Hausdorff dimension of repellors in low sensitive systems

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Abstract

Methods to estimate the Hausdorff dimension of invariant sets of scattering systems are presented. Based on the levels’ hierarchical structure of the time delay function, these techniques can be used in systems whose future-invariant-set codimensions are approximately equal to or greater than one. The discussion is illustrated by a numerical example of a scatterer built with four hard spheres located at the vertices of a regular tetrahedron.

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Usually, in a scattering process almost all particles outcome asymptotically free after interacting with a potential. Some particles, however, remain in the scattering region bouncing forever under the action of the potential. The nature of these trapped orbits is in general very intricate, including fractal dimensions and chaotic behaviour. The dimension seems to be the most fundamental quantity characterising this set. When the dimension is large enough, scattered particles may present sensitive dependence on initial conditions reminiscent of the chaotic dynamics of the trapped orbits. This phenomenon allows the computation of the uncertainty dimension of the bounded orbits, defined as follows. For a scattering system, colour by black initial conditions of particles scattered, for instance, to the right-hand side of the scattering centre and by white initial conditions corresponding to particles scattered to the left-hand side. An initial condition of a given colour at a distance less than $\varepsilon$ of initial conditions of a different colour is labelled $\varepsilon$-uncertain. The final state (left or right) of a particle associated to an $\varepsilon$-uncertain initial condition is uncertain if this point is determined only within a precision of order $\varepsilon$. In the limit of small $\varepsilon$, the fraction of such $\varepsilon$-uncertain points is $f(\varepsilon) \sim \varepsilon^{N-D_u}$, for $N$ denoting the dimension of the subspace where the initial conditions are taken, and $D_u$ the corresponding uncertainty dimension of the intersection of the trapped orbits with this subspace. Therefore $D_u$ can be computed by fitting $\ln f(\varepsilon)$ as a function of $\ln(\varepsilon)$. This procedure works in systems where the set of bounded orbits has dimension greater than $N-1$ in the $N$-dimensional subspace of initial conditions. That is supported by the fact that in this case $D_u$ is expected to be equal to a more general concept of dimension, the Hausdorff dimension.

The Hausdorff dimension of a set $A$ is defined as follows \[1\]: Let $S_j$ denote a countable collection of subsets of the Euclidean space such that the diameters $\epsilon_j$ of the $S_j$ are all less than or equal to $\delta$, and such that the $S_j$ are a covering of $A$. We define the Hausdorff sum

$$ K_\delta(d) = \inf \sum_{j=1}^\infty (\epsilon_j)^d, $$

where the infimum is taken on the set of all the possible countable coverings of $A$ satisfying $\epsilon_j \leq \delta$. Then we define the $d$-dimensional Hausdorff measure

$$ K(d) = \lim_{\delta \to 0} K_\delta(d). $$

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It can be shown that $K(d)$ is infinite if $d$ is less than some critical value $D_H$, and is zero if $d$ is greater than $D_H$. This critical value is the Hausdorff dimension of the set $A$.

Among the several existing concepts of dimension, the Hausdorff dimension is the one that better implement the intuitive notion of dimension that we have in mind. Unfortunately, the uncertainty methods cannot be used to estimate $D_H$ when its value is less than or equal to $N - 1$. Even when $D_H$ is slightly greater than $N - 1$, its evaluation through the numerical computation of the uncertainty dimension is highly inaccurate. The aim of these work is to present methods to compute the Hausdorff dimension of the set of trapped orbits - the future invariant set ($I_f$) - when uncertainty methods do not apply. The determination of this dimension is important, for instance, to understand the onset of chaos in scattering systems when a system parameter is varied.

First in this communication, we introduce a method to take into account the infimum requirement appearing in the definition of the Hausdorff dimension, that allows the direct computation of $D_H(I_f)$. Next, the Hausdorff dimension is estimated from the box-counting dimension computed by using a proper-interior-maximum-like procedure. Finally, we define a new dimension, the self-similarity dimension, which is also used to approximate $D_H(I_f)$. Our methods can be applied for $D_H(I_f) > N - 1$ as well as for $D_H(I_f) \leq N - 1$. The discussion is illustrated along the text by a numerical example of a simple scattering system presenting $D_H(I_f) \leq N - 1$ and $D_H(I_f) > N - 1$ for two ranges of values of its control parameter.

The example we shall consider is due to Chen et al. [3], who investigated a system consisting of a particle bouncing between four identical hard spheres placed at the vertices of a regular tetrahedron of unit edge. The centres of the spheres are located at the coordinates $(0, 0, \sqrt{2}/3)$, $(1/2, -1/2\sqrt{3}, 0)$, $(-1/2, -1/2\sqrt{3}, 0)$ and $(0, 1/\sqrt{3}, 0)$, and their radius $R$ is the variable parameter of the system. These authors contributed with a procedure to directly evaluate the Hausdorff dimension $\tilde{D}_H(R)$ on 1-dimensional lines. By taking lines on the plane $P = \{z = -k \; (k > R), p_x = p_y = 0, p_z = 1\}$, they computed the Hausdorff dimension $D_H(R)$ of the intersection of $I_f$ with $P$, obtaining $D_H(0.48) = 1 + \tilde{D}_H(0.48) = 1.4$. It is reasonable to presume that $D_H$ is an increasing function of $R$. Here we are interested in computing $D_H$ for small values of the radius, where the dimension of $I_f \cap P$ is expected to be less than one (codimension greater than one).
We consider initial conditions \((x_0, y_0)\) on \(P\), and we define the time delay function \(T(x_0, y_0)\) as the number of collisions of the particle with the spheres. We also introduce \(C_n = \{(x_0, y_0) \mid T(x_0, y_0) \geq n\}\). \(C_1\) is the union of 4 discs, the projection on \(P\) of the four spheres. \(C_2\) is the union of \(4 \cdot 3 = 12\) deformed discs, the projection on \(P\) of the reflection on each sphere of the other three spheres. \(C_3\) is the union of \(4 \cdot 3^2 = 36\) deformed discs, and so on. Therefore, for sufficiently small \(R\), \(C_n\) is the union of \(4 \cdot 3^{n-1}\) deformed discs. The construction of the Cantor structure of the set \(I_\cap P = \cap_{n=1}^\infty C_n\) can be followed in Fig. 1, where we show \(C_1, C_2, C_3\) and \(C_4\) for \(R = 0.37\).

Labelling the spheres by 1, 2, 3 and 4, the left shift symbolic dynamics of the future invariant set consists of sequences \(s_1s_2s_3...\) of 1, 2, 3 and 4, where \(s_n\) is the number of the sphere of the \(n^{th}\) collision. The particle cannot collide two successive times with the same sphere, and hence the only constraint is \(s_{n+1} \neq s_n\) (at least for \(R\) small enough). A relevant point here is that each one of the \(4 \cdot 3^{n-1}\) deformed discs of \(C_n\) can be identified by a sequence of collisions, \(c_{n,j} = [s_1s_2...s_n]\) for \(j = 1, 2, ..., 4 \cdot 3^{n-1}\). It allows us to define the Hausdorff sum

\[
K_n(d) = \sum_{j=1}^{4 \cdot 3^{n-1}} |c_{n,j}|^d, \tag{3}
\]

where \(|c_{n,j}|\) is the diameter of \(c_{n,j}\), \(|c_{n,j}| = \sup_{\vec{x}, \vec{y} \in c_{n,j}} |\vec{x} - \vec{y}|\), which can be easily estimated from a sample of initial conditions. The \(d\)-dimensional Hausdorff measure \(K(d)\) is supposed to be the limit of \(K_n(d)\) for \(n \to \infty\). \(K(d)\) is infinite for \(d\) less than the Hausdorff dimension \(D_H\), and is zero for \(d\) greater than \(D_H\). Since it is not known how to compute \(\lim_{n \to \infty} K_n(d)\) numerically, we generalise an argument due to [3]: For \(n\) sufficiently large, the sums \(K_n(d)\) for different values of \(n\) will all intersect with each other at approximately the same point \(d = D_H\). It provides a method to estimate the Hausdorff dimension.

In Fig. 2 we show \(\ln K_5(d)\), \(\ln K_6(d)\), \(\ln K_7(d)\) and \(\ln K_8(d)\) for \(R = 0.37\). The curves in fact intersect approximately at the same point giving \(D_H(0.37) = 0.87 \pm 0.01\). In Fig. 3 (boxes) we show a graph of \(D_H\) computed by this method for \(0.37 \leq R \leq 0.48\) (it includes regions with \(D_H > 1\) and with \(D_H \leq 1\)). In the same figure (stars) we also show the box-counting dimension \(D_c\) of \(\cap_{m=1}^\infty C_m\). \(D_c\) was calculated by approximating \(\cap_{m=1}^\infty C_m\) by \(C_n\) for a sufficiently large \(n\). The number of squares \(N(\varepsilon)\) needed to cover \(C_n\) was counted for different values of the edge length \(\varepsilon\), and the dimension \(D_c\)
was then obtained by fitting $\ln N(\varepsilon) = -D_c \ln \varepsilon$. The comparison between $D_c$ and $D_H$ in Fig. 3 suggests that $D_c(R) = D_H(R)$.

Some remarks about the computation of the box-counting dimension have to be made. The accurate evaluation of $D_c$ requires the use of relatively small values for $\varepsilon$. On the other hand, $C_n$ has to reflect the fractal property of $\bigcap_{m=1}^{\infty} C_m$, condition satisfied if $|c_{n,j}| < \varepsilon$ for all $j$. It implies the need of large values for $n$ (we used $n = 15$ in our computations), demanding great computational efforts in finding $C_n$ when $D_c$ is less than one. The remedy is based on the use of a modified PIM (proper-interior-maximum) procedure. In the first step, we start with a sample of initial conditions on $P$ taken at the corners of a grid. From this set we store those points that are in $C_1$ as well as their first neighbours. We denote the stored set by $\bar{C}_1$. In the second step, we reduce the edge length of the grid and iterate only those points of the new grid that are in the region covered by $\bar{C}_1$. Then we store the points that are in $C_2$ together with their first neighbours. We denote this stored set by $\bar{C}_2$, and so on. After $n$ steps we obtain the desired approximation for $C_n$.

Back to Fig. 1, in the centre of the figure we see an approximately self-similar structure. Each step of the construction of the Cantor set divides one disc in three smaller deformed discs. If we assume that the self-similarity is exact, we can introduce $\lambda_1$, $\lambda_2$ and $\lambda_3$, the linear scales by which the discs are reduced in one step. Under such hypothesis we have that Hausdorff and box-counting dimensions are equal and satisfy

$$\lambda_1^D + \lambda_2^D + \lambda_3^D = 1. \quad (4)$$

Even through the self-similarity is not exact in our case, (4) is expected to provide a good estimate for $D_H$ (and $D_c$). Fig. 1 also shows that the factors by which the discs are reduced are approximately the same. It allows us to take $\lambda_1 = \lambda_2 = \lambda_3 \equiv \lambda$, and we refer to the resulting dimension

$$D_s = -\frac{\ln 3}{\ln \lambda} \quad (5)$$

as the self-similarity dimension. The computation of $\lambda$ can be performed by a Monte Carlo method. We determine the areas of $C_n$ and $C_{n+1}$, for a sufficiently large $n$, by evolving a sample of random initial conditions. An

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1 This technique can also be employed in the computation of $|c_{n,j}|$, to calculate $D_H$. 

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estimate of $\lambda$ is then given by

$$\lambda_n = \sqrt{\frac{1}{3} \times \frac{\text{area}(C_{n+1})}{\text{area}(C_n)}}. \quad (6)$$

A better statistics is obtained by taking $\lambda$ as the average on $\lambda_n, \lambda_{n+1}, ..., \lambda_{n+k}$ for an adequate $k$. For the tetrahedron scatterer, the value of $\lambda$ is very stable in relation to $n$ and $k$, what allows us to compute a well defined $\lambda$ with not much computational effort. The resulting dimension is shown in Fig. 3 (triangles) for $0.36 \leq R \leq 0.49$ and is consistent with $D_H$ and $D_c$ computed directly from their definitions. We believe that $D_s$ can be used to estimate the common value of $D_H$ and $D_c$ in most systems where some kind of statistical self-similarity takes place. A rigorous statement in this direction requires, however, further investigations.

The dimension ($D$) that we computed corresponds to the intersection of the stable manifold of the invariant set (repellor) with the plane $P$. In the 5-dimensional energy surface, the dimension of the stable manifold will be $d_s = 3 + D$. The time reversibility of the dynamics implies that the dimension of the unstable manifold $d_u$ will be equal to $d_s$. Since the invariant set is the intersection of the stable and unstable manifolds, its dimension will be $d_i = d_s + d_u - 5 = 2D + 1$. Therefore, the dimensions $d_s$, $d_u$ and $d_i$ can be calculated by computing $D$ with the techniques employed here. In this procedure, the critical value of the radius ($R_c$) where $D = 1$ ($R_c \approx 0.41$, see Fig. 3) does not play any particular role. In this context, to claim that the dynamics of the scattering systems is chaotic for $D > 1$ ($d_i > 3$) and regular for $D \leq 1$ ($d_i \leq 3$) sounds largely a matter of semantics. What is sure is that there is a chaotic set of trapped orbits whose dimension increases with the radius $R$. The presence of this chaotic set prevents the existence of integrals of motion besides the energy (the system is non-integrable).

In the computation of $D_H$, $D_c$ and $D_s$, we explored the hierarchical structure of levels of the time delay function in order to infer the dimension of its set of singularities ($\cap_{m=1}^{\infty} C_m$). The dimension of the singularities of the time delay seems to be the most fundamental quantity that we can measure to characterise invariant sets of scattering systems. The result involves no ambiguity since it will lead unequivocally to the dimension of the future invariant set. The same is not true for basin boundaries, for instance. See Fig. 4, where we show the basins of the tetrahedron scatterer defined by particles.
scattered to \( x \to +\infty \) and particles scattered to \( x \to -\infty \), for \( R = 0.48 \) (a) and \( R = 0.37 \) (b). The basin boundaries present smooth 1-dimensional parts on arbitrarily fine scales. These smooth parts are not on the future invariant set and, although immaterial when \( R = 0.48 \), they do affect the basin boundary dimension when \( R = 0.37 \). In this case the dimension of the fractal part \( (I_f \cap P) \) is less than the dimension of the smooth parts. Smooth parts also forbid the use of uncertainty methods to estimate the dimension of the future invariant set from the time delay function. In computing the uncertainty dimension of the singularities, the uncertainty method effectively computes the box-counting dimension of the set of all discontinuities. The time delay is discontinuous on the (1-dimensional) frontiers of all \( C_n \) (see Fig. 1), what implies that the result will be always greater than or equal to 1. The same happens with scattering functions.

Finally, we remark that methods to directly estimate the Hausdorff dimension of attractor sets (taking into account the infimum in (1)) was already discussed (see \[\textnormal{[6]}\] and references therein). The main difficulty in adapting these methods to the case of nonattracting sets is that they require a sample of points on the set we want to measure. Even though a simple matter in the case of attractors, the computation of these points is nontrivial for nonattracting sets. A possibility would be the use of the PIM-triple procedure \[\textnormal{[5]}\] to find trajectories which stay near the invariant set for arbitrarily long periods of time. The resulting methods are, however, far more complicated than those introduced here.

In summary, we have presented, through an example, methods to estimate the Hausdorff dimension of nonattracting invariant sets of scattering systems. The methods apply, albeit not only, to systems with invariant set dimension so smaller that the uncertainty methods do not work. It includes cases where the codimension of the future invariant set is approximately equal to or greater than one. We stress that these methods are general and can be used in phase spaces of any dimension. And since they allow, in principle, the computation of arbitrarily small dimensions, these techniques should be useful to study how chaotic scattering comes about as a system parameter is varied \[\textnormal{[7]}\]. In particular, it may be interesting in investigations about routes to chaos in three dimensional scattering.

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Figure 1: $C_n$ for $R = 0.37$: $C_1$ (light grey), $C_2$ (grey), $C_3$ (dark grey) and $C_4$ (black).

Figure 2: $\ln K_n$ for $R = 0.37$: $n = 5$ (least inclined curve), $n = 6$, $n = 7$ and $n = 8$ (most inclined curve).

Figure 3: Estimates of the dimension of $\bigcap_{m=1}^{\infty} \mathcal{C}_m$ as a function of $R$: $D_H$ (boxes), $D_c$ (stars) and $D_s$ (triangles). The size of the boxes, stars and triangles corresponds approximately to the statistical uncertainty of the dimension.

Figure 4: Portrait of the basins of the tetrahedron scatterer for: (a) $R = 0.48$; (b) $R = 0.37$. The initial conditions were chosen on a grid of $400 \times 400$, on the plane $P$. Regions in black and white correspond to orbits that escape to $x \to +\infty$ and $x \to -\infty$, respectively. Regions in grey correspond to orbits not scattered.
