Computational Topology and Dynamics

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Homology of Nodal Domains

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Computational Homology Project

Computational Conley Theory

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Verified Homology of Nodal Domains

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Material microstructures -- binary alloys
Pb-Sn

Courtesy P. Voorhees (Northwestern)

[Kammer and Voorhees 2006]
Rayleigh-Benard convection
Spiral defect chaos -- RBC

Courtesy M. Schatz (Georgia Tech)

[Krishan, Gameiro, Mishaikow, Schatz 2006]
Cahn-Hilliard-Cook equation

\[ u_t = -\Delta (\epsilon^2 \Delta u + f(u)) + \sigma \cdot \xi \]

\( u \) is a phase variable and total mass is 0.

\( t / t_e = 0.000, \|U - \mu\|_\infty = 0.00010 \)
FitzHugh-Nagumo equation

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

\[ v_t = u^3 - v. \]

\[ \Omega = [0, 80] \times [0, 80] \quad \gamma = 0.06 \quad \alpha = 0.75 \]

\[ \epsilon = 1/14 \quad \epsilon = 1/12 \]
Homology of Cahn-Hilliard microstructures

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

\[ \beta_0 = 26 \]
\[ \beta_1 = 4 \]
Cubical approximation

dark: \( \beta_0 = 11 \)
\( \beta_1 = 3 \)

\( \beta_0 = 9 \)
\( \beta_1 = 4 \)
Nodal domains and accuracy of homology

- The patterns and microstructures of interest are nodal domains, i.e. sublevel sets of smooth functions, and hence are manifolds generically—though not at all times.

- Often the patterns involve some stochasticity or chaos, and we are interested in typical behavior.

- To study the homology of nodal domains computationally, some finite discretization must be introduced.

- How can we be sure that the computations provide the correct homology for the underlying nodal domain? Is it enough to choose a sufficiently fine discretization? Can we determine the discretization size a-priori?
Time series of Betti numbers

In all three settings:

(1) Cahn-Hilliard simulations of material microstructures,
(2) spatial-temporal chaos in FitzHugh-Nagumo,
(3) experimental spiral defect chaos

we find information from a direct topological study of the patterns that can be difficult to obtain or not noticed otherwise.

The main idea is to study the Betti numbers as a time series of data by thresholding the data on a finite grid to extract a cubical approximation to the pattern. Note that rectangular grids arise naturally in images and numerical solutions to PDE’s.
What is the goal?

CHC is one of several phenomenological models -- would like a quantitative measurement to make comparisons with experiments and between models.

SDC in RBC is easier to study experimentally than numerically, but then your data is a movie of a pattern of some observable, not values for fluid velocity. How do we quantitatively compare different experiments?

Spatial-temporal chaos is difficult to define and quantify precisely. The dynamics can be high-dimensional.

Computing Betti numbers is a huge reduction in information, is there any info left?
Cahn-Hilliard-Cook simulations

\[ \epsilon = 0.005 \]
\[ \sigma = 0 \]
\[ \sigma = 0.01 \]

\[ N^+(t) = \{ x \in \Gamma \mid u(x, t) \geq 0 \} \]
\[ N^-(t) = \{ x \in \Gamma \mid u(x, t) \leq 0 \} \]

[Gameiro, Mischaikow, Wanner 2005]
Cahn-Hilliard-Cook averages

Average of 500 simulations with random initial conditions for various levels of noise.

The non-monotone curves for CH are not boundary effects nor can they be seen with Euler characteristic.

[Gameiro, Mischaikow, Wanner 2005]
Gray-Scott equations

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

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
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 $\mathbb{T}_{m,b} = \{V_{i,k} \in E \mid m \leq k \leq m + b\}$ 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 $\mathbb{T}_{a(n-1),b}$ 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, \(H_i(\mathbb{T}_{a(n-1),b}, \mathbb{Z}) \equiv \mathbb{Z} \beta_i\). The integers \(\beta_i \geq 0\) are the **Betti numbers** of the time block.

We then generate a time series from each Betti number \(\beta_i(n)\).

For \(d\)-dimensional complexes, \(\beta_i = 0\) for all \(i \geq d\).
First Betti number of $\mathbb{T}_{300(n-1),10000}$ for Gray-Scott

Maximal Lyapunov exponent was computed to be 0.037 using TISEAN. [Heggar, Kantz, Schreiber].
**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 $n = 1, ..., N$. 
FitzHugh-Nagumo equation

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

\[ \Omega = [0, 80] \times [0, 80] \quad \gamma = 0.06 \quad \alpha = 0.75 \]

\[ \epsilon = 1/14 \quad \epsilon = 1/12 \]
First Betti number of $\mathbb{T}_{10(n-1),1000}$ for FitzHugh-Nagumo

$\epsilon = 1/11.5$ and numerical simulations used EZ-spiral. [Barkley]
Maximal Lyapunov exponent for $\beta_1$ time series for FN
Observations

The Lyapunov exponent is constant so not a good measurement to do parameter estimation.

The Lyapunov exponent for the Betti number time series drops to 0 before the time series of values at a fixed point in the domain.
Mean of first Betti number for FitzHugh-Nagumo

![Graph showing the mean value of B_1(\varepsilon, 1000) vs. \varepsilon^{-1}}
Time series of Betti numbers for SDC in RBC

[Krishan, Gameiro, Mischaikow, Schatz 2006]

[Krishan, Kurtuldu, Schatz, Gameiro, Mischaikow, Madruga 2007]

More cold downflow components and hot upflow has more holes. Not observed using standard statistics.
Asymmetry suggests breakdown in Boussinesq approximation.
Cubical approximation

dark: $\beta_0 = 11$
$\beta_1 = 3$

$\beta_0 = 9$
$\beta_1 = 4$
Errors due to discretization

Discretization errors in homology computations can occur at all levels of refinement.

In time-dependent nodal domains this effect occurs when the topology changes and is therefore more-or-less unavoidable.

From *Computational Homology* by Kaczynski, Mischaikow, and Mrozek 2003.
A probabilistic analysis

In the setting of evolutionary PDE like CHC, there is an element of stochasticity introduced via explicit noise in the PDE and/or random initial conditions.

So we can think of the solution at some fixed time as a random Fourier series of the form:

\[ u(x, \omega) = \sum_{n=0}^{\infty} \alpha_k \cdot g_k(\omega) \cdot \varphi_k(x) \]

where \( \alpha_k \) are real constants, \( g_k \) are independent random variables on a common probability space, and \( \varphi_k \) are a complete orthogonal set of basis functions.

Mischaikow and Wanner (2007) give estimates on the probability that the homology of a cubical approximation from an equidistant grid is the same as the homology of the nodal domain.
1d trigonometric polynomials

\[ u(x, \omega) = \sum_{k=1}^{K} (g_{2k}(\omega) \cdot \cos(2\pi kx) + g_{2k-1}(\omega) \cdot \sin(2\pi kx)) \]

**Theorem** [Mischaikow and Wanner (2007)] Suppose \( Q^+ \) is the cubical approximation of \( N^+ \) determined by \( M \) equally-spaced points in \( \Gamma = [0, 1] \). Then the probability that \( H_*(N^+) = H_*(Q^+) \) satisfies

\[
P \geq 1 - \frac{2\sqrt{3}\pi^2}{135} \cdot \frac{K^3}{M^2} + O \left( \frac{1}{M^4} \right)
\]

so that asymptotically \( M \sim K^{3/2} \) to obtain the correct homology.
This asymptotic estimate is sharp even for small values of $K$.

Computed values for 95% correctness

Predicted values for 95% correctness

Inverse of expected minimal distance between zeroes

Expected number of zeros
Application to 1d linear Cahn-Hilliard

Solutions to the linearized Cahn-Hilliard equation with initial data in a Gaussian random field have the form

\[ u(x, \omega) = \sum_{k=1}^{K} e^{\lambda_k t} \cdot \alpha_k \cdot (g_{2k}(\omega) \cdot \cos(2\pi kx) + g_{2k-1}(\omega) \cdot \sin(2\pi kx)) \]

In this setting, the probability estimate becomes

\[ P \geq 1 - \frac{\pi^2}{6\epsilon^3 M^2} \cdot C \left( \frac{t}{\epsilon^2} \right) + O \left( \frac{1}{M^4} \right) \]

where the function \( C \) is \( \epsilon \)-independent, decreasing.
Application to 1d linear Cahn-Hilliard

Linear

Nonlinear

\[ M = 25 \quad M = 50 \quad M = 100 \]
2d trigonometric polynomials

\[ u(x, \omega) = \sum_{k, \ell = 0}^{K} \left( g_{k, \ell, 1}(\omega) \cos(2\pi k x_1) \cos(2\pi \ell x_2) + g_{k, \ell, 2}(\omega) \cos(2\pi k x_1) \sin(2\pi \ell x_2) \right. \]
\[ \left. + g_{k, \ell, 3}(\omega) \sin(2\pi k x_1) \cos(2\pi \ell x_2) + g_{k, \ell, 4}(\omega) \sin(2\pi k x_1) \sin(2\pi \ell x_2) \right) \]

**Theorem [Mischaikow and Wanner (2007)]** Suppose \( Q^+ \) is the cubical approximation of \( N^+ \) determined from an equi-spaced grid of size \( M \). Then the probability that \( H_*(N^+) = H_*(Q^+) \) satisfies

\[ P \geq 1 - \frac{1067\pi^2}{18M^2} \cdot \frac{1}{900} \cdot \left( 46K^2 + 51K - 7 \right)^2 + O \left( \frac{1}{M^3} \right) \]

so that asymptotically \( M \sim K^2 \) to obtain the correct homology.

Not so easy to see that this estimate is sharp for small \( K \).
Verified homology computation

In [Day, K., Wanner (2009)], we develop an algorithm to compute the homology of the nodal domain of a function \( f : [0, 1]^2 \to \mathbb{R} \) in a verified way, i.e. the algorithm will either return the correct homology or stop when a preset maximum level of refinement is reached.

For values of \( K = 2, \ldots, 16 \) we computed the correct homology of the nodal domains of between 300 and 1000 random trig polynomials. We then calculated the homology obtained from equi-spaced grids of sizes \( M = 4, \ldots, 4096 \) to obtain for each value of \( K \) the probability of a correct homology computation as a function of \( M \).
\[ \mathcal{E}(t, M_h, M_{\text{max}}) = \{ u_0 : \text{verification with size } M \leq M_{\text{max}} = 50,000 \text{ is possible, and the Betti numbers are correctly computed via the } M_h\text{-grid} \} \]
Using interval arithmetic for all floating point calculations, the basic algorithm is as follows:

(0) Subdivide into some initial equi-spaced grid.

(1) For each box determine the signs at the vertices.

(2) Try to verify that the nodal line cuts through the box in the simplest way, i.e. homeomorphic to

(3) If unsuccessful subdivide the box by bisection and repeat.

(4) Fail if maximum subdivision is attained.
Conclusions

Computing a time series of Betti numbers directly from patterned images from experiment or simulation can give new insight into dynamics of systems with complicated spatial and temporal dynamics.

One can estimate how fine a cubical approximation is needed to compute homology of nodal domains with a specified confidence depending on computable properties of the function.

It is often possible to correctly compute the homology of a nodal domain with verified numerical techniques.
Thank You!

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