Topological Characterization of Spatial-Temporal Chaos

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We introduce a new technique based on algebraic topology for quantifying spatio-temporally chaotic dynamics. The technique is illustrated using the FitzHugh-Nagumo equations.

INTRODUCTION

It is well established both numerically and experimentally that nonlinear systems involving diffusion, chemotaxis, and/or convection mechanisms can generate complicated time-dependent patterns. Specific examples include the Belousov-Zhabotinskii reaction, the oxidation of carbon-monoxide on platinum surfaces, slime mold, and excitable media. Because this phenomenon is global in nature, obtaining a quantitative mathematical characterization that to some extent records or preserves the geometric structures of the complex patterns is difficult. In this paper we propose a new technique aimed at this problem. More precisely we show that using algebraic topology, in particular homology, we can measure Lyapunov exponents that imply the existence of spatial-temporal chaos and suggest a tentative step towards the classification and/or identification of patterns within a particular system.

Since the emphasis of this paper is on the presentation of the technique, we have chosen to work with a well-studied system in two dimensions. However, the technique is system and dimension independent. Consider the particular form of the FitzHugh-Nagumo equations

$$\begin{aligned} u_t &= \Delta u + \epsilon^{-1} u(1-u)(u - \tfrac{v+\gamma}{\alpha}) \\ v_t &= u^3 - v \end{aligned} \tag{1}$$

with Neumann boundary conditions on the domain $\Omega = [0, 80] \times [0, 80]$. In all of what follows we fix $\alpha = 0.75$, $\gamma = 0.06$ and vary the parameter ϵ.

We numerically solved (1) using code of Barkley [1–3]. The dynamics of the patterns of the variable u is most easily observed by producing a movie. Since the FitzHugh-Nagumo system is meant to model an excited media, a standard technique is to threshold the data. In particular, a point (x_i, y_j) is declared to be *excited* at time t_k if $u(x_i, y_j, t_k) \geq 0.9$ and is shaded light gray. The dark gray pixels correspond to the quiescent region ($u \leq 0.1$), and black corresponds to the reaction zone ($0.1 < u < 0.9$). Figure 1 shows some snapshots of such a movie.

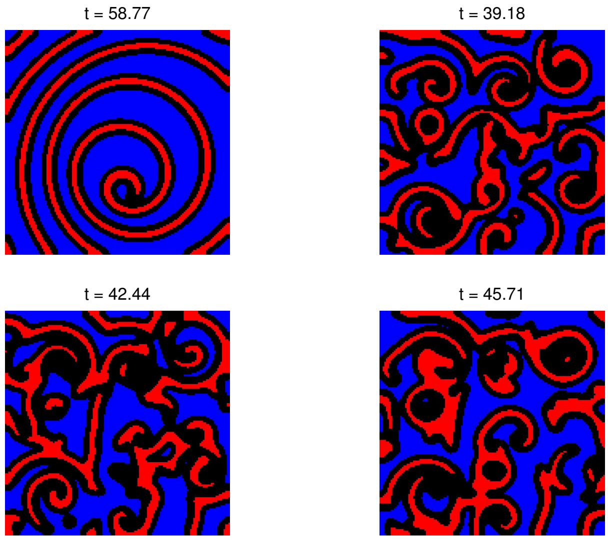

FIG. 1: Wave patterns generated by (1). The light gray (red) region corresponds to excited points ($u \geq 0.9$), dark gray (blue) to the quiescent region ($u \leq 0.1$), and black to the reaction zone ($0.1 < u < 0.9$). In the top left figure we used $1/\epsilon = 14$ (in which case the pattern consists of a single spiral wave), and in the other three $1/\epsilon = 12$ was used. Sampling times are shown.

An important point is that this thresholded movie provides the input data for the technique we are about to describe. Thus, in principle this method can be applied in exactly the same manner to a thresholded movie produced from experimental as opposed to numerical data.

EXCITED SPACE-TIME GEOMETRY

As indicated above, our goal is to understand and quantify the spatial and temporal geometry of the patterns generated by (1). For this purpose it is useful to think of the excited media as a subset of $\Omega \times [0, \tau]$ where the third direction represents time and τ is the length of the movie. To be more precise, as indicated above, the excited media is defined to be the set of light gray pixels.

Since we are now working with a subset of $\mathbb{R}^3$, we view each pixel as a voxel, i.e. a three dimensional cube. Thus the excited media is now represented by a set E in $\mathbb{R}^3$ consisting of a finite union of voxels. If we let $V_{i,j,k}$ denote the voxel corresponding to the pixel (x_i, y_j) for the k^{th} frame of the movie, then $E = \{V_{i,j,k} \mid u(x_i, y_j, t_k) \geq 0.9\}$. Observe that viewed as a finite collection of voxels E provides for a combinatorial representation of the excited media. At the same time we can consider E to be a subset of $\Omega \times [0, \tau]$ that approximates the geometry of the excited media in both space and time.

In the next section we will discuss how algebraic topology can be used to measure the complexity of the geometry of the patterns. Before doing so, recall that we are trying to quantify both the spatial structures of the patterns and how they change with time. Conceptually, the simplest way to do this is to compute the topology of each frame of the movie and then measure the change. Unfortunately, this approach cannot measure the global interactions between the fronts of the patterns that occur at different points in time. The other extreme is to consider the topology of E itself. However, if the dynamics of the original system is chaotic, then it is recurrent, and hence for large τ much of the structure should be redundant.

For these reasons we introduce the notion of a *time block* $T_{n,b} := \{V_{i,j,k} \in E \mid n \leq k \leq n + b\}$. Observe that $T_{n,0}$ represents the n^{th} frame of the movie. For fixed b, $T_{n,b}$ captures the geometry of the pattern interactions over a given time range. We can see how this evolves by studying a sequence of time blocks of the form $\{T_{a(m-1),b} \mid m = 1, 2, \ldots, M\}$.

COMPUTING HOMOLOGY

Algebraic topology is employed to measure the topological complexity of the excited patterns. In particular we make use of the fact that to any topological space X one can assign homology groups $H_i(X)$, $i = 0, 1, 2, \ldots$ (see [4]). Clearly, this is not the venue in which to discuss homology theory, however there are two issues that need to be considered: the geometric information that these groups contain and how they can be computed.

Returning to the very restricted setting of this paper, for any time block $T_{n,b}$, $H_i(T_{n,b}) \cong \mathbb{Z}^{\beta_i}$ where $\mathbb{Z}$ is the group of integers. The nonnegative integer β_i is called the i^{th} Betti number of $T_{n,b}$. A simple argument shows that $\beta_i = 0$ for $i \geq 3$. The remaining Betti numbers give the following geometric information: β_0 equals the number of connected components that make up the space, β_1 indicates the number of tunnels, and β_2 corresponds to the number of enclosed cavities.

To compute the Betti numbers we make use of the fact that homology remains invariant under scaling and translation. For each $V_{i,j,k} \in E$ define $Q_{i,j,k} := [i, i+1] \times [j, j+1] \times [k, k+1]$. Let $\mathbb{T}_{n,b} := \{Q_{i,j,k} \mid V_{i,j,k} \in T_{n,b}\}$. Then $H_i(\mathbb{T}_{n,b}) \cong H_i(T_{n,b})$. Because $\mathbb{T}_{n,b}$ is the union of unit cubes defined in terms of an integer lattice, it is a *cubical set*. Algorithms for the computation of the homology of cubical sets can be found in [5, 6], and their implementation can be found at [7].

BENCH MARK RESULTS

As was mentioned in the introduction we will use the existence of a positive Lyapunov exponent to conclude the existence of spatial-temporal chaos. Since our approach is new, we feel it is important to compare it against the following more standard Lyapunov exponent computation.

Consider a time series $\{s_n \in \mathbb{R} \mid n = 0, \ldots, N\}$ obtained from some nonlinear dynamical system. We make use of the following algorithm (see [8]) to compute the maximal Lyapunov exponent. Let

$$S(k) = \frac{1}{N} \sum_{n_0=1}^{N} \ln \left[\frac{1}{|B_{n_0}|} \sum_{y_n \in B_{n_0}} |y_{n_0+k} - y_{n+k}| \right] \quad (2)$$

where $y_n = (s_n, s_{n+1}, \ldots, s_{n+d-1})$ is a vector in the d-dimensional reconstructed space, and B_{n_0} is a η-neighborhood of y_{n_0}. If $S(k)$ exhibits a linear increase with identical slope for k greater than a given k_0 and for a reasonable range of η, then this slope can be taken to be an estimate for the maximal Lyapunov exponent.

Returning to the system being considered in this paper, we fixed (i, j) such that $(x_i, y_j) = (11.4286, 21.4286)$ and produced a time series $\{u(x_i, y_j, t_k) \mid k = 0, \ldots, K\}$ by numerically solving (1). Applying the above mentioned method, using the TISEAN package [9], we obtained estimates for the maximal Lyapunov exponents as indicated in Figure 2. We obtained essentially the same result for several grid points (x_i, y_j).

From these computations we conclude that, for those values of ϵ at which the maximal Lyapunov exponent is positive, (1) exhibits temporally chaotic dynamics. However, it is important to observe that this computation completely ignores the spatial complexity of this system.

TOPOLOGICAL RESULTS

To produce a time series that incorporates the spatial structure, we computed the Betti numbers of various $\mathbb{T}_{n,b}$. More precisely, we computed $\{H_*(\mathbb{T}_{10(m-1),1000}) \mid m = 1, 2, \ldots, 10{,}000\}$ and hence obtained the Betti numbers $\beta_i(m)$ for $H_i(\mathbb{T}_{10(m-1),1000})$.

Our first observation was that $\beta_2(m) \equiv 0$ and that $\beta_0(m)$ is piece-wise constant taking on a limited number of fairly small values. However, the time series

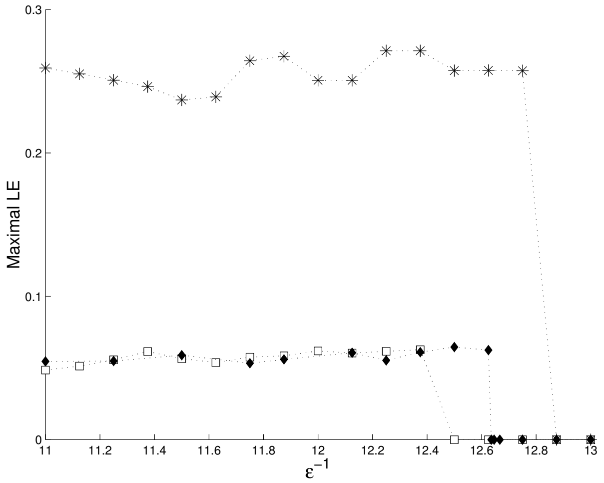

FIG. 2: Maximal Lyapunov exponents, as a function of $1/\epsilon$, from the time series generated by fixing the point $(x_i, y_j) = (11.4286, 21.4286)$ in the domain and solving (1) for 30,000 time steps (stars). The diamonds and the squares are the Lyapunov exponents of time series of Betti numbers $B_{(10,1000)}$ computed using different initial conditions. For points where (2) did not show a clear linear increase, the Lyapunov exponents were set to zero.

$B_{(10,1000)} := \{\beta_1(m) \mid m = 1, 2, \ldots, 10{,}000\}$ proved to be quite interesting. Typical plots for various values of ϵ are indicated in Figure 3.

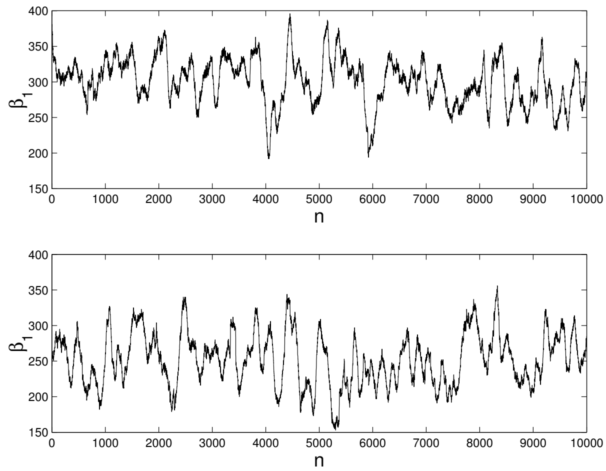

FIG. 3: Plot of the time series $\{\beta_1(m) \mid m = 1, 2 \ldots, 10{,}000\}$ of Betti numbers, for $1/\epsilon = 11.5$ (top) and $1/\epsilon = 12$ (botton).

Using the method described in the previous section, we computed the maximal Lyapunov exponent for the time series $B_{(10,1000)}$. Figure 2 provides a plot of the maximal Lyapunov exponent as a function of $1/\epsilon$. There are three important points to be made. The first is the near agreement between the ranges of ϵ on which the maximal Lyapunov exponents are positive and zero. This suggests computing the Lyapunov exponent from homological data is an acceptable approach. The second is that we can now conclude that the system exhibits *spatial-temporal chaotic* behavior. This follows from the fact that this chaotic time series is defined in terms of the Betti numbers β_1, since $\beta_1(m) \neq 0$ implies that the topology of $T_{m,1000}$ is non-trivial and $\beta_1(m) \neq \beta_1(m')$ implies that the topology of $T_{m,1000}$ differs from that of $T_{m',1000}$. The fact that the Lyapunov exponent from the homological data goes to zero sooner than that computed from a single point can be explained by the fact that the latter measures temporal chaos only and the homological data measures spatial structures as well. Thus it is possible that the spatial-temporal chaos disappears before the purely temporal chaos does. The third point is the observation that, as in the case of a fixed (x_i, y_i), the maximal Lyapunov exponent appears to be essentially constant as a function of $1/\epsilon$ until it drops to zero. This implies that Lyapunov exponents do not provide a useful measurement for characterizing the value of ϵ at which the simulation is being performed. On the other hand plotting the average value of β_1 as is done in Figure 4 results in an almost monotone curve. Thus, in principle by computing the average of the Betti numbers we can determine the parameter value ϵ at which the simulation is being performed. Computing the average of the Betti numbers is much cheaper than computing the maximal Lyapunov exponent, because, as is indicated in Figure 4, it can be computed with a shorter time series.

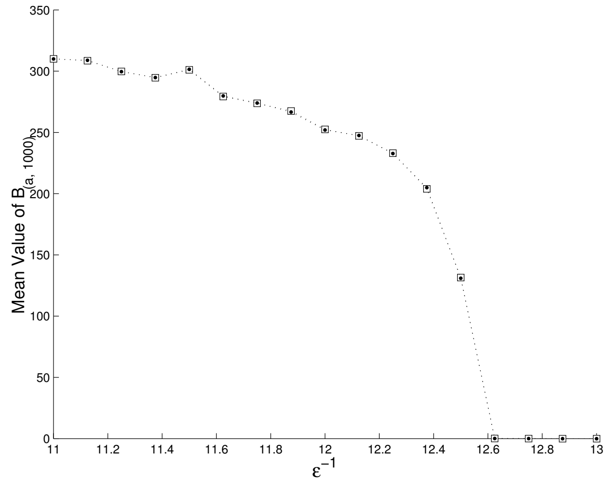

FIG. 4: Mean values of the time series $B_{(10,1000)}$ used to compute the Lyapunov exponents in Figure 2 (squares), and the mean values of the time series $B_{100,1000} = \{\beta_1(m) \mid m = 1, 2, \ldots, 100\}$ (dots), as functions of $1/\epsilon$.

COMPUTATIONAL COMMENTS

The above mentioned results depend upon the choice of b and a for the time blocks $T_{a(m-1),b}$. For the examples presented in this paper $a = 10$ and $b = 1000$ seems to be a satisfactory solution. However, we cannot at this point in time suggest useful heuristics for a particular choice. The principal issues are as follows. If b is small, then β_1 is small. Since the Betti numbers are integers this implies that we do not have enough significant figures to compute Lyapunov exponents. If b is large then the cost of computing $H_1(\mathbb{T}_{n,b})$ becomes impractical. Since the system is chaotic, choosing a too large results in decorollation of subsequent Betti numbers. On the other hand if a is too small the local change in the Betti numbers is insignificant. It should be noted that for computing the mean value of the Betti numbers we were able to use $a = 100$ because strong correlation is not necessary.

The typical running time for generating one of the 10,000 point time series is about 12 CPU hours or 52 wall time hours in a Beowulf cluster with 30 Pentium 4, 2.4GHz processors. On the other hand each data point in Figure 4 (using 100 points time series) requires only 0.12 CPU hours or 0.5 wall time hours.

The homology algorithm [6] used for these computations takes advantage of the fact that homology can be determined by means of local spatial computations. The code makes use of a binary tree data structure to store the data into memory, and this data structure is implemented in such a way that it is not necessary to read the whole data set into memory at once. In this way it is possible to compute with data sets that do not fit into memory. This feature is of particular importance in higher dimensional problems.

The numerical method used to solve (1) consists of a semi-implicit finite difference algorithm, on a equally spaced grid $\{(x_i, y_j) \mid i, j = 0, \ldots, N\}$ covering Ω. We used $N = 280$ in the computations of Lyapunov exponents for a fixed grid point (x_i, y_j), and $N = 140$ in all the other computations. This algorithm uses the fact that if the solution at a point (x_i, y_j) is small, it will remain small in the next step to speed up the algorithm. So there is a small numerical parameter δ such that $u(x_i, y_j, t_{k+1}) = 0$ if $u(x_i, y_j, t_k) < \delta$. A implementation of this algorithm, EZ-Spiral, can be found at [3]. In this paper we use a modified version of this program. We used $\delta = 10^{-4}$, and the time step $\Delta t = 0.0653$. Given the coarse grid (with $N = 140$) this method can not be guaranteed to accurately solve (1). On the other hand sample calculations at slightly finer grids did not result in qualitatively different results. In part this is due to the fact that homology is fairly robust with respect to small perturbations. Therefore, small numerical errors are not expected to lead to changes in the homology groups.

CONCLUSION

We have proposed the use of computational homology to measure the spatial-temporal complexity of patterns. In addition we have shown that this technique can be used as a means of discriminating different patterns at different parameter values. Furthermore, although it is computationally expensive to measure spatial-temporal chaos, the computations necessary to do such discrimination are relatively cheap. One important feature of the proposed method is that it is fairly automated and can be applied to experimental data.

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