Stochastic modeling of diffusion in dynamical systems: three examples

Rainer Klages

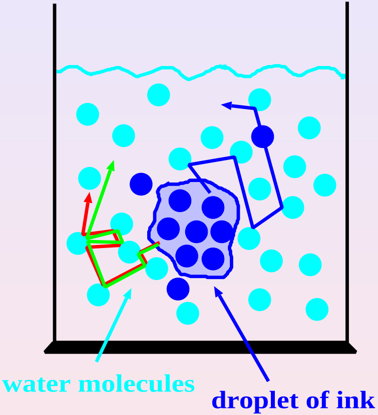
School of Mathematical Sciences, Queen Mary University of London
Institute of Theoretical Physics, Technical University of Berlin

School of Mathematical Sciences, QMUL
26 February 2019

Outline

1. **Motivation:**
   dynamical systems, diffusion and stochastic modeling
2. **Diffusion in three random walk-like examples:**
   1. non-chaotic ‘slicer’ map
   2. randomly perturbed dissipative standard map
   3. a simple random dynamical system
3. **Conclusion:**
   successes, failures and pitfalls for these three examples when relating the above three layers to each other

Microscopic chaos in a glass of water?



- dispersion of a droplet of ink by diffusion
- chaotic collisions between billiard balls
- **chaotic hypothesis:**

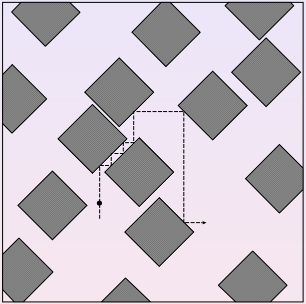
microscopic chaos
$\Downarrow$
macroscopic diffusion

Gallavotti, Cohen (1995)

P.Gaspard et al. (1998): experiment on small colloidal particle in water; diffusion due to microscopic chaos based on positive *pattern entropy per unit time* $h(\epsilon, \tau) \leq h_{KS} = \sum_{\lambda_i > 0} \lambda_i$

The random wind tree model

counterexample:



Ehrenfest, Ehrenfest (1959)

no positive Lyapunov exponent, hence non-chaotic dynamics

Dettmann et al. (1999): generates trajectories and $h(\epsilon, \tau)$ *indistinguishable from the colloidal particle dynamics*

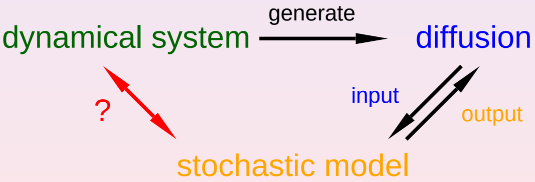
Microscopic chaos, diffusion and stochastic modeling

conclusion:

- **theory:** (chaotic) model $\rightarrow$ diffusion
- **experiment:** diffusion $\rightarrow$ (chaotic) model?

$\Rightarrow$ non-trivial interplay microscopic model $\leftrightarrow$ diffusion

theme of this talk:
add yet a third layer of stochastic modeling



two questions:

1. what type of diffusion is generated by a dynamical system?
2. can it be reproduced by some stochastic model?

Basic diffusive setup

- in the following only diffusion in one dimension
- key quantity: **mean square displacement**

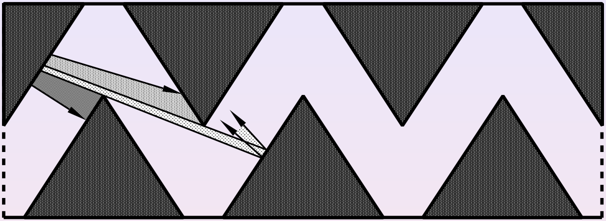
$$< x^2 > := \int dx\ x^2 \rho(x,t) \sim t^\gamma$$

- **note:** three basic types of diffusion
  1. there is not only 'Brownian' (normal) diffusion with $\gamma = 1$
     but also anomalous diffusion:
  2. subdiffusion with $\gamma < 1$
     and
  3. superdiffusion with $\gamma > 1$

(plus more exotic types)

I. The slicer map

Motivation: diffusion in polygonal billiards

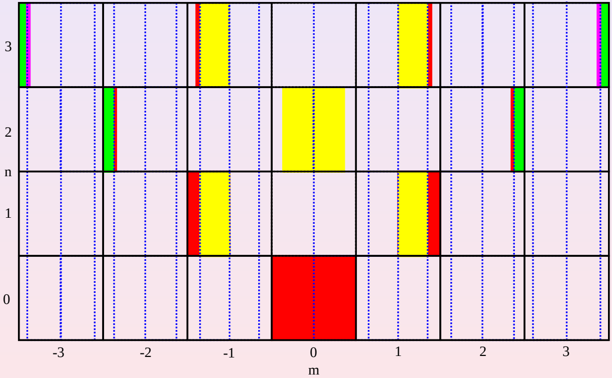


Zaslavsky et al. (2001), Jepps et al. (2006)

- zero Lyapunov exponent: different points separate *linearly* but not *exponentially* in time, hence non-chaotic dynamics
- mean square displacement from simulations: sub-, super- or normal diffusion depending on parameters, with partially conflicting results (Alonso / Jepps / Sanders et al., 2002ff)

Pictorial construction

a one-dimensional ‘random walk-like’ but fully deterministic system; diffusion of a density of points from uniform initial density in **space (m) - discrete time (n) diagram**:



‘slicers’ at points (of Lebesgue measure zero) split the density; no stretching, hence zero Lyapunov exponent: **no chaos!**

Formal definition

- consider a chain of intervals $\widehat{M} := M \times \mathbb{Z}$, $M := [0,1]$ with point $\widehat{X} = (x, m)$ in $\widehat{M}$, where $\widehat{M}_m := M \times \{m\}$ is the m-th cell of $\widehat{M}$

- subdivide each $\widehat{M}_m$ in subintervals, separated by points called slicers: $\{1/2\} \times \{m\}$, $\{\ell_m\} \times \{m\}$, $\{1-\ell_m\} \times \{m\}$, where $0 < \ell_m < 1/2$ for every $m \in \mathbb{Z}$ with

power law $\ell_m(\alpha) = \frac{1}{(|m|+2^{1/\alpha})^\alpha}$, $\alpha > 0$

- slicer map: $S : \widehat{M} \to \widehat{M}$, $\widehat{X}_{n+1} = S(\widehat{X}_n)$, $n \in \mathbb{N}$ with

$$S(x,m) = \begin{cases} (x, m-1) & \text{if } 0 \le x < \ell_m \text{ or } \frac{1}{2} < x \le 1-\ell_m, \\ (x, m+1) & \text{if } \ell_m \le x \le \frac{1}{2} \text{ or } 1-\ell_m < x \le 1. \end{cases}$$

$\Rightarrow$ interval exchange transformation lifted onto the real line

Main result: diffusive properties

Proposition: Salari et al., 2015

Given $\alpha \geq 0$ and a uniform initial distribution in $\widehat{M}_0$, we have

1. $\alpha = 0$: ballistic motion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^2$
2. $0 < \alpha < 1$: superdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
3. $\alpha = 1$: normal diffusion with linear MSD $\langle \widehat{X}_n^2 \rangle \sim n$
   non-chaotic normal diffusion with non-Gaussian density
4. $1 < \alpha < 2$: subdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim n^{2-\alpha}$
   subdiffusion with ballistic peaks
5. $\alpha = 2$: logarithmic subdiffusion with MSD $\langle \widehat{X}_n^2 \rangle \sim \log n$
   a bit exotic
6. $\alpha > 2$: localisation in the MSD with $\langle \widehat{X}_n^2 \rangle \sim const.$
   non-trivial phenomenon

Higher order moments

Theorem: Salari et al., 2015

For $\alpha \in (0, 2]$ the moments $\langle \widehat{X}_n^p \rangle$ with $p > 2$ even and uniform initial distribution in $\widehat{M}_0$ have the asymptotic behavior

$$\langle \widehat{X}_n^p \rangle \sim n^{p-\alpha}$$

while the odd moments ($p = 1, 3, ...$) vanish.

Matching to stochastic dynamics?

- one-dimensional stochastic Lévy Lorentz gas:

point particle moves ballistically between static point scatterers on a line from which it is transmitted / reflected with probability $1/2$

distance r between two scatterers is a random variable iid from the Lévy distribution

$$\lambda(r) := \beta r_0^{\beta} \frac{1}{r^{\beta+1}} \ , \ r \in [r_0, \infty) \ , \ \beta > 0$$

with cutoff r_0

$\rightarrow$ model exhibits only *superdiffusion*

$\rightarrow$ *all moments scale with the slicer moments* for $\alpha \in (0, 1]$ (piecewise linearly depending on parameters)

Matching to stochastic dynamics?

- Lévy walk modeled by CTRW theory:

$\rightarrow$ *moments* calculated to $\sim t^{p+1-\beta}$ for $p > \beta$, $1 < \beta < 2$:
match to slicer *superdiffusion* with $\beta = 1 + \alpha$

$\rightarrow$ but conceptually a totally *different process*

- correlated Gaussian stochastic processes:

modeled by a generalized Langevin equation with a power law memory kernel

$\rightarrow$ formal analogy in the *subdiffusive* regime

$\rightarrow$ but Gaussian distribution and a *conceptual mismatch*

$\Rightarrow$ slicer might help to explain a **controversy about different stochastic models for diffusion in polygonal billiards**

II. The dissipative randomly perturbed standard map

The standard map and diffusion

- paradigmatic Hamiltonian dynamical system:

standard map

$$x_{n+1} = x_n + y_n \mod 2\pi$$
$$y_{n+1} = y_n + K \sin x_{n+1}$$

derived from kicked rot(at)or where $x_n \in \mathbb{R}$ is an angle, $y_n \in \mathbb{R}$ the angular velocity with $n \in \mathbb{N}$ and $K > 0$ the kick strength

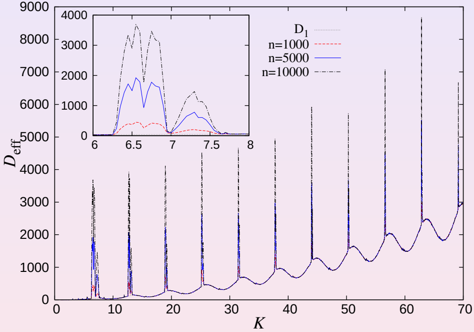
- define **diffusion coefficient** as

$$D(K) = \lim_{n\to\infty} \frac{1}{n} < (y_n - y_0)^2 >$$

with ensemble average over the initial density
$< \ldots >= \int dx\, dy\, \varrho(x,y) \ldots \;,\; x \in [0,2\pi)\;,\; y = y_0 \in [0,2\pi)$

Diffusion in the standard map

analytical (Rechester, White, 1980) and numerical studies of parameter-dependent diffusion $D_{eff}(K)$:



Manos, Robnik, PRE (2014)

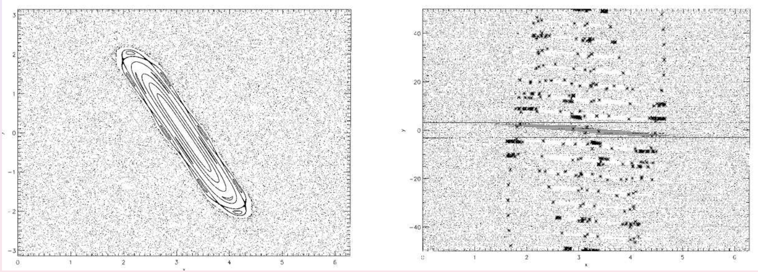
- $D(K)$ is highly irregular
- for some K there is superdiffusion with mean square displacement $< y_n^2 > \sim n^\gamma$, $\gamma > 1$ due to accelerator modes

The dissipative standard map

model damping in the standard map by

$$x_{n+1} = x_n + y_n \mod 2\pi$$
$$y_{n+1} = (1-\nu)y_n + f_0 \sin x_{n+1}$$

with $\nu \in [0,1]$:



Feudel, Grebogi, Hunt, Yorke, PRE (1996)

- islands in phase space for $\nu = 0$ (left) become coexisting periodic attractors (right): 150 found for $\nu = 0.02$, $f_0 = 4$
- simple argument yields $|y_n| < y_{max}$: quick trapping

Dissipative dynamics and random perturbations

Question: What happens to dissipative deterministic dynamics $\mathbf{x}_{n+1} = \mathbf{f}(\mathbf{x}_n)$ under random perturbations?

Consider the dissipative standard map with additive noise:

$$\begin{aligned} x_{n+1} &= x_n + y_n + \epsilon_{x,n} \mod 2\pi \\ y_{n+1} &= (1-\nu)y_n + f_0 \sin x_{n+1} + \epsilon_{y,n} \end{aligned}$$

with iid random variables $\boldsymbol{\epsilon}_n = (\epsilon_{x,n}, \epsilon_{y,n})$ drawn from uniform distribution bounded by $||\boldsymbol{\epsilon}_n|| < \xi$ of noise amplitude ξ

• beyond a noise threshold $\xi \geq \xi_0$ the noise induces a hopping process between all coexisting pseudo attractors

• the resulting dynamics is intermittent because of stickiness to pseudo attractors

Continuous time random walk theory

match simulation results to **CTRW theory** (Montroll, Weiss, Scher, 1973): define stochastic process by master equation with *waiting time distribution* $w(t)$ and *jump distribution* $\lambda(x)$

$$\varrho(x,t) = \int_{-\infty}^{\infty} dx' \lambda(x-x') \int_0^t dt' \; w(t-t') \; \varrho(x',t') + \\ +(1 - \int_0^t dt' w(t'))\delta(x)$$

structure: jump + no jump for points starting at $(x,t)=(0,0)$

$\hat{\text{F}}$ourier-$\tilde{\text{L}}$aplace transform yields **Montroll-Weiss eqn (1965)**

$$\hat{\tilde{\varrho}}(k,s) = \frac{1-\tilde{w}(s)}{s} \frac{1}{1-\hat{\lambda}(k)\tilde{w}(s)}$$

with mean square displacement $\tilde{\langle x^2(s) \rangle} = -\left.\frac{\partial^2 \hat{\tilde{\varrho}}(k,s)}{\partial k^2}\right|_{k=0}$

Predictions of CTRW theory

according to CTRW theory solving the MW eqn. for

1. a power law waiting time distribution $w(t) \sim t^{-(\gamma+1)}$

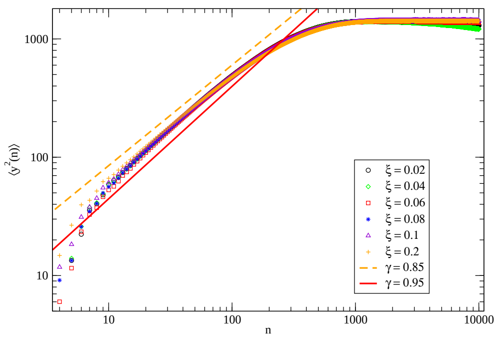
   with jump distribution $\lambda(x) = \delta(|x| - const.)$
2. yields a mean square discplacement of $< x^2(t) >\sim t^\gamma$

   and
3. a stretched exponential position pdf, approximately given by $P_n(y) \sim \exp\left(-cx^{2/(2-\gamma)}\right)$

crucial fit parameter: γ; check these three predictions in numerical experiments

CTRW theory and mean square displacement

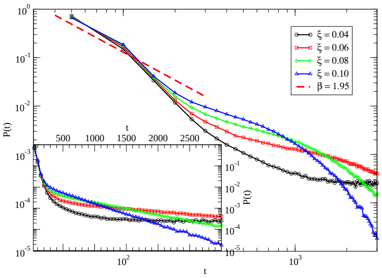
$< y^2(n) >$ for different noise amplitudes ξ at $\nu = 0.002$:



- transient subdiffusion $< y^2(n) > \sim n^\gamma$ up to $n < 1000$
- only small variation of $0.85 < \gamma < 0.95$ for different ξ; for $\xi = 0.06$ we have $\gamma \simeq 0.95$

CTRW theory and escape time distribution

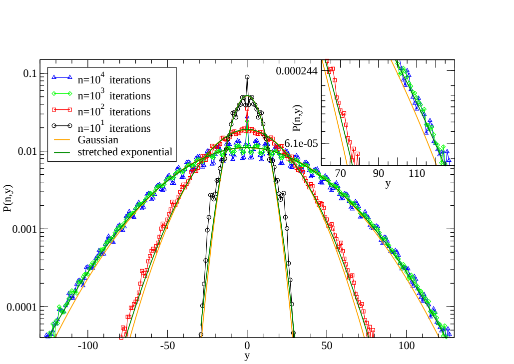
probability distributions $P(t)$ of escape times t from pseudo attractors; dissipation $\nu = 0.002$ with different noise strength ξ:



- transition from power law (stickiness) to exponential
- transition takes longer when $\xi \to 0$
- the dashed red line represents the CTRW theory prediction of $P(t) \sim t^{-1.95}$ corresponding to $< y^2(n) > \sim n^{0.95}$

CTRW theory and position pdf

$P_n(y)$ for position y at different time steps n:



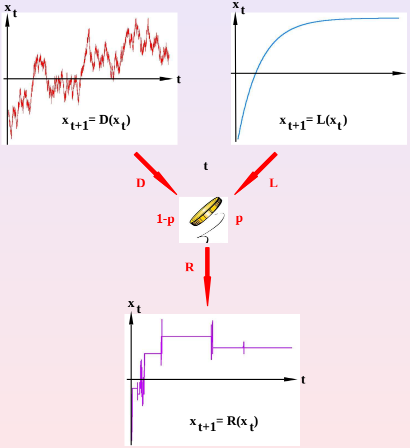
$\xi = 0.06\ ,\ \nu = 0.002$

- ‘Gaussian-like’ diffusive spreading up to $n < 1000$
- localization trivially due to boundedness of pseudo attractors
- CTRW theory pdf (green lines) for $\gamma = 0.95$ corrects mismatch in tails

III. A random dynamical system

Constructing a random dynamical system

three time series for position x_t of a particle at discrete time t:



- *upper left:* deterministic dynamical system D yielding normal diffusion
- *upper right:* deterministic dynamical system L where all particles localize in space.
- *bottom:* **random dynamical system** R that mixes these two types of dynamics at time t with probability p; the result is intermittent motion

Our model

equation of motion

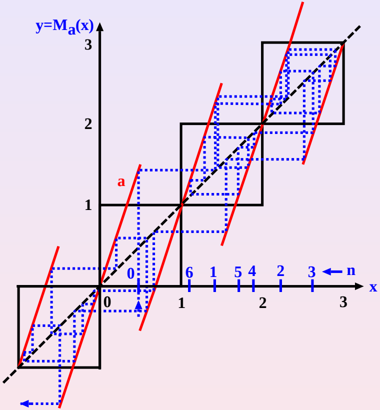
$x_{t+1} = M_a(x_t)$ with discrete time $t \in \mathbb{N}_0$, $a > 0$ and

one-dimensional piecewise linear map

$$M_a(x) = \begin{cases} ax \, , 0 \le x < \frac{1}{2} \\ ax + 1 - a \, , \frac{1}{2} \le x < 1 \end{cases}$$

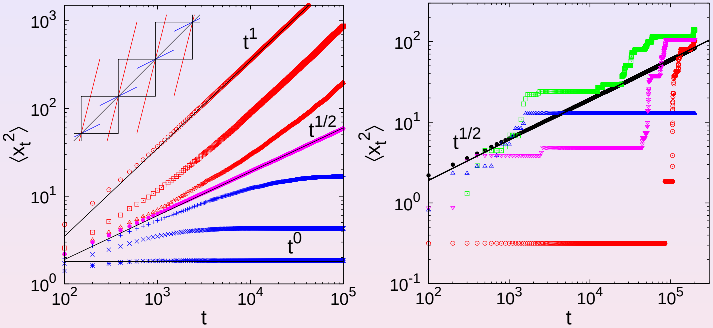
lift $M_a(x+1) = M_a(x) + 1$;

Lyapunov exponent $\lambda(a) = \ln a$



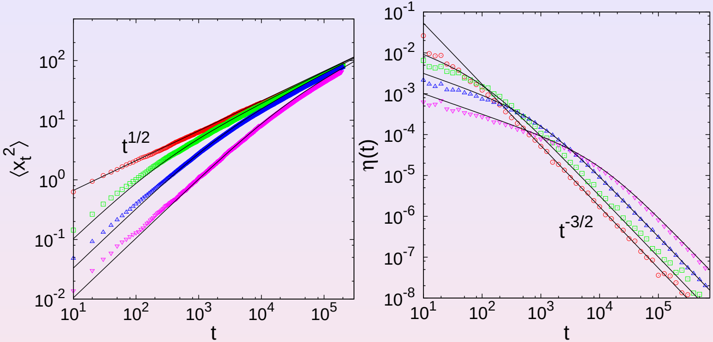
random map $R = M_a(x)$: at any t choose a iid with probability $p \in [0, 1]$ from $a = 1/2$ and with $1 - p$ from $a = 4$

Diffusion in a simple random dynamical system



- *left:* $\langle x_t^2 \rangle$ for $p = 0.6, \ldots, 0.7$ (top to bottom); subdiffusion with zero Lyapunov exponent at $p_c = 2/3$
- *right:* $\langle x_t^2 \rangle$ at p_c with *same* random sequence for *each* particle (colors), cp. to *different* random sequence (**black**); MSD is a random variable breaking self-averaging and ergodicity

Ageing and weak ergodicity breaking



- *left:* $\langle x_t^2 \rangle$ at p_c by starting the computations after different ageing times $t_a = 0, 10^2, 10^3, 10^4$ (top to bottom) displays ageing, cp. to CTRW theory (Barkai, 2003; bold lines)
- *right:* corresponding waiting time distribution $\eta(t)$ (for particles leaving a unit cell at t_a), again matching to CTRW theory
- both results imply weak ergodicity breaking (Bouchaud, 1992)

Connection with dynamical systems theory

- mixing 'expanding'/chaotic with contracting/non-chaotic dynamics randomly in time generates intermittent motion
- the underlying microscopic mechanism is called on-off intermittency (Pikovsky (1984), Fujisaka et al. (1985)); transition called blowout bifurcation (Ott et al. (1994))

Summary

- **central theme:** interplay between *dynamical systems, diffusion and stochastic modeling*
- **main results:**
  1. dynamical systems can feature *novel types of (anomalous) diffusion*
  2. naive matching to stochastic models can be misleading and difficult
- **outlook:** perhaps dynamical systems theory can inspire stochastic theory to invent new stochastic processes?

Acknowledgement and references

work performed with all authors on the following references:

- slicer: L.Salari, L.Rondoni, C.Giberti, RK, Chaos **25**, 073113 (2015)
- standard map: C.S.Rodrigues A.V.Chechkin, A.P.S. de Moura, C.Grebogi, RK, Europhys.Lett. **108**, 40002 (2014)
- random dynamical system: Y.Sato, RK, arXiv:1810.02674; resubmitted to PRL