Understanding fractal diffusion coefficients: Approximation methods.

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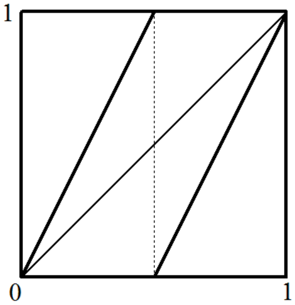
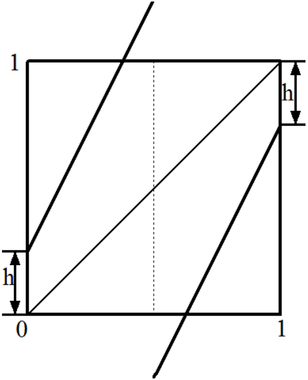
Outline

1. Introduce the map being studied and the phenomenon of chaotic diffusion.
2. Look at three different methods for approximating the diffusion coefficient of the map.
3. Compare the different methods and see what they tell us about the structure.
4. Motivation: To understand parameter dependent diffusion coefficients in a general setting.

The lifted Bernoulli shift map

The Bernoulli shift with a lift parameter h defines a *"box map"*:



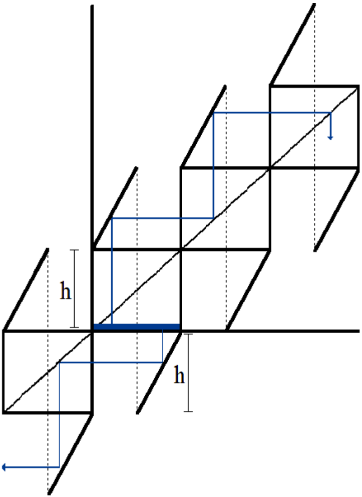


$$M(x) = \begin{cases} 2x & 0 \leq x < \frac{1}{2} \\ 2x - 1 & \frac{1}{2} \leq x < 1 \end{cases}$$

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

The lifted Bernoulli shift map

The box map is copied with a *lift of degree one* onto the real line:



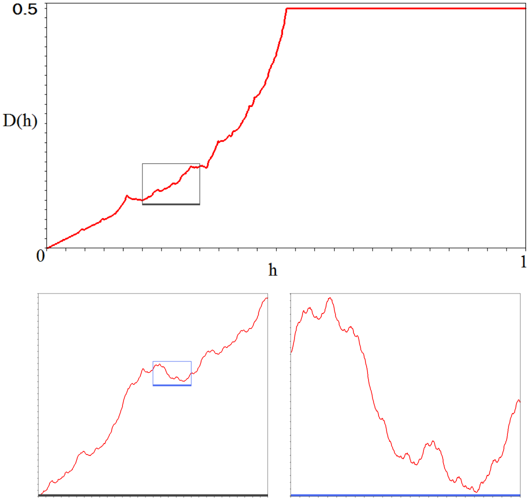
$$M_h(x+1) = M_h(x) + 1.$$

A probability density function will diffuse out under iteration. We will consider how to approximate the diffusion coefficient,

$$D = \lim_{n\to\infty} \frac{\left\langle (x_n - x_0)^2 \right\rangle}{2n}$$

as a function of the parameter.

Complicated fractal structure.



We have an exact analytical solution for $D(h)$ and for $0 \leq h \leq \frac{1}{2}$, it is a fractal function in terms of non-trivial fine scale structure and regions of self similarity.

Georgie Knight and Rainer Klages, 2011 Nonlinearity **24** 227 *Linear and fractal diffusion coefficients in a family of one-dimensional chaotic maps*

Taylor-Green-Kubo formula

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

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

- $v_j(x) = \lfloor x_{j+1} \rfloor - \lfloor x_j \rfloor$
- $\left\langle (x_n - x_0)^2 \right\rangle := \int_0^1 (x_n - x_0)^2 \rho^*(x) dx$

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*.

Approximation

If we truncate the Taylor-Green-Kubo formula at a given n, we get a time dependent diffusion coefficient

$$D_n(h) = \sum_{k=0}^{n} \int_0^1 v_0(x) v_k(x) dx - \frac{1}{2} \int_0^1 (v_0(x))^2 dx.$$

We see that

$$D_0(h) = \frac{h}{2}$$

which is the random walk solution.

We move the summation inside the integral and define a '*jump function*' $J^n(x) : [0,1] \rightarrow \mathbb{R}$ as

$$J^n(x) = \sum_{k=0}^{n-1} v_k(x). \quad n \geq 1. \quad J^0(x) := 0$$

giving

$$D_n(h) = \int_0^1 v_0(x) J^n(x) dx - \frac{1}{2} \int_0^1 (v_0(x))^2 dx$$

We then define the integral as $T_h^n(x) : [0,1] \rightarrow \mathbb{R}$,

$$T_h^n(x) := \int_0^x J^n(y) dy. \quad n \geq 1. \quad T^0(x) := 0$$

Recursive relation

We then use the recursive relation

$$J^n(x) = v_0(x) + J^{n-1}\left(\tilde{M}_h(x)\right),$$

where $\tilde{M}_h(x) = M_h(x)$ modulo 1 to define $T_h^n(x)$ recursively.
$T_h^n(x) =$

$$\begin{cases} \frac{1}{2}T_h^{n-1}(2x+h) & -\frac{1}{2}T^{n-1}(h) & 0 \le x < \frac{1-h}{2} \\ \frac{1}{2}T_h^{n-1}(2x+h-1) & -\frac{1}{2}T^{n-1}(h) + x + \left(\frac{h-1}{2}\right) & \frac{1-h}{2} \le x < \frac{1}{2} \\ \frac{1}{2}T_h^{n-1}(2x-h) & -\frac{1}{2}T^{n-1}(h) - x + \left(\frac{h+1}{2}\right) & \frac{1}{2} \le x < \frac{1+h}{2} \\ \frac{1}{2}T_h^{n-1}(2x-1-h) & -\frac{1}{2}T^{n-1}(h) & \frac{1+h}{2} \le x < 1 \end{cases}$$

Where the constants of integration can be evaluated using the continuity of the function, and the fact that $T_h^n(0) = T_h^n(1) = 0$.

Evaluating

Evaluating the diffusion coefficient using these functions we obtain

$$D_n(h) = \frac{h}{2} + T_h^n(h).$$

After a bit of wrangling we obtain

$$T_h^n(h) = \sum_{k=0}^{n-1} \frac{1}{2^k} t\left(\tilde{M}_h^k(h)\right) - \sum_{k=0}^{n-2} \frac{1}{2^{k+1}} t\left(\tilde{M}_h^k(h)\right),$$

where

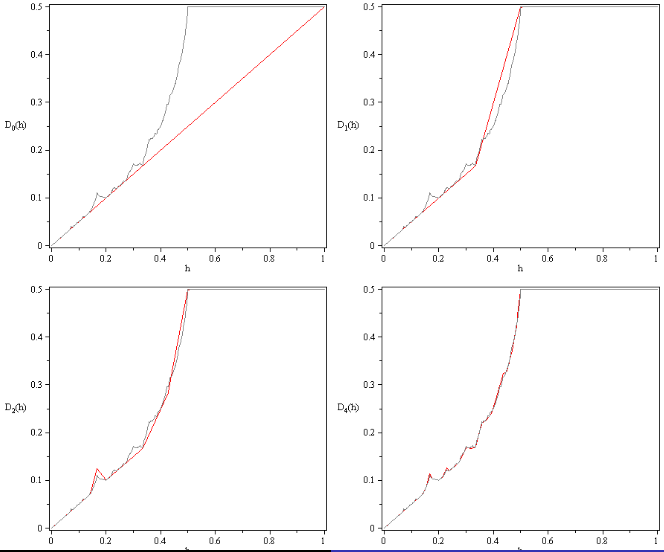
$$t(x) := \begin{cases} 0 & 0 \leq x < \frac{1-h}{2} \\ x + \frac{h-1}{2} & \frac{1-h}{2} \leq x < \frac{1}{2} \\ -x + \frac{h+1}{2} & \frac{1}{2} \leq x < \frac{1+h}{2} \\ 0 & \frac{1+h}{2} \leq x < 1 \end{cases}.$$

Results

Writing $D_n(h)$ in this way furnishes us with a simple sum to evaluate the approximations:

$$\begin{aligned}
D_0(h) &= h/2 \\
D_1(h) &= h/2 + t(h) \\
D_2(h) &= h/2 + \frac{1}{2}t(h) + \frac{1}{2}t\left(\tilde{M}_h(h)\right) \\
D_3(h) &= h/2 + \frac{1}{2}t(h) + \frac{1}{4}t\left(\tilde{M}_h(h)\right) + \frac{1}{4}t\left(\tilde{M}_h^2(h)\right) \\
D_4(h) &= h/2 + \frac{1}{2}t(h) + \frac{1}{4}t\left(\tilde{M}_h(h)\right) + \frac{1}{8}t\left(\tilde{M}_h^2(h)\right) + \frac{1}{8}t\left(\tilde{M}_h^3(h)\right)
\end{aligned}$$

Results



Results

Positive points:

1. **Analytical with relatively little input.**
2. **Shows clearly how the fractal builds up.**

Negative point:

1. **Restricted to one-dimensional systems.**
2. **You get overshooting at some of the extrema.**

Restricting the memory with exponential decay

We now evaluate our diffusion coefficient by restricting the memory of our system and not taking the full correlations into account[2].We again use the Taylor-Green-Kubo formula

$$D(h) = \lim_{n\to\infty} \sum_{k=0}^{n} \langle v_k(x) v_0(x) \rangle - \frac{1}{2} \langle v_0(x)^2 \rangle$$

but we take the limit and approximate $\langle v_k(x) v_0(x) \rangle$.For example if we do not include any memory effects, $\langle v_k(x) v_0(x) \rangle = 0, k > 0$, and we reproduce a simple random walk solution.

[2] Gilbert T and Sanders D P 2009 *Diffusion coefficients for multi-step persistent random walks on lattices* J. Phys. A: Math. Theor.

One-step

We now use one step of memory, i.e. the behaviour of a point at the n^{th} step is only dependent on the $(n-1)^{th}$ step. We now have to find an expression for the n^{th} velocity auto correlation

$$\langle v_0 \cdot v_n \rangle = \sum_{v_0,\ldots,v_n} v_0 \cdot v_n \mu\left(\{v_0 \ldots v_n\}\right),$$

where μ is the invariant probability density function or measure of our system. The sum is taken over all possible combinations of paths from v_0 to v_n.

Evaluating the correlations as a matrix

Let $P(\mathbf{b}|\mathbf{a})$ be the probability that a point takes the velocity $\mathbf{b}$ given that at the previous step it had velocity $\mathbf{a}$. Given a one step memory approximation, we can write our velocity auto correlation function as

$$\langle v_0 \cdot v_n \rangle = \sum_{v_0,\ldots,v_n} v_0 \cdot v_n \cdot p(v_0) \prod_{i=1}^{n} P(v_i | v_{i-1}),$$

where $p(v_0)$ is the probability that a point takes the velocity v_0 at the first step with $v_0 \in [0, 1, -1]$. In order to deal with the sum we rewrite it as a matrix equation

$$\langle v_0 \cdot v_n \rangle = \begin{pmatrix} 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} P_{00} & P_{01} & P_{0-1} \\ P_{10} & P_{11} & P_{1-1} \\ P_{-10} & P_{-11} & P_{-1-1} \end{pmatrix}^{n} \begin{pmatrix} 0 \\ p(1) \\ -p(-1) \end{pmatrix}$$

Simplifying

Using the symmetries of our system and the fact that any path with a '*0*' state will be canceled out we can write the expression as

$$\langle v_0 \cdot v_n \rangle = \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} P_{11} & P_{1-1} \\ P_{1-1} & P_{11} \end{pmatrix}^n \begin{pmatrix} 1 \\ -1 \end{pmatrix} p(1),$$

which is in a simple quadratic form and hence our expression for the n^{th} velocity auto correlation function is

$$\langle v_0 \cdot v_n \rangle = 2p(1) \left(P_{11} - P_{1-1} \right)^n$$

where $P_{ij} = P(v_i | v_j)$.

Hence our expression for $D_1(h)$ from the Taylor-Green-Kubo formula is

$$\begin{aligned} D_1(h) &= \sum_{n=0}^{\infty} \langle v_0 \cdot v_n \rangle - \frac{1}{2} \left\langle v_0^2 \right\rangle \\ &= h \left(\sum_{n=0}^{\infty} (P_{11} - P_{1-1})^n \right) - \frac{h}{2} \\ &= \frac{h}{1 - P_{11} + P_{1-1}} - \frac{h}{2}. \end{aligned} \quad (1)$$

Two steps of memory

We now include two steps of memory so the behaviour of a point at the n^{th} step depends on what has happened at the $(n-1)^{th}$ and $(n-2)^{th}$ step. Let $P(\mathbf{c}|\mathbf{b},\mathbf{a})$ be the probability that a point has velocity $\mathbf{c}$ given that it had velocity $\mathbf{b}$ at the previous step and $\mathbf{a}$ at the step before that. With $\mathbf{a},\mathbf{b},\mathbf{c} \in [0,1,-1]$. Given this two step approximation, the velocity auto correlations are given by

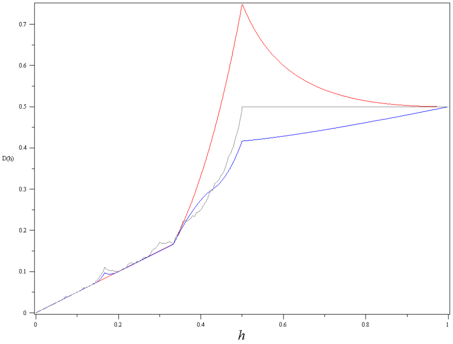
$$\langle v_0 \cdot v_n \rangle = \sum_{v_0,\ldots,v_n} v_0 \cdot v_n \cdot p(v_0, v_1) \prod_{i=2}^{n} P(v_i | v_{i-1}, v_{i-2}),$$

Again we rewrite the problem as a matrix equation where,

$$\langle v_0 \cdot v_n \rangle = \underline{a} \cdot \underline{A}^n \cdot \underline{b},$$

where $\underline{a}$ evaluates v_n, $\underline{b}$ evaluates v_0 and $\underline{A}$ is the 9×9 probability transition matrix for the system. However, due to the inclusion of the '*0*' state, we have to resort to numerically evaluating the diffusion coefficient.

Results



one step, two step.

Positive points:

1. **Can be used analytically in a wide class of systems.**
2. **Retains the exponential decay.**

Negative points:

1. **Requires a lot more input.**
2. **Does not give information about the fractal structure.**

Transition matrix method

The final method we consider is to approximate the Markov transition matrix for the system.[3]. This method involves evaluating the second largest eigenvalue of the transition matrix for the system $\chi_1(h)$, as this can be used to evaluate the decay rate for the system

$$\gamma_{dec}(h) = \ln(2/\chi_1(h))$$

which in turn can be used to evaluate the diffusion coefficient

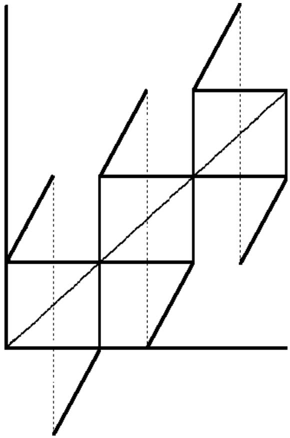
$$D(h) = \lim_{L\to\infty} \frac{L^2}{4\pi^2}\gamma_{dec}(h)$$

where L is the '*chain length*' of the system.

[3] Klages R, Dorfman J R 1999 Phys. Rev. E. **59** 5361 *Simple deterministic dynamical systems with fractal diffusion coefficients*

Approximating the transition matrix

This method relies on having a Markov transition matrix for the system. We don't use the full Markov matrix, rather we approximate it with $1, 2, 4\ldots$ partition parts per box map and introduce stochasticity to account for any overlap or non Markov behaviour. So for 1 part, the box maps themselves act as the partition parts



h=1,L=3

The approximate transition matrix for this system as a function of the parameter is a cyclic matrix

$$\begin{pmatrix} 2-2h & h & 0 & \dots & h \\ h & 2-2h & h & \dots & 0 \\ 0 & h & 2-2h & h & \dots \\ \vdots & \vdots & h & \ddots & h \\ h & 0 & \dots & h & 2-2h \end{pmatrix}$$

whose eigenvalues can be evaluated analytically.[4]

$$\chi_1(h) = 2-2h+2hcos(2\pi/L) \simeq 2-2h+2h\left(1-\frac{2\pi^2}{L^2}\right), (L \to \infty)$$

hence the decay rate

$$\gamma_{dec}(h) = \ln\left(\frac{1}{1-h+hcos(2\pi/L)}\right) \simeq \frac{h2\pi^2}{L}\,(L \to \infty)$$

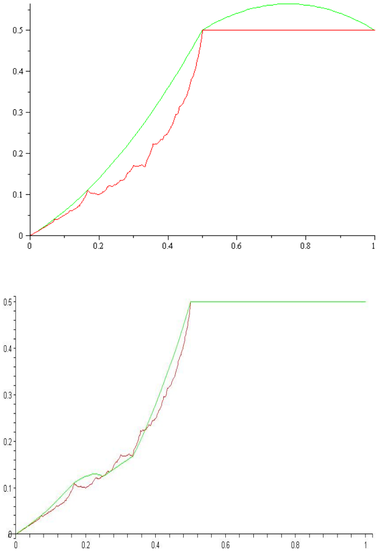
[4] Berlin T H, Kac M, 1952 Phys. Rev. **86** 821 *The spherical model of a ferromagnet*

Hence the diffusion coefficient evaluates to

$$D(h) = \frac{L^2}{4\pi^2}\frac{2\pi^2 h}{L^2} = \frac{h}{2}$$

which is the random walk approximation again.

The next stage of approximation involves two partition parts, for this we simply pick the critical point $x = 0.5$. To get four partition parts we use the iterate of $x = 0.5$ and it's mirror image about $x = 0.5$. However, we again have to resort to numerics to evaluate the diffusion coefficient.



Positive points:

1. **Highlights the self similarity of the fractal.**
2. **Quick, quantifiable convergence.**

Negative points:

1. **Again, requires a lot of input.**
2. **We don't have a method to obtain fully analytical results.**

Thank you for listening!