^2 \gamma(4) \to \frac{1}{4} \quad (L \to \infty)$$

exact method to calculate $D(4)$; value is identical to random walk solution

Escape rate formula for diffusion

establish relation between diffusion coefficient and dynamical systems quantities: it was

$$D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 \gamma$$

with

$$\gamma = \ln |M'(x)| - \ln \chi_{max}$$

cp. with escape rate formula derived previously:

$$\gamma = \lambda(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)$$

general result:

$$\boxed{D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 [\lambda(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)]}$$

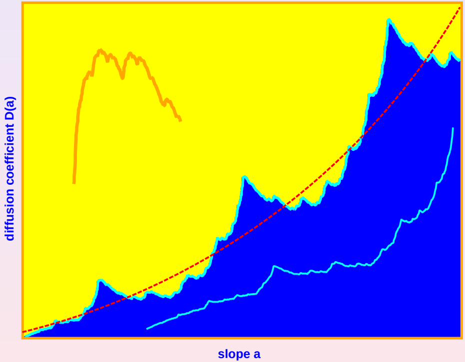
escape rate formula for diffusion

Gaspard, Nicolis, Dorfman (1990ff)

Parameter-dependent deterministic diffusion

result for the parameter dependent diffusion coefficient $D(a)$:

$D(a)$ exists and is a **fractal function of a control parameter**



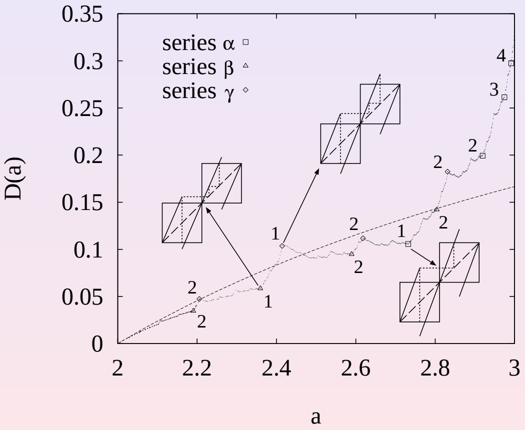
compare diffusion of drunken sailor with chaotic model:

$\exists$ **fine structure beyond simple random walk solution**

R.K., Dorfman (1995)

Physical explanation of the fractal structure

blowup of the initial region of $D(a)$:



local extrema are generated by specific sequences of **correlated microscopic scattering processes**

Reference

R.Klages,

From Deterministic Chaos to Anomalous Diffusion

book chapter in:

Reviews of Nonlinear Dynamics and Complexity, Vol. 3

H.G.Schuster (Ed.), Wiley-VCH, Weinheim, 2010

based on 6-hour first-year PhD course

lecture notes available on

http://www.maths.qmul.ac.uk/˜klages