Computational Topology and Dynamics

I. Topological Characterization of Spatial-Temporal Chaos

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FitzHugh-Nagumo equations

\[ u_t = \Delta u + \epsilon^{-1} u(1 - u)(u - \frac{v + \gamma}{\alpha}) \]
\[ v_t = u^3 - v. \]

on the rectangular domain \( \Omega = [0,80] \times [0,80] \) with parameter values \( \alpha = 0.75, \gamma = 0.06, \) and varying \( \epsilon > 0. \)

Depending on \( \epsilon, \) this system demonstrates relatively simple spiral wave patterns (\( \epsilon = 1/14 \)) and complicated spatial-temporal patterns (\( \epsilon = 1/12 \)).
\( \epsilon = \frac{1}{14} \)

\( t = 58.77 \)

\( \epsilon = \frac{1}{12} \)

\( t = 39.18 \)
Is there a way to quantify the spatial-temporal dynamics by directly measuring the patterns generated by the system?

First we extract the excited region by thresholding the data, i.e. identify the red pixels.

The thresholded pattern is realized by a set of cubes in space-time— a **combinatorial** representation.

**Numerical simulation:** finite differences on a rectangular grid

**Experimental data:** movies of pixelated images
Gray-Scott equations

\[ u_t = d_1 u_{xx} - uv^2 + F(1 - u) \]
\[ v_t = d_2 v_{xx} + uv^2 - (F + k)v \]

on \([0, 1.6]\) with parameter values \(d_1 = 2 \times 10^{-5}\), \(d_2 = 10^{-5}\), \(F = 0.035\), and \(k = 0.05632\).

This system displays complicated time-dependent patterns at these parameter values. [Nishiura, Ueyama]
Gray-Scott simulation in space-time
**Idea:** measure the topological characteristics of the pattern, i.e. the number of components, holes, enclosed cavities...

[1] Measure the change in topology between time slices—this method will not measure the global interactions between fronts/waves that occur at different points in time. Also, the topology of one time slice is often too simple.

[2] Compute the topology of the entire excited region in spacetime over a long time interval— if the system is chaotic, then much of this structure should be redundant.

[3] Study the evolution of the topology over a sliding time window.
Time blocks

Let $V_{i,k}$ denote the 2-d cube centered at $(x_i, t_k)$.

Then the excited region is $E = \{V_{i,k} \mid v(x_i, t_k) \geq 0.23\}$.

Define $T_{m,b} = \{V_{i,k} \in E \mid m \leq k \leq m + b\}$ which captures the geometry of the pattern over a fixed time range.

We will study the evolution of the topology over a sequence of time blocks $T_{a(n-1),b}$ for $n = 1, \ldots, N$. 
$T_{1500,2000}$ for Gray-Scott, $\beta_0 = 3, \beta_1 = 20$
Betti numbers

To every topological space $X$, one can assign a sequence of homology groups $H_i(X, \mathbb{Z})$.

In this setting of full cubical complexes, $H_i(T_{a(n−1),b}, \mathbb{Z}) \equiv \mathbb{Z}^{β_i}$. The integers $β_i \geq 0$ are the **Betti numbers** of the time block.

We then generate a time series from each Betti number $β_i(n)$.

For $d$-dimensional complexes, $β_i = 0$ for all $i \geq d$.

http://www.math.gatech.edu/~chomp [K., Pilarczyk]
Homology is a tool to measure connectivity and holes in a topological space.

How can we distinguish (computationally) between a cylinder, sphere, and torus?

Topological space $\xrightarrow{\text{Combinatorial description}}$ Cellular decomposition $\xrightarrow{\text{e.g. triangles or cubes}}$ (linear) Algebra
\[ \partial_1 e = A + B \]
\[ \partial_2 S = e + f + g + h \]

\[ \partial_1(e + f + g + h) = \]
\[ A + B + B + C + C + D + D + E = A + 2B + 2C + 2D + E = A + E \]

\[ \partial_1(e + f + g + h) = \]
\[ A + B + B + C + C + D + D + A = 2A + 2B + 2C + 2D = 0 \]

so \[ \partial_1 \partial_2 S = 0 \]
An $n$-chain is a sum of $n$-dimensional cells.

A cycle is a chain $C$ whose boundary $\partial C = 0$.

A boundary is a chain $B$ for which there is a chain $C$ such that $\partial C = B$.

Two cycles $C$ and $D$ are homologous if they differ by a boundary, i.e. there exists a chain $E$ such that $C = D + \partial E$.

$I$, $J$, and $K$ are cycles. $K$ is a boundary, but $I$ and $J$ are not. $I$ and $J$ are homologous, but $K$ is not homologous to $I$ or $J$. 
The set of all $n$-cycles $Z_n$ and the set of all $n$-boundaries $B_n$ are vector spaces over $\mathbb{Z}_2$.

Since $\partial^2 = 0$, we have $B_n \subset Z_n$.

The homology is then defined by $H_n = Z_n / B_n$.

The homology of a space is a sequence of vector spaces.

A choice of basis elements for $H_n$ are called $n$-generators.
The dimensions of the vector spaces $H_n$ are the Betti numbers $\beta_n$.

The Betti numbers represent the number of non-homologous cycles which are not boundaries = \textit{“$n$-dimensional holes”}.

In 3-dimensional complexes made from full 3-dimensional cubes:

the zeroth Betti number, $\beta_0$, counts the number of connected components,
the first Betti number, $\beta_1$, counts the number of tunnels, and
the second Betti number, $\beta_2$, counts the number of enclosed cavities.
\[\beta_0 = 1\]
\[\beta_1 = 1\]
\[\beta_n = 0 \text{ for } k \geq 2\]

\[\beta_0 = 1\]
\[\beta_1 = 0\]
\[\beta_2 = 1\]
\[\beta_n = 0 \text{ for } k \geq 3\]

\[\beta_0 = 1\]
\[\beta_1 = 2\]
\[\beta_2 = 1\]
\[\beta_n = 0 \text{ for } k \geq 3\]
The Betti numbers are:

\[ \beta_0 = 1 \]
\[ \beta_1 = 1059 \]
\[ \beta_2 = 0 \]

This space is connected, has no enclosed cavities, and has 1059 tunnels.
First Betti number of $T_{300(n-1),10000}$ for Gray-Scott

Maximal Lyapunov exponent was computed to be 0.037 using TISEAN. [Heggar, Kantz, Schreiber].
Time series - Phase space reconstruction

Given as sequence \( \{s_m \mid m = 1 \ldots M\} \) of scalars.

**Idea:** \( s_m \) is a scalar measurement at \( x(t_m) \) where \( x(t) \) is an orbit of some dynamical system.

Pick an **embedding dimension** \( n \) and a **lag/delay** \( \tau \) in \( \mathbb{Z}^+ \).

\[
y_m = (s_{m-(n-1)\tau}, s_{m-(n-2)\tau}, \ldots, s_{m-2\tau}, s_{m-\tau}, s_m) \in \mathbb{R}^n
\]

Think of \( \{y_m\} \) as a finite orbit in \( \mathbb{R}^n \). Note there are **finitely many** states, \( M - (n-1)\tau \).
Theorems [Takens] [Sauer, Yorke] If \( \{s_n\} \) is a continuous measurement of a dynamical system, then generically for \( n \) large enough, there is a injective map from PSR into the real system.

Idea: Measure dynamical quantities on PSR to estimate them for the real system.

Problems: Finiteness, noise, and Betti numbers are discrete.

Have really measured the underlying (infinite-dimensional) system?
Measures of chaos

**Maximal Lyapunov exponent:** measure of sensitive dependence on initial conditions.

$$
\lambda_i = \lim_{t \to \infty} \frac{1}{t} \log \left| \frac{dl_i}{dr} \right|
$$

so

$$
|\Delta x(t)| \sim e^{\lambda t} |\Delta x(0)|
$$

**Entropy:** measure of randomness / amount of information in a finite system.

$$
E = - \sum_{i}^{N} p_i \log(p_i) \\
\bar{E} = \frac{E}{\log(N)}
$$
Time blocks for FitzHugh-Nagumo

Let $V_{i,j,k}$ denote the 3-d cube centered at $(x_i, y_j, t_k)$.

Then the excited region is $E = \{V_{i,k} \mid u(x_i, y_j, t_k) \geq 0.9\}$.

Define $T_{m,b} = \{V_{i,j,k} \in E \mid m \leq k \leq m + b\}$ which captures the geometry of the pattern over a fixed time range.

We will study the evolution of the topology over a sequence of time blocks $T_{a(n-1),b}$ for $n = 1, \ldots, N$. 
First Betti number of $T_{10(n-1),1000}$ for FitzHugh-Nagumo

$\epsilon = 1/11.5$ and numerical simulations used EZ-spiral. [Barkley]
Sample maximal Lyapunov exponent calculation

Slop = 0.053311, eps = 11.75
Observations

There is near agreement on the range of $\epsilon$ values for which the Lyapunov exponent is positive.

The fact that the LE from homological data goes to zero sooner than that from a single point can be explained by the fact that the latter measures temporal chaos only and the homological data measure spatial structures as well. Spatial-temporal chaos disappears before the purely temporal chaos does.

The Lyapunov exponent is essentially constant in $\epsilon$ before dropping to zero, so they are not a useful measurement for parameter identification.
Mean of first Betti number for FitzHugh-Nagumo
Observations

In principle we can determine the value of $\epsilon$ from the mean value of the first Betti number.

Moreover, this is a much cheaper computation since many fewer time blocks are needed to compute the mean than to compute the Lyapunov exponent.
Bar-Eiswirth equations

\[ u_t = \Delta u + \epsilon^{-1} u(1 - u)(u - \frac{v + \gamma}{\alpha}) \]
\[ v_t = f(u) - v. \]

on the rectangular domain \( \Omega = [0, 450] \times [0, 450] \) with

\[ f(u) = \begin{cases} 
0 & 0 \leq u \leq \frac{1}{3} \\
1 - 6.75u(u - 1)^2 & \frac{1}{3} \leq u \leq 1 \\
1 & u \geq 1
\end{cases} \]
Can we distinguish between the eventual chaotic patterns? [Sandstede and Scheel] with EZSPIRAL by [Barkley]
2D reversible Gray-Scott equations

\[ u_t = D_u \Delta u + a(1 - u) - buv^2 + cv^3 \]
\[ v_t = D_v \Delta v - (a + d)v + buv^2 - cv^3 + cp \]
\[ p_t = D_p \Delta p - ap - cp + dv \]

on the rectangular domain \( \Omega = [0, 128] \times [0, 128] \) with Neumann boundary conditions and

\[ D_u = 2.0 \times 10^{-5} \quad D_v = 10^{-5} \quad D_p = 10^{-6} \]
\[ a = 0.015 \quad b = 1 \quad c = 10^{-3} \quad d = 0.058 \]
Can we detect chaos from these patterns?
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