Coarse graining: lessons from simple examples

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Abstract

We assess Coarse Graining by studying different partitions of the phase space of the Baker transformation and the periodic torus automorphisms. It turns out that the shape of autocorrelation functions for the Baker transformation is more or less reproduced. However, for certain partitions the decay rates turn out to be irrelevant, even decay may stop in a finite time. For the periodic torus automorphisms, Coarse Graining introduces artificial dumping.

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1 Introduction

Coarse graining is a simple way to explain the manifest irreversibility from the underlying entropy preserving dynamical laws. The idea which goes back to Ehrenfests [1], see also Tolman [2], is that fine measurements at the fundamental level are unattainable, therefore we can and should observe only averages over microstates. The averaging is introduced by the observer in addition to the dynamical evolution. The resulting loss of information gives rise to entropy increase. In fact all other conventional explanations of irreversibility are inventions of extra-dynamical mechanisms to lose dynamical information. Boltzmann’s Stossalanzats [1, 3] amounts to loss of postcollisional correlations, von Neumann’s [4] measurement projection postulate amounts to loss of quantum correlations described by the off-diagonal matrix elements of the representation of the pure state in terms of a basis of common eigenvectors of a complete system of commuting observables, resulting in the collapse of the wave function. Decoherence amounts to loss of information through transfer to an unknown and uncontrollable environment [5].

We shall not discuss here the details of these approaches which involve assumptions additional to the dynamical evolution of a more or less subjectivistic character. For a recent discussion see for example [3]. In contradistinction Prigogine and coworkers have stressed [7, 8, 9] that irreversibility should be an intrinsic property of dynamical systems which admit time asymmetric representations of evolution, without any loss of information. These time asymmetric representations can be obtained by extending the evolution to suitable Rigged Hilbert Space or by intertwining the evolution with Markov processes. These intrinsically irreversible systems include for example Large Poincaré Non-Integrable systems and chaotic systems. We shall not discuss further these interesting direction of research. Our objective is to see how coarse graining works for simple systems where calculations are controllable
and then draw more general conclusions. In Section 2 we define the coarse graining projections and the coarse grained evolution. We study coarse graining projection of the Baker transformation in Section 3 and of the periodic torus automorphisms in Section 4.

2 Coarse graining projections

We introduce the basic concepts and notations that will later be used in the description of particular systems. Let us consider the configuration space \( X \) with the measure \( \mu \). The partition \( \zeta \) is the finite set \( \{ Z_k \}_{k=1}^M \) of the cells \( Z_k \) which satisfy the following properties:

\[
\bigcup_{k=1}^M Z_k = X, \\
\mu(Z_i \cap Z_k) = \delta_{ik} \mu(Z_i),
\]

where \( \delta_{ik} \) is the Kroneker symbol.

Coarse graining is implemented through the averaging projection over the cells of the partition \( \zeta \) known also in probability theory \([10, 11]\) as the conditional expectation operator \( P \) over \( \zeta \):

\[
P f(x) = \sum_{k=1}^M f_k 1_{Z_k}(x).
\]

Here \( 1_{Z_k}(x) \) is the indicator of the set \( Z_k \):

\[
1_{Z_k}(x) = \begin{cases} 
1, & x \in Z_k \\
0, & x \notin Z_k
\end{cases}
\]

and the average value \( f_k \) of the function \( f(x) \) in the cell \( Z_k \) is

\[
f_k = \frac{1}{\mu(Z_k)} \int_{Z_k} d\mu(x)f(x).
\]

Let us define by \( Q \) the orthocomplement of \( P \):

\[
P + Q = I
\]

\( Q \) projects onto the fine/detail information eliminated by \( P \). The simplest dynamics are cascades of automorphisms \( S \) of the phase space \( X \). The observables are usually
square integrable phase functions in \( L^2(X) \) and they evolve according to the iterated Koopman operator

\[
V : L^2(X) \to L^2(X) \text{ such that } V f(x) = f(Sx).
\]

The coarse grained evolution is described by the projected evolution by \( P \) (2):

\[
V^n_P = (PVP)^n, \quad n = 0, 1, 2 \ldots.
\] (3)

In general however

\[
VP = PVP + QVP.
\] (4)

Therefore starting with a coarse grained observable \( Pf \), the evolution may regenerate the fine detail \( QVPf \), which is eliminated by the repeated application of the projection \( P \). Therefore arbitrary projections \( P \) destroy the dynamical evolution. In fact as the Koopman operators of chaotic systems are shifts [12], their coarse grained projections can be whatever contractive evolution one wishes (Structure theorem of bounded operators) [12, 13] with any desired decay rates. A condition which guarantees the reliability of the coarse grained description is that the evolution \( V \) should not destroy the cells of the coarse graining partition. In this way minimal dynamical information is lost by averaging and the resulting symbolic dynamics is very close to the original evolution. Such coarse-graining projections compatible with the dynamics should be distinguished from arbitrary coarse grainings because they are not imposed by the external observer but are intrinsic properties of the system. To our knowledge only three types of such intrinsic coarse grainings have been proposed. Namely, projections onto the \( K \)-partition [7, 14], onto the generating partition [15] of Kolmogorov dynamical systems and onto Markov partitions [16].

We shall not discuss further this interesting subject related also to the symbolic representation of dynamics [17] but consider arbitrary coarse grainings as so far no
a priori reason to decide over the proper natural partition has been proposed to our knowledge.

The influence of the coarse graining to the approach to equilibrium will be studied through the decay rates of the autocorrelation functions of the observable phase functions \( f \):

\[
C^{(n)}(f) = \frac{\int_X (V^n f)(x) f(x) d\mu(x)}{\int_X f^2(x) d\mu(x)}.
\] (5)

The coarse grained autocorrelation function \( C_P^{(n)}(f) \) is

\[
C_P^{(n)}(f) = \frac{\int_X (V^n_P f)(x) P f(x) d\mu(x)}{\int_X (P f(x))^2 d\mu(x)}.
\] (6)

However, in the following we shall see that the autocorrelation functions are not sensitive enough to discriminate results of different approaches. In order to analyze a system in more detail, we introduce the decay rate \( \tau^{(n)}(f) \) at time (stage) \( n \):

\[
\tau^{(n)}(f) = -\log \frac{C^{(n+1)}(f) - C^{(n)}(f)}{C^{(n)}(f) - C^{(n-1)}(f)}.
\] (7)

This definition is motivated by the following observation. If the autocorrelation function decreases (or increases) monotonically at the points \( n - 1, n, n + 1 \), it can be written as

\[
C^{(n)} = A(n) + B(n) \exp(-\kappa(n)n)
\] (8)

at these points. In this case the decay rate is \( \tau^{(n)} = \kappa(n) \). As we can usually expect that the representation \( (8) \) is the leading term of the asymptotics for sufficiently large \( n \) and that \( A(n), B(n), \text{and} \kappa(n) \) become independent of \( n \) for large \( n \), the decay rate \( \tau^{(n)} \) converges to the decay rate of the system \( \kappa(\infty) \). Physically speaking, in most cases one needs information about the widths and the lifetimes of the system, i.e. \( \tau^{(n)} \), rather than just the decaying profile \( C^{(n)} \).
3 Coarse graining the Baker transformation

We shall apply the coarse graining to the Baker transformation defined [18] on the torus \([0, 1] \times [0, 1]\) by the formula

\[
B(x, y) = \begin{cases} 
(2x, \frac{y}{2}), & \text{for } 0 \leq x \leq 1/2 \\
(2x - 1, \frac{y + 1}{2}), & \text{for } 1/2 \leq x \leq 1.
\end{cases}
\]  

(9)

In order to study the applicability of the coarse graining for this transformation, we introduce two different partitions \(\zeta^s\) and \(\zeta^t\) such that \(\mu(Z^s_i) = \mu(Z^t_j)\) for all \(i, j\). As these partitions have cells of the same measure, the role of geometry is manifested in the clearest way. It is worth noticing here that we cannot use for this study an one-dimensional map as we cannot choose two different partitions with the same measure in one dimension. In Fig. 1, we present both partitions for the number of the cells in each direction \(M = 4\).

The calculation of autocorrelation functions (5,6) involves integration over each cell. The numerical realization of this integration results in loss of accuracy. To avoid this problem, we use the fact that the function \(f^{(n)} = (PBP)^n f\) is piece-wise constant for \(n \geq 1\). For such functions, the successive iterations can be written as

\[
f_k^{(n+1)} = \frac{1}{\mu(Z_k)} \sum_i f_i^{(n)} \mu(Z_k \cap B(Z_i)).
\]  

(10)

It is worth noticing that the latter representation is rather effective from the computational point of view as the sum in Eq. (10) involves very few terms. The only remaining integration in Eq. (10) is the calculation of \(Pf\). We use the rectangular quadrature formula for this integration. The numerical investigation shows that the number of integration points 40 by 40 for each cell is enough to reach the convergence.

Now, after the description of the method, we present the results. We start with the initial function

\[
f(x, y) = x + y.
\]
With this particular choice, it is possible to calculate the autocorrelation function explicitly. A straightforward analytical calculation gives:

\[ C^{(n)} = \frac{6}{7}(1 + \frac{1}{8}n2^{-n} + \frac{1}{6}2^{-n}). \]  

(11)

It is interesting to point out that the second term in expression (11) corresponds to the Jordan block of the second order in the generalized spectral decomposition [19].

With expression (11), the decay rate can be obtained exactly:

\[ \tau^{(n)} = \log 2 - \log \left(1 + \frac{3}{3n - 2}\right). \]  

(12)

The exact expressions (11,12) are used for the comparison with the coarse graining results.

The autocorrelation function and the local decay rates for both partitions with \(M = 200\), and analytical results are presented in Fig. 2. The first conclusion we can make here is that coarse graining reproduces the correlation function with accuracy better than \(10^{-4}\). Hence, if one is interested only in similar integral characteristics, coarse graining can be used.

However, in many cases one needs more detailed characteristics of the evolution, for example the decay rates. Here the situation is changed as different partitions result in significantly different decay rates. While in this particular case the square partition \(\zeta^s\) produces results that are surprisingly close to the exact ones, the results for the triangle partition \(\zeta^t\) differ drastically although they agree up to 11 iterations.

The decay rates for the partitions with \(M = 800\) are presented in Fig. 3. For these partitions the results agree very well in a wider region, up to about 20 iterations. However, further iterations again show huge disagreement between the results for the triangle partition and the exact results.

The square partitions may also give irrelevant results. Namely, if we consider the rectangle partitions with \(2^N\) subdivisions of the \(x\) axis and \(2^M\) subdivisions of
the $y$ axis, than after $N + M - 1$ iterations the coarse grained correlation function reaches equilibrium exactly. Hence, there is no decay after this number of stages. This statement is also true for the square partition when $N = M$. However, there exists rectangle partition with the same cell area that results in the proper decay curve. We illustrate this discussion in Fig. 4. Therefore the decay rates are very sensitive to the choice of the type of the partition.

One may expect that despite the big variations of the decay rates, an average of them might be stable. To analyze this possibility, we present in Fig. 5 the average decay rates

$$\tau_{av}^{(n)} = \frac{1}{10} \sum_{i=n+1}^{n+10} \tau^{(i)}$$

for $n = 10$ and $n = 20$. However also in this case the previous conclusions remain valid: while the square partition produces decay rates robust with respect to changes of the cell area, the triangle partition gives results which change irregularly with respect to changes of the cell area. However, the average decay rate $\tau_{av}^{(10)}$ for the triangle partition is stabilized when $M$ is rather big. But we cannot restrict ourselves to this small number of iterations ($n \sim 10$) as the decay rates reach their asymptotics much later. The results for the $\zeta^s$ show this clearly as the difference of $\tau_{av}^{(10)}$ and $\tau_{av}^{(20)}$ is rather pronounced.

We have already mentioned that our results do not depend on the choice of the observable function $f(x, y)$. To illustrate this, we present in Fig. 6 the autocorrelation function and the local decay rates for both partitions with $M = 800$, and the initial function $f(x, y) = x\sqrt{x+y}$. Analytical results are not available for this function. One can see that the results have the same qualitative behavior as previous ones. Calculations for other initial functions also give the similar results, so our conclusions are valid and independent of the initial function.
4 Coarse graining the periodic torus automorphisms

In the previous section we discussed coarse graining applied for the Baker transformation. One could see that, despite the problems with the decay rates, the method reproduces the autocorrelation functions rather well. Here we shall show that this is not always the case, and coarse graining applied to some dynamical systems may produce even qualitatively wrong autocorrelation functions.

Let us consider the periodic automorphisms $T$ of the torus $[0,1] \times [0,1]$:

$$T \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} (T_{11}x + T_{12}y) \mod 1 \\ (T_{21}x + T_{22}y) \mod 1 \end{pmatrix}.$$  

The coefficients $T_{ij}$ are integers with the property

$$T^k = I \quad \text{for some } k \in \mathbb{N}. \quad (13)$$

There exist few families of periodic torus automorphisms $T$ with only possible periods $k = 2, 3, 4, \text{ and } 6$ (Appendix 1). As described in the previous section, we construct the autocorrelation functions (5,6). Due to the periodicity of the transformation $T$, the exact autocorrelation function is also periodic. However, the coarse grained autocorrelation functions may show damping as a result of information loss. We present two such examples in Fig. 7. For the transformation

$$T = \begin{pmatrix} 1 & 2 \\ -1 & -1 \end{pmatrix}$$

we used the partition $\zeta^s$ with $M = 20$. This type of the partition gives reasonable results for the Baker transformation. Here, however, one can see that the autocorrelation function approaches equilibrium as if there was damping. Hence, the periodicity is not preserved. Moreover, for the simple transformation

$$T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$
there exist also partitions giving rise to damping. As an example, we plot in Fig. 7 the autocorrelation function for the rectangle partition with 5 subdivisions for the $x$ axis and 7 subdivisions for the $y$ axis.

5 Conclusions

For the Baker transformation, coarse graining reproduces the shape of the autocorrelation functions (Figs. 2,6), but decay rates are hardly reproduced (Figs. 2-6). Moreover, some partitions like in Fig. 4 give rise to exact approach of equilibrium after a finite time while others may give the correct asymptotic behaviour. For the periodic torus automorphisms, coarse graining introduces artificial damping of the autocorrelation functions.

The above mentioned conclusions illustrate once more the subjectivistic character of coarse graining. Therefore when employed, coarse graining should be chosen with care, for example by selecting partitions intrinsic to the dynamics, as discussed at the end of section 2. In fact the answer to the inverse problem of statistical physics is [15] that all stationary Markov processes arise as exact projections onto the generating partitions of Kolmogorov dynamical systems, in the spirit of Misra-Prigigine-Courbage theory of irreversibility [7, 14]. In fact such intrinsic partitions are not defined by any observations but they are objective properties of the dynamical evolution.

Concerning the general issue of irreversibility, the possibilities opened by extending the dynamical evolution or by intertwining the dynamical evolution with Markov processes [4, 8, 9] are a challenging physical and mathematical research direction.

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Appendix 1. The periodic torus automorphisms.

The periodic torus automorphisms

\[ T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \]

with integer coefficients satisfy the equation

\[ T^k = I, \]

where \( k = 2, 3, \ldots \) is the period. As \(|\det T| = 1\), we have \( \det T = \pm 1 \). Let us transform the matrix \( T \) to the diagonal or the Jordan form with the unitary transformation. As the identity matrix is unchanged, we can conclude that the eigenvalues of the matrix \( T \) satisfy \(|\lambda_{1,2}| = 1\). Let us examine all possible cases corresponding to real and complex eigenvalues.

I. The eigenvalues are real. In this case we have three possibilities:

1. \( \lambda_1 = \lambda_2 = 1 \). As the Jordan block cannot be unitarily equivalent to the identity matrix, the only possible transformation is the trivial one, \( T = I \).

2. \( \lambda_1 = \lambda_2 = -1 \). As in the first case, the only possible transformation is \( T = -I \) which has the period \( k = 2 \).

3. \( \lambda_1 = 1, \lambda_2 = -1 \). In this case we have a family of periodic automorphisms. In order to describe them, we may use two invariants: the determinant \( \det T = -1 \) and trace \( \text{tr} T = 0 \), and write down the family as

\[ \begin{pmatrix} a & b \\ c & -a \end{pmatrix} \quad \text{with} \quad \det T = -a^2 - bc = -1. \quad (14) \]

These automorphisms have the period \( k = 2 \).

II. The eigenvalues are complex. As the matrix has real coefficients, the eigenvalues are conjugated to each other and can be written as \( \lambda_1 = e^{i\varphi}, \lambda_2 = e^{-i\varphi}, \varphi \in \mathbb{R} \). Using the invariants of the matrix, \( \det T = 1 \) and \( \text{tr} T = 2 \cos \varphi \), we may write the
corresponding family as

$$\begin{pmatrix} a & b \\ c & 2 \cos \varphi - a \end{pmatrix} \quad \text{with} \quad \det T = a(2 \cos \varphi - a) - bc = 1. \quad (14)$$

The cases when $\varphi = 0$ and $\varphi = \pi$ give in fact real coefficients and are already analyzed. The only remaining cases when the matrix has integer coefficients are:

1. $\cos \varphi = 0$, $\varphi = \pi/2$. Here we have the family

$$\begin{pmatrix} a & b \\ c & -a \end{pmatrix} \quad \text{with} \quad \det T = -a^2 - bc = 1. \quad (15)$$

These automorphisms have the period $k = 4$.

2. $\cos \varphi = 1/2$, $\varphi = \pi/3$. The corresponding family is

$$\begin{pmatrix} a & b \\ c & 1 - a \end{pmatrix} \quad \text{with} \quad \det T = a(1 - a) - bc = 1. \quad (16)$$

These automorphisms have the period $k = 6$.

3. $\cos \varphi = -1/2$, $\varphi = 2\pi/3$. The corresponding family is

$$\begin{pmatrix} a & b \\ c & -1 - a \end{pmatrix} \quad \text{with} \quad \det T = -a(1 + a) - bc = 1. \quad (17)$$

These automorphisms have the period $k = 3$.

All possible periodic torus automorphisms are given by (14) – (17).
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Figure captions

Fig. 1. The partitions used in calculations for $M = 4$. Fig. 1a shows the square partition $\zeta^s$, and Fig. 1b shows the triangle partition $\zeta^t$.

Fig. 2. The correlation function $C^{(n)}$ (the solid line) and decay rates $\tau^{(n)}$ for squares (the long-dashed line), triangles (the dot-dashed line), and analytical results (the short-dashed line). The number of cells is 200 by 200.

Fig. 3. Decay rates $\tau^{(n)}$ for squares (the short-dashed line), triangles (the long-dashed line), and analytical results (the solid line). The number of cells is 800 by 800.

Fig. 4. Decay rates $\tau^{(n)}$ for squares (the dashed line) with number of cells 256 by 256 (the cell area $1.52588 \cdot 10^{-5}$), for 254 by 258 rectangles (the dot-dashed line, the cell area $1.52597 \cdot 10^{-5}$), and analytical results (the solid line). The second and the third lines practically coincide.

Fig. 5. Average values $\tau_{av}^{(n)}$ for $n = 10$ and $n = 20$ as the function of number of cells $M$ for squares and triangles. The solid line is for $\tau_{av}^{(10)}$ for triangles, the long-dashed line is for $\tau_{av}^{(20)}$ for triangles, the short-dashed line is for $\tau_{av}^{(10)}$ for squares, and the dot-dashed line is for $\tau_{av}^{(20)}$ for squares.

Fig. 6. The correlation function $C^{(n)}$ (the solid line) and decay rates $\tau^{(n)}$ for squares (the long-dashed line) and triangles (the short-dashed line). The initial function is $f(x, y) = x\sqrt{x + y}$. The number of elements is 800 by 800.

Fig. 7. The correlation function $C^{(n)}$ for the periodic torus automorphisms $T = \begin{pmatrix} 1 & 2 \\ -1 & -1 \end{pmatrix}$ with the partition $\zeta^s$ and $M = 20$ (line 1), and for the $T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ with the partition of 5 intervals for $x$ and 7 intervals for $y$ (line 2).
