Appendix S

Projects

OU ARE URGED to work through the essential steps in a project that combines the techniques learned in the course with some application of interest to you for other reasons. It is OK to share computer programs and such, but otherwise each project should be distinct, not a group project. The essential steps are:

• Dynamics

- 1. construct a symbolic dynamics
- 2. count prime cycles
- 3. prune inadmissible itineraries, construct transition graphs if appropriate
- 4. implement a numerical simulator for your problem
- 5. compute a set of the shortest periodic orbits
- 6. compute cycle stabilities

• Averaging, numerical

- 1. estimate by numerical simulation some observable quantity, like the escape rate,
- 2. or check the flow conservation, compute something like the Lyapunov exponent

• Averaging, periodic orbits

- 1. implement the appropriate cycle expansions
- 2. check flow conservation as function of cycle length truncation, if the system is closed
- 3. implement desymmetrization, factorization of zeta functions, if dynamics possesses a discrete symmetry

- 4. compute a quantity like the escape rate as a leading zero of a spectral determinant or a dynamical zeta function.
- 5. or evaluate a sequence of truncated cycle expansions for averages, such as the Lyapunov exponent or/and diffusion coefficients
- 6. compute a physically intersting quantity, such as the conductance
- 7. compute some number of the classical and/or quantum eigenvalues, if appropriate

S.1 Deterministic diffusion, zig-zag map

To illustrate the main idea of chapter 25, tracking of a globally diffusing orbit by the associated confined orbit restricted to the fundamental cell, we consider a class of simple 1-dimensional dynamical systems, chains of piecewise linear maps, where all transport coefficients can be evaluated analytically. The translational symmetry (25.10) relates the unbounded dynamics on the real line to the dynamics restricted to a "fundamental cell" - in the present example the unit interval curled up into a circle. An example of such map is the sawtooth map

$$\hat{f}(x) = \begin{cases} \Lambda x & x \in [0, 1/4 + 1/4\Lambda] \\ -\Lambda x + (\Lambda + 1)/2 & x \in [1/4 + 1/4\Lambda, 3/4 - 1/4\Lambda] \\ \Lambda x + (1 - \Lambda) & x \in [3/4 - 1/4\Lambda, 1] \end{cases}$$
(S.1)

The corresponding circle map f(x) is obtained by modulo the integer part. The elementary cell map f(x) is sketched in figure S.1. The map has the symmetry property

$$\hat{f}(\hat{x}) = -\hat{f}(-\hat{x}),$$
 (S.2)

so that the dynamics has no drift, and all odd derivatives of the generating function (25.3) with respect to β evaluated at $\beta = 0$ vanish.

The cycle weights are given by

$$t_p = z^{n_p} \frac{e^{\beta \hat{n}_p}}{|\Lambda_p|} \,. \tag{S.3}$$

The diffusion constant formula for 1-dimensional maps is

$$D = \frac{1}{2} \frac{\left\langle \hat{n}^2 \right\rangle_{\zeta}}{\left\langle n \right\rangle_{\zeta}} \tag{S.4}$$

where the "mean cycle time" is given by

$$\langle n \rangle_{\zeta} = \left. z \frac{\partial}{\partial z} \frac{1}{\zeta(0, z)} \right|_{z=1} = -\sum' (-1)^k \frac{n_{p_1} + \dots + n_{p_k}}{|\Lambda_{p_1} \cdots \Lambda_{p_k}|}, \tag{S.5}$$

the mean cycle displacement squared by

$$\left\langle \hat{n}^2 \right\rangle_{\zeta} = \left. \frac{\partial^2}{\partial \beta^2} \frac{1}{\zeta(\beta, 1)} \right|_{\beta=0} = -\sum' (-1)^k \frac{(\hat{n}_{p_1} + \dots + \hat{n}_{p_k})^2}{|\Lambda_{p_1} \cdots \Lambda_{p_k}|}, \tag{S.6}$$

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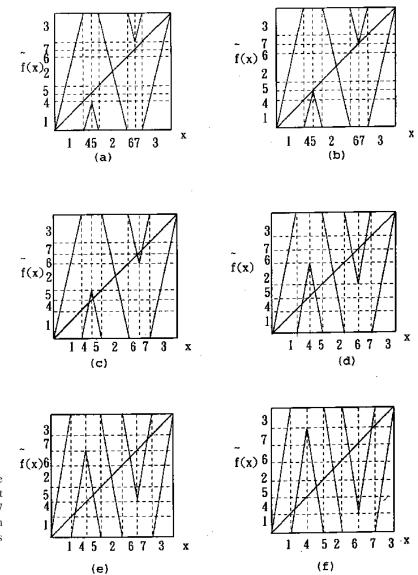


Figure S.1: (a)-(f) The sawtooth map (S.1) for the 6 values of parameter *a* for which the folding point of the map aligns with the endpoint of one of the 7 intervals and yields a finite Markov partition (from ref. [S.1]). The corresponding transition graphs are given in figure S.2.

and the sum is over all distinct non-repeating combinations of prime cycles. Most of results expected in this projects require no more than pencil and paper computations.

Implementing the symmetry factorization (25.35) is convenient, but not essential for this project, so if you find sect. 21.1.1 too long a read, skip the symmetrization.

S.1.1 The full shift

Take the map (S.1) and extend it to the real line. As in example of figure 25.3, denote by *a* the critical value of the map (the maximum height in the unit cell)

$$a = \hat{f}(\frac{1}{4} + \frac{1}{4\Lambda}) = \frac{\Lambda + 1}{4}.$$
 (S.7)

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Describe the symbolic dynamics that you obtain when *a* is an integer, and derive the formula for the diffusion constant:

$$D = \frac{(\Lambda^2 - 1)(\Lambda - 3)}{96\Lambda} \quad \text{for } \Lambda = 4a - 1, \ a \in \mathbb{Z}.$$
 (S.8)

If you are going strong, derive also the fromula for the half-integer a = (2k+1)/2, $\Lambda = 4a + 1$ case and email it to DasBuch@nbi.dk. You will need to partition \mathcal{M}_2 into the left and right half, $\mathcal{M}_2 = \mathcal{M}_8 \cup \mathcal{M}_9$, as in the derivation of (25.21).

exercise 25.1

S.1.2 Subshifts of finite type

We now work out an example when the partition is Markov, although the slope is not an integer number. The key step is that of having a partition where intervals are mapped *onto* unions of intervals. Consider for example the case in which $\Lambda = 4a - 1$, where $1 \le a \le 2$. A first partition is constructed from seven intervals, which we label { \mathcal{M}_1 , \mathcal{M}_4 , \mathcal{M}_5 , \mathcal{M}_2 , \mathcal{M}_6 , \mathcal{M}_7 , \mathcal{M}_3 }, with the alphabet ordered as the intervals are laid out along the unit interval. In general the critical value *a* will not correspond to an interval border, but now we choose *a* such that the critical point is mapped onto the right border of \mathcal{M}_1 , as in figure S.1 (a). The critical value of f() is $f(\frac{\Lambda+1}{4\Lambda}) = a - 1 = (\Lambda - 3)/4$. Equating this with the right border of \mathcal{M}_1 , $x = 1/\Lambda$, we obtain a quadratic equation with the expanding solution $\Lambda = 4$. We have that $f(\mathcal{M}_4) = f(\mathcal{M}_5) = \mathcal{M}_1$, so the transition matrix (14.1) is given by

$$\phi' = T\phi = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_4 \\ \phi_5 \\ \phi_2 \\ \phi_6 \\ \phi_7 \\ \phi_3 \end{pmatrix}$$
(S.9)

and the dynamics is unrestricted in the alphabet

 $\{1, \underline{41}, \underline{51}, 2, \underline{63}, \underline{73}, 3, \}.$

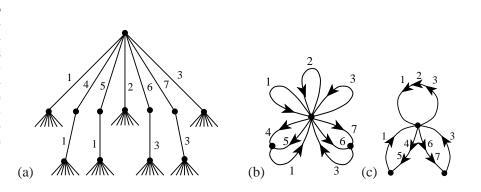
One could diagonalize (S.9) on the computer, but, as we saw in chapter 14, the transition graph figure S.2 (b) corresponding to figure S.1 (a) offers more insight into the dynamics. The dynamical zeta function

$$1/\zeta = 1 - (t_1 + t_2 + t_3) - 2(t_{14} + t_{37})$$

$$1/\zeta = 1 - 3\frac{z}{\Lambda} - 4\cosh\beta\frac{z^2}{\Lambda^2}.$$
(S.10)

follows from the loop expansion (15.15) of sect. 15.3.

Figure S.2: (a) The sawtooth map (S.1) partition tree for figure S.1 (a); while intervals $\mathcal{M}_1, \mathcal{M}_2, \mathcal{M}_3$ map onto the whole unit interval, $f(\mathcal{M}_1) =$ $f(\mathcal{M}_2) = f(\mathcal{M}_3) = \mathcal{M}$, intervals $\mathcal{M}_4, \mathcal{M}_5$ map onto \mathcal{M}_1 only, $f(\mathcal{M}_4) = f(\mathcal{M}_5) = \mathcal{M}_1$, and similarly for intervals $\mathcal{M}_6, \mathcal{M}_7$. An initial point starting out in the interval $\mathcal{M}_1, \mathcal{M}_2$ or \mathcal{M}_3 can land anywhere on the unit interval, so the subtrees originating from the corresponding nodes on the partition three are similar to the whole tree and can be identified (as, for example, in figure 14.5), yielding (b) the transition graph for the Markov partition of figure S.1 (a). (c) the transition graph in the compact notation of (25.26).



The material flow conservation sect. 20.3.2 and the symmetry factorization (25.35) yield

$$0 = \frac{1}{\zeta(0,1)} = \left(1 + \frac{1}{\Lambda}\right) \left(1 - \frac{4}{\Lambda}\right)$$

which indeed is satisfied by the given value of Λ . Conversely, we can use the desired Markov partition topology to write down the corresponding dynamical zeta function, and use the $1/\zeta(0, 1) = 0$ condition to fix Λ . For more complicated transition matrices the factorization (25.35) is very helpful in reducing the order of the polynomial condition that fixes Λ .

The diffusion constant follows from (25.36) and (S.4)

$$\langle n \rangle_{\zeta} = -\left(1 + \frac{1}{\Lambda}\right)\left(-\frac{4}{\Lambda}\right), \quad \left\langle \hat{n}^2 \right\rangle_{\zeta} = \frac{4}{\Lambda^2}$$
$$D = \frac{1}{2}\frac{1}{\Lambda+1} = \frac{1}{10}$$

Think up other non-integer values of the parameter for which the symbolic dynamics is given in terms of Markov partitions: in particular consider the cases illustrated in figure S.1 and determine for what value of the parameter *a* each of them is realized. Work out the transition graph, symmetrization factorization and the diffusion constant, and check the material flow conservation for each case. Derive the diffusion constants listed in table S.1. It is not clear why the final answers tend to be so simple. Numerically, the case of figure S.1 (c) appears to yield the maximal diffusion constant. Does it? Is there an argument that it should be so?

The seven cases considered here (see table S.1, figure S.1 and (S.8)) are the 7 simplest complete Markov partitions, the criterion being that the critical points map onto partition boundary points. This is, for example, what happens for unimodal tent map; if the critical point is preperiodic to an unstable cycle, the grammar is complete. The simplest example is the case in which the tent map critical

| figure S.1 | Λ | D |
|------------|----------------------------|---|
| | 3 | 0 |
| (a) | 4 | $\frac{1}{10}$ |
| (b) | $\sqrt{5} + 2$ | $\frac{1}{2\sqrt{5}}$ |
| (c) | $\frac{1}{2}(\sqrt{17}+5)$ | $\frac{\frac{2}{\sqrt{17}}}{\sqrt{17}}$ |
| (c') | 5 | <u>Z</u> |
| (d) | $\frac{1}{2}(\sqrt{33}+5)$ | $\frac{1}{8} + \frac{5}{88}\sqrt{33}$ |
| (e) | $2\sqrt{2} + 3$ | $\frac{1}{2\sqrt{2}}$ |
| (f) | $\frac{1}{2}(\sqrt{33}+7)$ | $\frac{1}{4} + \frac{1}{4\sqrt{33}}$ |
| | 7 | $\frac{2}{7}$ |

Table S.1: The diffusion constant as function of the slope Λ for the a = 1, 2 values of (S.8) and the 6 Markov partitions of figure S.1

point is preperiodic to a unimodal map 3-cycle, in which case the grammar is of golden mean type, with _00_ substring prohibited (see figure 14.5). In case at hand, the "critical" point is the junction of branches 4 and 5 (symmetry automatically takes care of the other critical point, at the junction of branches 6 and 7), and for the cases considered the critical point maps into the endpoint of each of the seven branches.

One can fill out parameter *a* axis arbitrarily densely with such points - each of the 7 primary intervals can be subdivided into 7 intervals obtained by 2-nd iterate of the map, and for the critical point mapping into any of those in 2 steps the grammar (and the corresponding cycle expansion) is finite, and so on.

S.1.3 Diffusion coefficient, numerically

(optional:)

Attempt a numerical evaluation of

$$D = \frac{1}{2} \lim_{n \to \infty} \frac{1}{n} \left\langle \hat{x}_n^2 \right\rangle.$$
(S.11)

Study the convergence by comparing your numerical results to the exact answers derived above. Is it better to use few initial \hat{x} and average for long times, or to use many initial \hat{x} for shorter times? Or should one fit the distribution of \hat{x}^2 with a Gaussian and get the *D* this way? Try to plot dependence of *D* on Λ ; perhaps blow up a small region to show that the dependence of *D* on the parameter Λ is fractal. Compare with figure 25.5 and figures in refs. [S.1, S.2, 25.9, 25.8, 25.10].

S.1.4 *D* is a nonuniform function of the parameters

(optional:)

The dependence of D on the map parameter Λ is rather unexpected - even though

for larger Λ more points are mapped outside the unit cell in one iteration, the diffusion constant does not necessarily grow. An interpretation of this lack of monotonicity would be interesting.

You can also try applying periodic orbit theory to the sawtooth map (S.1) for a random "generic" value of the parameter Λ , for example $\Lambda = 6$. The idea is to bracket this value of Λ by the nearby ones, for which higher and higher iterates of the critical value $a = (\Lambda + 1)/4$ fall onto the partition boundaries, compute the exact diffusion constant for each such approximate Markov partition, and study their convergence toward the value of D for $\Lambda = 6$. Judging how difficult such problem is already for a tent map (see sect. 15.5 and appendix D.1), this is too ambitious for a week-long exam.

References

- [S.1] H.-C. Tseng, H.-J. Chen, P.-C. Li, W.-Y. Lai, C.-H. Chou and H.-W. Chen, "Some exact results for the diffusion coefficients of maps with pruned cycles," *Phys. Lett.* A 195, 74 (1994).
- [S.2] C.-C. Chen, "Diffusion Coefficient of Piecewise Linear Maps," *Phys. Rev.* E51, 2815 (1995).
- [S.3] H.-C. Tseng and H.-J. Chen, "Analytic results for the diffusion coefficient of a piecewise linear map," *Int. J. Mod. Phys.*B 10, 1913 (1996).

S.2 Deterministic diffusion, sawtooth map

To illustrate the main idea of chapter 25, tracking of a globally diffusing orbit by the associated confined orbit restricted to the fundamental cell, we consider in more detail the class of simple 1-dimensional dynamical systems, chains of piecewise linear maps (25.9). The translational symmetry (25.10) relates the unbounded dynamics on the real line to the dynamics restricted to a "fundamental cell" - in the present example the unit interval curled up into a circle. The corresponding circle map f(x) is obtained by modulo the integer part. The elementary cell map f(x) is sketched in figure 25.3. The map has the symmetry property

$$\hat{f}(\hat{x}) = -\hat{f}(-\hat{x}),$$
 (S.12)

so that the dynamics has no drift, and all odd derivatives of the generating function (25.3) with respect to β evaluated at $\beta = 0$ vanish.

The cycle weights are given by

$$t_p = z^{n_p} \frac{e^{\beta \hat{n}_p}}{|\Lambda_p|} \,. \tag{S.13}$$

The diffusion constant formula for 1-dimensional maps is

$$D = \frac{1}{2} \frac{\left\langle \hat{n}^2 \right\rangle_{\zeta}}{\left\langle n \right\rangle_{\zeta}} \tag{S.14}$$

where the "mean cycle time" is given by

$$\langle n \rangle_{\zeta} = \left. z \frac{\partial}{\partial z} \frac{1}{\zeta(0, z)} \right|_{z=1} = -\sum' (-1)^k \frac{n_{p_1} + \dots + n_{p_k}}{|\Lambda_{p_1} \cdots \Lambda_{p_k}|}, \tag{S.15}$$

the mean cycle displacement squared by

$$\left\langle \hat{n}^2 \right\rangle_{\zeta} = \left. \frac{\partial^2}{\partial \beta^2} \frac{1}{\zeta(\beta, 1)} \right|_{\beta=0} = -\sum' (-1)^k \frac{(\hat{n}_{p_1} + \dots + \hat{n}_{p_k})^2}{|\Lambda_{p_1} \cdots \Lambda_{p_k}|}, \tag{S.16}$$

and the sum is over all distinct non-repeating combinations of prime cycles. Most of results expected in this projects require no more than pencil and paper computations.

S.2.1 The full shift

Reproduce the formulas of sect. 25.2 for the diffusion constant D for Λ both even and odd integer.

| figure 25.4 | Λ | D |
|---------------------------------|--|--|
| (a) (b) (c) (d) (e) | 4 $2 + \sqrt{6}$ $2\sqrt{2} + 2$ 5 $3 + \sqrt{5}$ $3 + \sqrt{7}$ 6 | $ \frac{\frac{1}{4}}{1 - \frac{3}{4}\sqrt{6}} \\ \frac{15 + 2\sqrt{2}}{16 + 4\sqrt{2}} \\ \frac{5}{1} \\ \frac{5}{3\Lambda - 4} \\ \frac{5\Lambda - 4}{3\Lambda - 2} \\ \frac{5}{5} \\ \frac{5}{6} $ |

Table S.2: The diffusion constant as function of the slope Λ for the $\Lambda = 4, 6$ values of (25.20) and the 5 Markov partitions like the one indicated in figure 25.4.

S.2.2 Subshifts of finite type

We now work out examples when the partition is Markov, although the slope is not an integer number. The key step is that of having a partition where intervals are mapped *onto* unions of intervals.

Start by reproducing the formula (25.28) of sect. 25.2.2 for the diffusion constant *D* for the Markov partition, the case where the critical point is mapped onto the right border of I_{1_+} .

Think up other non-integer values of the parameter Λ for which the symbolic dynamics is given in terms of Markov partitions: in particular consider the remaining four cases for which the critical point is mapped onto a border of a partition in one iteration. Work out the transition graph symmetrization factorization and the diffusion constant, and check the material flow conservation for each case. Fill in the diffusion constants missing in table S.2. It is not clear why the final answers tend to be so simple. What value of Λ appears to yield the maximal diffusion constant?

The 7 cases considered here (see table S.2 and figure 25.4) are the 7 simplest complete Markov partitions in the $4 \le \Lambda \le 6$ interval, the criterion being that the critical points map onto partition boundary points. In case at hand, the "critical" point is the highest point of the left branch of the map (symmetry automatically takes care of the other critical point, the lowest point of the left branch), and for the cases considered the critical point maps into the endpoint of each of the seven branches.

One can fill out parameter a axis arbitrarily densely with such points - each of the 6 primary intervals can be subdivided into 6 intervals obtained by 2-nd iterate of the map, and for the critical point mapping into any of those in 2 steps the grammar (and the corresponding cycle expansion) is finite, and so on.

S.2.3 Diffusion coefficient, numerically

(optional:)

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Attempt a numerical evaluation of

$$D = \frac{1}{2} \lim_{n \to \infty} \frac{1}{n} \left\langle \hat{x}_n^2 \right\rangle.$$
(S.17)

Study the convergence by comparing your numerical results to the exact answers derived above. Is it better to use few initial \hat{x} and average for long times, or to use many initial \hat{x} for shorter times? Or should one fit the distribution of \hat{x}^2 with a Gaussian and get the *D* this way? Try to plot dependence of *D* on Λ ; perhaps blow up a small region to show that the dependance of *D* on the parameter Λ is fractal. Compare with figure 25.5 and figures in refs. [S.1, S.2, 25.9, 25.8, 25.10].

S.2.4 *D* is a nonuniform function of the parameters

(optional:)

The dependence of D on the map parameter Λ is rather unexpected - even though for larger Λ more points are mapped outside the unit cell in one iteration, the diffusion constant does not necessarily grow. Figure 25.5 taken from ref. [25.9] illustrates the fractal dependence of diffusion constant on the map parameter. An interpretation of this lack of monotonicity would be interesting.

You can also try applying periodic orbit theory to the sawtooth map (25.9) for a random "generic" value of the parameter Λ , for example $\Lambda = 4.5$. The idea is to bracket this value of Λ by the nearby ones, for which higher and higher iterates of the critical value $a = \Lambda/2$ fall onto the partition boundaries, compute the exact diffusion constant for each such approximate Markov partition, and study their convergence toward the value of D for $\Lambda = 4.5$. Judging how difficult such problem is already for a tent map (see sect. 15.5 and appendix D.1), this is too ambitious for a week-long exam.