Linear and fractal diffusion coefficients for a family of shifted, one-dimensional maps.

Georgie Knight and Rainer Klages

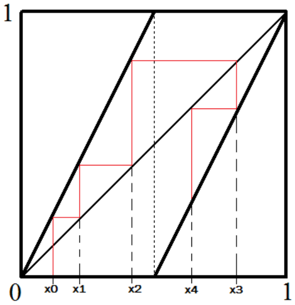
School of Mathematical Sciences
Queen Mary, University of London

Open Statistical Physics 10/03/2010

Outline

- **Introduce the three discrete time dynamical systems modeling diffusion.**
- **Explain how to obtain an analytical expression for the parameter dependent diffusion coefficient.**
- **Compare and explain the structure of the parameter dependent diffusion coefficients.**

Discrete time dynamical system



$$M(x) = \begin{cases} 2x & 0 \leq x < \frac{1}{2} \\ 2x - 1 & \frac{1}{2} \leq x < 1 \end{cases}$$

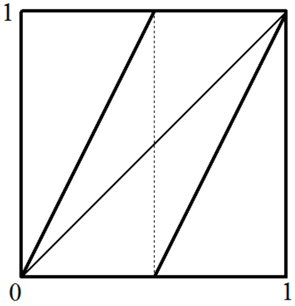
A dynamical system consists of a *phase space* X and a map $M := X \to X$ such that for all $x \in X$

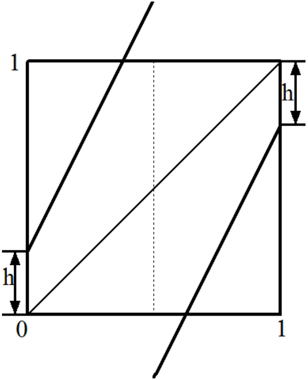
$$x_{n+1} = M(x_n).$$

This *dynamical system* determines the movement of the particles, or the iterates of the points according to the equations of motion.

The lifted Bernoulli shift map

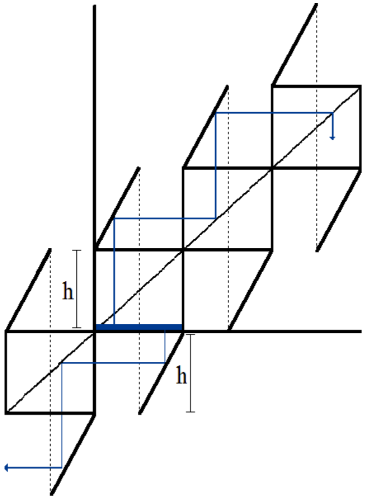
The Bernoulli shift with a lift parameter $h \in [0,1]$ defines a box map:





$$M(x) = \begin{cases} 2x & 0 \leq x < \frac{1}{2} \\ 2x-1 & \frac{1}{2} \leq x < 1 \end{cases} \qquad M_h(x) = \begin{cases} 2x+h & 0 \leq x < \frac{1}{2} \\ 2x-1-h & \frac{1}{2} \leq x < 1 \end{cases}$$

The box map is copied such that $M_h(x+1) = M_h(x) + 1$.

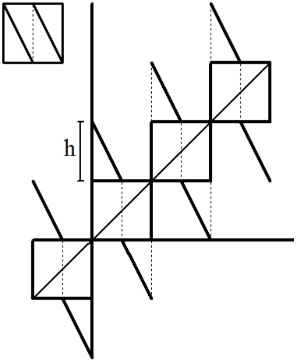


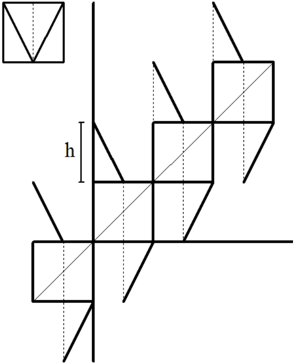
We construct a probability density function from an ensemble of points which will spread out when iterated. Hence we talk about *deterministic diffusion*. We will consider:

- **How to evaluate the diffusion coefficient.**
- **The behavior of the diffusion coefficient under parameter variation.**

The other maps

We also consider the two following variations:





$$W_h(x) = \begin{cases} -2x + h + 1 & 0 \leq x < \frac{1}{2} \\ -2x + 2 - h & \frac{1}{2} \leq x < 1 \end{cases}$$

$$W_h(x+1) = W_h(x) + 1.$$

$$V_h(x) = \begin{cases} -2x + 1 + h & 0 \leq x < \frac{1}{2} \\ 2x - 1 - h & \frac{1}{2} \leq x < 1 \end{cases}$$

$$V_h(x+1) = V_h(x) + 1.$$

Evaluating the Diffusion coefficient

We rewrite Einstein's formula as the Taylor-Green-Kubo formula:

$$\begin{aligned} D &= \lim_{n\to\infty} \frac{\left\langle (x_n - x_0)^2 \right\rangle}{2n} \\ &= \lim_{n\to\infty} \sum_{k=0}^{n} \langle v_k(x) v_0(x) \rangle - \frac{1}{2} \left\langle v_0(x)^2 \right\rangle . \end{aligned}$$ [1]

- $v_j(x) = \lfloor x_{j+1} \rfloor - \lfloor x_j \rfloor$.
- $\langle \ldots \rangle := \int_0^1 \ldots \rho^*(x) dx$.

where $\rho^*(x) = 1$ is the invariant probability density function of the box map mod 1.

[1] For a full derivation see Dorfman, *An Introduction to Chaos in Nonequilibrium Statistical Mechanics*.

Takagi functions

Taylor-Green-Kubo formula for diffusion:

$$D = \lim_{n\to\infty} \int_0^1 \sum_{k=0}^{n} v_k(x)v_0(x)dx - \frac{1}{2}\int_0^1 (v_0(x))^2 dx.$$

Define a function which gives the integer displacement of a point at the n^{th} iteration:

$$J^n(x) = \sum_{k=0}^{n} v_k(x).$$

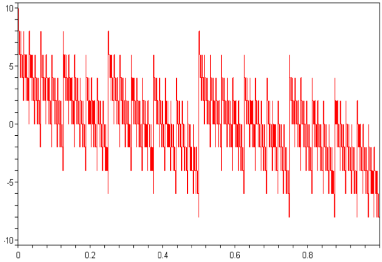
Define a cumulative function for $J^n(x)$ [2]:

$$T^n(x) = \int_0^x J^n(y)dy.$$

[2] T. Takagi, *A simple example of the continuous function without derivative*. Proc. Phys. Math. Soc. Jpn. **1** (1903) pp 176-177

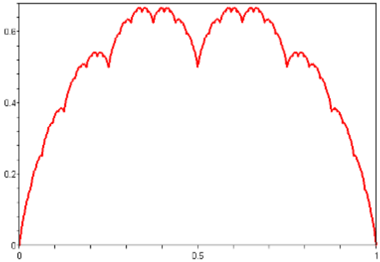
Takagi functions

$J^n(x)$ becomes erratic for large n:



$J^{10}(x)$ for $M_1(x)$

Hence the Takagi functions become fractal in the limit:



$T(x)$ for $M_1(x)$

Recursion relation

We calculate the Takagi functions recursively:

$$\begin{aligned} J^n(x) &= \sum_{k=0}^{n} v_k(x) \\ &= v_0(x) + J^{n-1}(\tilde{M}_h(x)). \end{aligned}$$

$$\begin{aligned} T(x) = \lim_{n\to\infty} T^n(x) &= \lim_{n\to\infty} \int_0^x J^n(y)dy \\ &= \lim_{n\to\infty} \int_0^x v_0(y) + J^{n-1}(\tilde{M}_h(y))dy \\ &= t(x) + \frac{1}{2} T^{n-1}\left(\tilde{M}_h(x)\right), \end{aligned}$$

where $t(x) = xv_0(x) + c$. We evaluate c by using the continuity of the Takagi functions and that $T(0) = T(1) = 0$.

Infinite sum

Takagi functions as an infinite sum:

$$T(x) = \lim_{n\to\infty} \sum_{k=0}^{n} \frac{1}{2^k} t\left(\tilde{M}^k(x)\right).$$

Hence we can evaluate the diffusion coefficient as an infinite sum.

$D(h)$

We can now use these elements to obtain the parameter dependent diffusion coefficient:

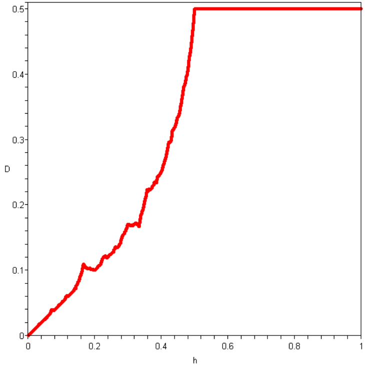
$$\begin{aligned} D(h) &= \lim_{n\to\infty} \int_0^1 J^n(x) v_0(x) dx - \frac{1}{2}\int_0^1 (v_0(x))^2 \, dx. \\ &= \frac{h}{2} + \frac{1}{2} T_h(h) + \frac{1}{2} T_h(1-h). \end{aligned}$$

Which for the maps $M_h(x)$ and $W_h(x)$ simplifies to,

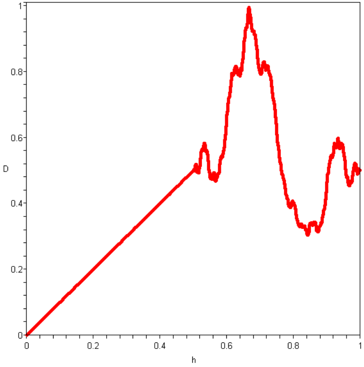
$$D(h) = \frac{h}{2} + T_h(h).$$

$D(h)$

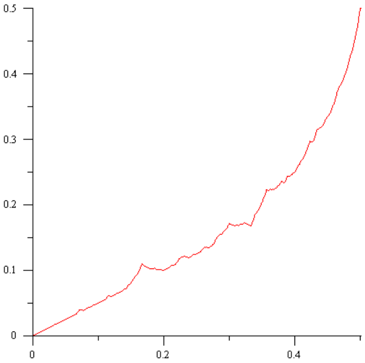
For $M_h(x)$:



For $W_h(x)$:



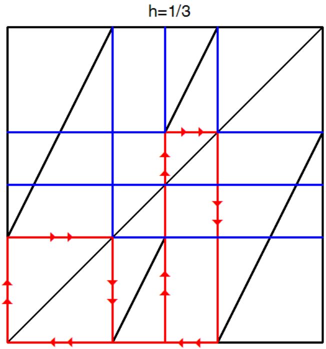
The fractal regions

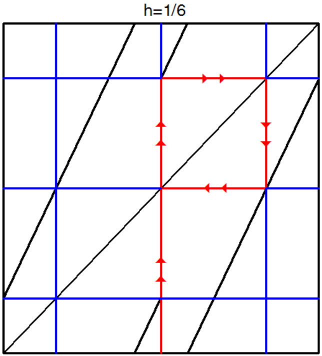


- Fractal structure indicates topological instability under parameter variation.
- The partition generating orbit of the mod 1 map will help us understand the instability.

Markov partitions

The orbit of the critical point generates the Markov partition:

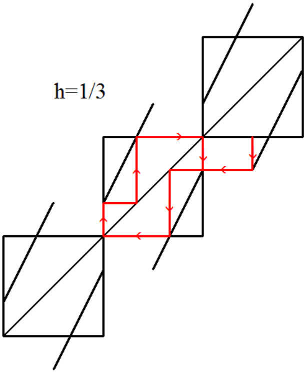




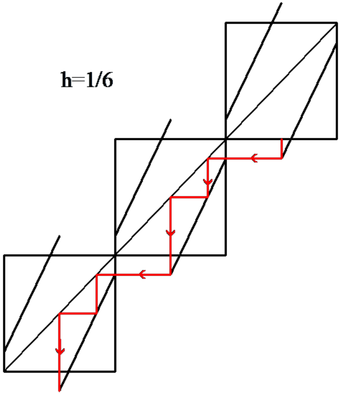
We can prove that these finite Markov partitions are dense in the parameter space. Their behaviour varies greatly under arbitrarily small variations. However, here we isolate two topological types.

Markov partitions

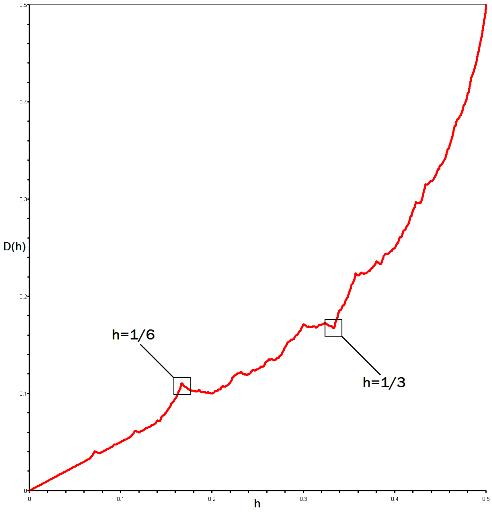
Restrictive:



Unrestrictive:



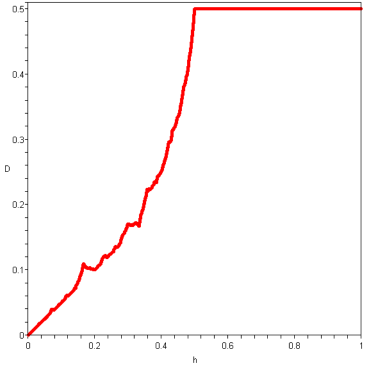
h values that promote and restrict diffusion.



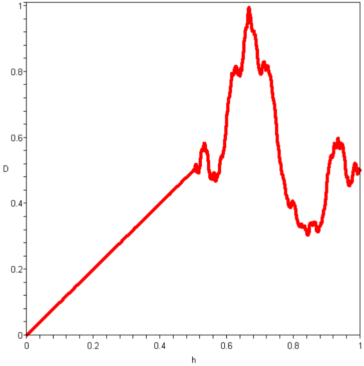
- $h = 1/6$ promotes diffusion.
- $h = 1/3$ restricts diffusion.

$D(h)$

For $M_h(x)$:

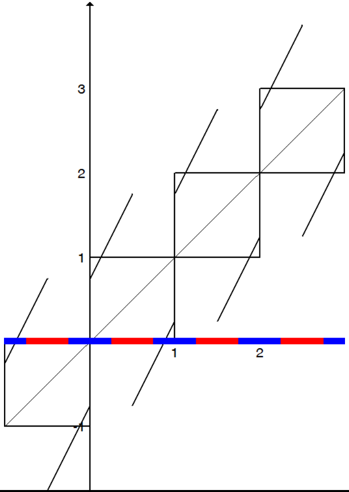


For $W_h(x)$:

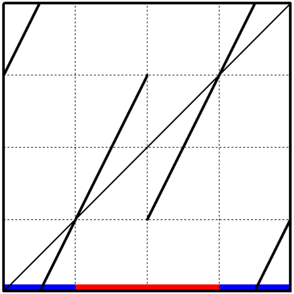


The linear regions

For $0.5 \leq h \leq 1$ in $M_h(x)$ the ergodicity of the map is broken:



The phase space is split up into two invariant sets. It's clear in the mod 1 map:



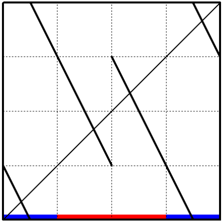
The linear regions

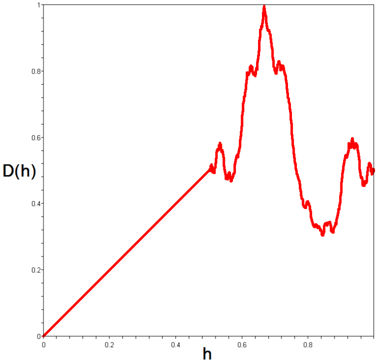
Our invariant density $\rho * (x) = \rho *_1 (x) + \rho *_2 (x)$:

$$
\begin{aligned}
D(h) &= \lim_{n\to\infty} \frac{\left\langle (x_n - x_0)^2 \right\rangle}{2n} \\
&= \lim_{n\to\infty} \frac{1}{2n} \int_0^1 \rho^*(x)(x_n - x_0)^2 dx \\
&= \lim_{n\to\infty} \frac{1}{2n} \left(\int_0^1 \rho_1^*(x)(x_n - x_0)^2 dx + \int_0^1 \rho_2^*(x)(x_n - x_0)^2 dx \right). \\
&\vdots \\
&= (1 - h) + (h - \frac{1}{2}) \\
&= \frac{1}{2}.
\end{aligned}
$$

The linear regions

For $0 \leq h \leq 0.5$ in $W_h(x)$ we have ergodicity breaking:

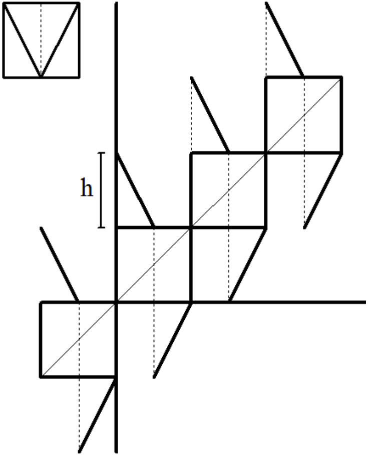




Topological instability $\Leftrightarrow$ Fractal diffusion coefficient.

Non-ergodicity $\Leftrightarrow$ Linear diffusion coefficient.

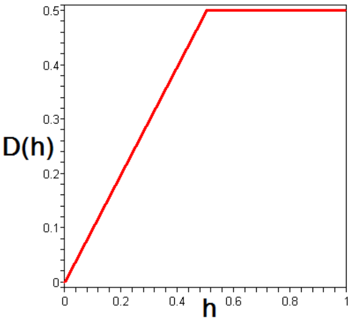
The lifted V-map



- The behaviour of the Markov partitions suggests topological instability across the entire parameter range.
- The map remains ergodic across the entire parameter range.

However...

The lifted V-map



- For the lifted V-map we observe a piecewise linear diffusion coefficient, similar to the linear parts found in the two Bernoulli maps.
- Why do we have this similarity, despite the difference in the microscopic dynamics?

'*Time-dependent*' diffusion coefficient

For the lifted Bernoulli shift map $D(h) =$

$$\frac{h}{2} + \lim_{n\to\infty}\left(\sum_{k=1}^{n-1}\frac{1}{2^k}t_M(\tilde{M}_h(h)) + \frac{t_M(h)}{2^{n-1}}\right).$$

For the lifted V map $D(h) =$

$$\frac{h}{2} + \lim_{n\to\infty}\left(\sum_{k=1}^{n}\frac{1}{2^k}t_V(\tilde{V}_h(h)) + \frac{1}{2}T_V^n(1-h) - \sum_{k=1}^{n-1}\frac{1}{2^{k+1}}T_V^{n-1-k}(1-h)\right).$$

dominating branch

$$t_M(x) := \begin{cases} 0 & 0 \le x < \frac{1-h}{2} \\ \frac{h-1}{2} + x & \frac{1-h}{2} \le x < \frac{1}{2} \\ \frac{1+h}{2} - x & \frac{1}{2} \le x < \frac{1+h}{2} \\ 0 & \frac{1+h}{2} \le x \le 1 \end{cases}$$

$$t_V(x) := \begin{cases} x & 0 \le x < \frac{h}{2} \\ \frac{h}{2} & \frac{h}{2} \le x < \frac{1}{2} \\ \frac{1+h}{2} - x & \frac{1}{2} \le x < \frac{1+h}{2} \\ 0 & \frac{1+h}{2} \le x \le 1 \end{cases}$$

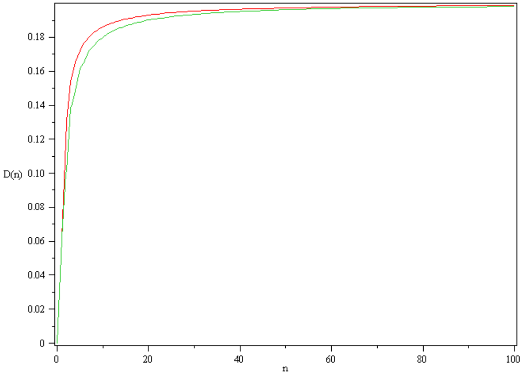
- For $0.5 \le x \le 1$ these two functions are identical.
- $h \ge 0.5$ is a fixed point of both $\tilde{M}_h(x)$ and $\tilde{V}_h(x)$.

Hence the diffusion coefficients are identical in the limit. The common branch is dominating the diffusion process.

We see a similar phenomenon in $W_h(x)$ for $0 \le h \le 0.5$.

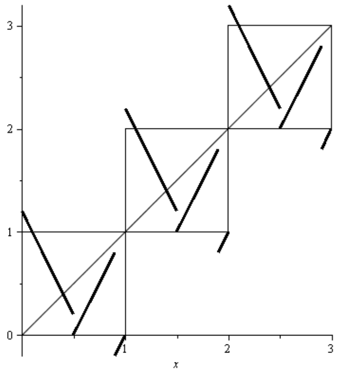
'*Time-dependent*' diffusion coefficient

This is seen in the time-dependent diffusion coefficient:

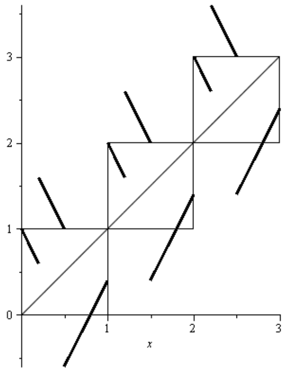


Here T.D.C is plotted for the negative Bernoulli shift and the V-map at $h = 0.2$

Distorting the maps



For $0 \leq h \leq 0.5$ $D(h) = h$



For $0.5 \leq h \leq 1$ $D(h) = 0.5$

Summary

- **We obtained an analytical expression for the parameter dependent diffusion coefficient in terms of generalised Takagi functions for a family of one dimensional maps.**
- **We explained the structure of the diffusion coefficient in terms of Markov partitions and non-ergodicity.**
- **We discovered a third effect whereby one branch of the map dictates the process of diffusion.**
- **This effect makes the diffusion coefficient very stable against changes in the microscopic dynamics.**