Homology of the Gray-Scott Model of Reaction-Diffusion

A Thesis

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Introduction

The study of pattern formation is incredibly diverse and certainly one of the most compelling aspects of nonlinear phenomenology. Scientists from many disciplines have analyzes patterns on the scale of the entire universe all the way down to the microscopic[1]. Just a cursory glance at the structure of a wind-swept sand dune, a snowflake, or even our own galaxy reveals something interesting. Observation of these patterns might lead a scientist to ask what causes the pattern and wonder why there are patterns at all. This question gets complicated quickly because whether it's God in the patterns or the result of a non-equilibrium universe, there is still the question of what it means to have "structure" or "complexity" or to be "interesting".

Fortunately, the theoretical model of pattern formation discussed here allows me to sidestep all of these questions while focusing primarily on the method of analysis. There are many mathematical tools available to help understand pattern formation but applying new methods and techniques is essential, especially when analyzing a tired system like the Gray-Scott model.

[1] See the introduction of Cross & Greenside for an overview of the study of pattern formation.

Chapter 1

Reaction-Diffusion Systems

Reaction-diffusion (RD) systems are models that determine how concentrations of substances change in space. These systems are driven by two processes: chemical reaction and spatial diffusion. RD systems are partial differential equations, the most basic of which might look something like (1.1). This is sometimes called the Kolmogorov-Petrovsky-Piskounov equation in which u is a generic chemical species, d is a diffusion coefficient, $\nabla^2 u$ is the Laplace operator, and $r(u)$ is a general reaction term.

$$\frac{\partial u}{\partial t} = d\nabla^2 u + r(u) \tag{1.1}$$

What makes RD systems interesting, however, is the wide variety of patterns they form and how many of those patterns resemble patterns of nature such as spirals, stripes, and spots. In 1952, Alan Turing suggested that RD systems of morphogens may be able to explain the presence of spots or stripes on an organism [10]. Although the science behind animal patterns is more complicated, Turing laid the framework by which patterns form from minor perturbations of otherwise homogenous systems. Since then, many others have noted the similarity between RD patterns and patterns in nature [1, 2, 8, 7, 3, 11, 12] [1].

1.1 The Gray-Scott Model

The Gray-Scott system models the reaction of two generic chemical species, U and V, whose concentration in space is represented by u and v respectively [5]. The

[1] Among others, Bard, 1974 or 1981; Murray, 1981; Meinhardt, 1982; Young, 1984; Meinhardt and Klinger, 1987; or Turk, 1991.

model is based on the chemical reaction in (1.2).

$$\begin{aligned} U + 2V &\rightarrow 3V \\ V &\rightarrow P \end{aligned} \tag{1.2}$$

V is converted to inert product, P, which doesn't interfere with the reaction of the system. V appears on both sides of the chemical reaction and thus catalyzes its own production. Gray, Scott developed the following non-dimensional PDE:

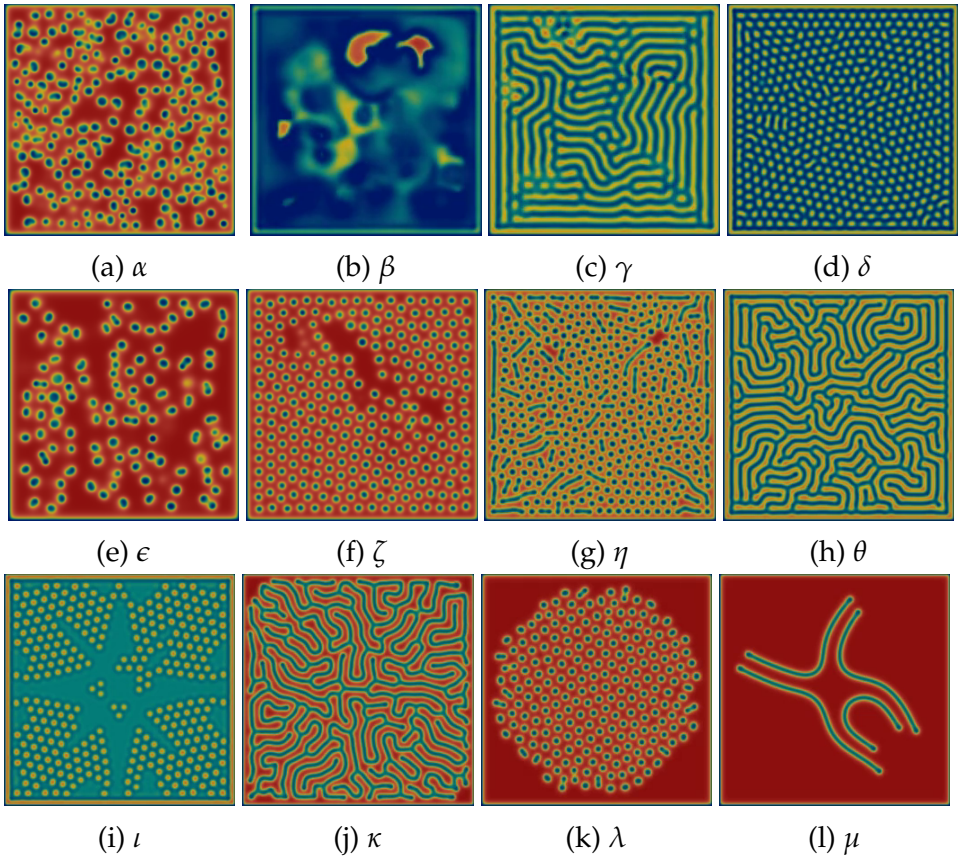
$$\frac{\partial u}{\partial t} = d_u \nabla^2 u - uv^2 + f(1-u) \tag{1.3}$$

$$\frac{\partial v}{\partial t} = d_v \nabla^2 v + uv^2 - (f+k)v \tag{1.4}$$

We see that both equations take the form of (1.1) only they are coupled. For simplicity, d_u, d_v, f, and k are taken to be constants. The first term in each equation, $d_u \nabla^2$ and $d_v \nabla^2$, are the diffusion terms. The Laplace operator, ∇^2, is responsible for the diffusion of each chemical in space (like the diffusion of heat in the more familiar heat equation) while the *diffusion coefficients*, d_u and d_v, govern the rate. The $\pm uv^2$ term is the *reaction term* which converts U into V: an increase in v is equal to the decrease in u, hence $+uv^2$ in the second equation. Since U will eventually get used up to generate V, the term $f(1-u)$ is the *replenishment term* which reintroduces chemical U into the system (u has a maximum value of 1). Similarly, chemical V would increase without limit except for the *diminishment term*, $(f+k)v$, which serves to remove chemical V from the system. One can imagine this system as two chemicals interacting in a cell where the bloodstream carries chemicals in and out.

The Grey-Scott system is particularly notable for the wide range of irregular patterns it produces. Previous analysis of the system by Pearson [9] identified at least 12 different pattern types, all of which occur at different points in k, f parameter space. Figure 1.1 shows the 12 quantifiably different patterns observed in this system. The figures, which plot the concentration of chemical U over a 256 by 256 grid, reveal the extremely variable behavior of this system[2]. One of the most compelling qualities of these patterns is their resemblance to patterns of nature, e.g. κ (figure 1.1j) looks like coral and λ (figure 1.1k) resembles the growth of bacteria. Other patterns, like β (figure 1.1b), exhibit turbulence.

[2]A concentration plot of V would resemble the inverse of U so only one is shown.



(a) α (b) β (c) γ (d) δ

(e) ϵ (f) ζ (g) η (h) θ

(i) ι (j) κ (k) λ (l) μ

Figure 1.1: Patterns of chemical concentration U identified in [9]. Each pattern, figure 1.1a—figure 1.1l, is designated by a Greek letter which corresponds to the plot in figure 1.2. Red and blue indicate $U = 1$ and $U \approx 0.2$ respectively.

1.2 Numerical Solution

The system in (1.3) is solved by forward Euler integration of the discrete Laplacian obtained by the finite difference method. A spacial grid of 256×256 points constitutes the mesh with a time step of 1[3]. The system was initialized with the state $U = 1$, $V = 0$ with a 20×20 area located in the center perturbed with $U = 0.5$, $V = 0.25$. The 20×20 area is then further perturbed with 1% random noise to catalyze the reaction. The patterns in figure 1.1 were generated this method and depict the concentration of chemical U. A plot of chemical V would appear as the inverse.

[3] [9] notes no qualitative differences on mesh sizes up to 1024×1024 and time steps as low as 0.01.

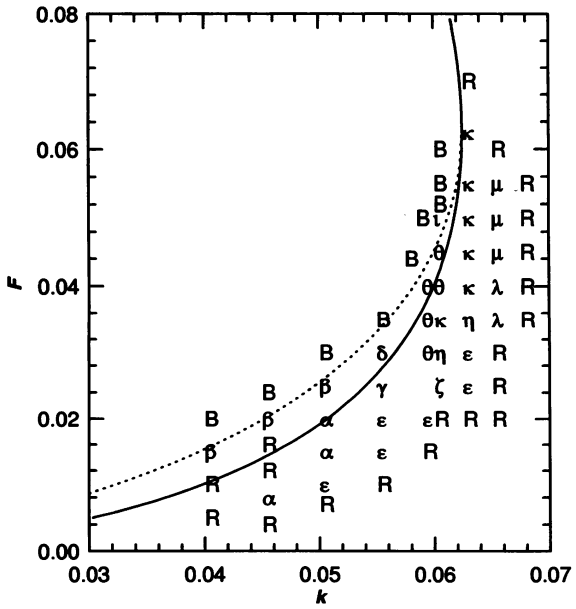


Figure 1.2: The mapping of Greek letters in figure 1.1 to their location in k, f parameter space. R and B indicate that the system evolved to uniform red and blue states respectively. This figure also represents a phase diagram of the reaction kinetics. Between the solid and dotted line, the system is bistable for which there are two linearly stable steady states. As f passes below the dotted line, the non-trivial steady state becomes unstable through Hopf bification giving stable periodic orbit for $k < 0.035$ and unstable for $k > 0.035$. The trivial state, ($U = 1$, $V = 0$) exists for all (f, k) outside the solid line [9].

Chapter 2

Computational Homology

Homology is one way of analyzing *local* properties in order to extract information about *global* phenomena. As large amounts of data become available, it becomes more difficult to determine what information is relevant. There are, of course, high and low-level approaches. A high-level approach like a fingerprint scanner or handwriting recognition might be the end-goal of one's analysis, but lower-level approaches like homology look at the geometric makeup of an object and is often a requisite step toward building higher-level processes.

At this time, computational homology is a relatively new field and its application in physics has only recently been explored. Although homology is a field of algebraic topology, it combines the mathematics of several other fields including combinatorics and computation. The mathematical formalism behind homology is difficult to grasp so only the relevant information will be detailed in Sect. 2.1. Sect. 2.2 on cubical homology presents a more thorough discussion of the mathematical background of the topic while LATER SECTIONS to be written provide an example of an algorithm to compute the homology.

2.1 Image analysis

To put it simply, homology is concerned with *holes* and *pieces*. Mathematically, how does one define a "hole"? What does it mean to be part of a "connected piece"? It's best to think about this in one dimension first. Figure 2.1 shows two simple topological spaces, X and Y. Although X and Y are spaces with one and two line segments respectively, in terms of homology one would say X consists of a single *connected piece* while Y has two distinct pieces. The fact that the line segments are straight or of different length is not important for the homology. In this one-dimensional example, the *zeroth homology groups* of each are

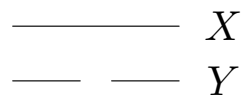


Figure 2.1: Topological spaces X and Y. X consists of one connected line segment and Y has two disconnected line segments.

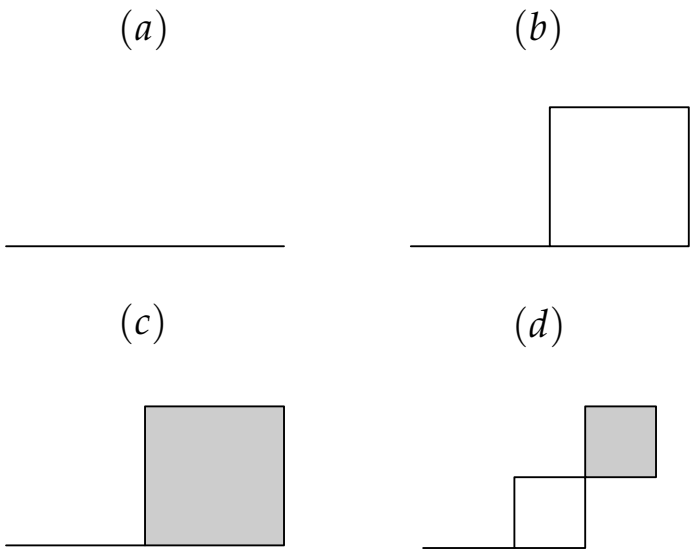


Figure 2.2: Topological spaces X_a, X_b, X_c, and X_d.

$$H_0(X) \cong \mathbf{Z}^1 \qquad \text{and} \quad H_0(Y) \cong \mathbf{Z}^2 \tag{2.1}$$

where $\mathbf{Z}$ is the group of integers. The homology pairs a topological space (e.g. X and Y) with an *abelian group*, a set of elements combined with operations that satisfy five axioms (closure, associativity, identity, invertibility, and commutativity). Notice, however, that the *zeroth homology group* of Y is $\mathbf{Z}^2$; the rank of the group, 2, is what accounts for the two (2) distinct pieces, but more on this later.

Since there is a *zeroth homology group*, it makes sense that there would be a *first homology group*. Looking at the two-dimensional example in Figure 2.2, the homology of each space X_a, X_b, X_c, and X_d is

$$H_1(X_a) \cong 0 \quad H_1(X_b) \cong \mathbf{Z} \qquad H_1(X_c) \cong 0 \quad H_1(X_d) \cong \mathbf{Z} \tag{2.2}$$

$$H_0(X_i) \cong \mathbf{Z} \qquad \text{for} \qquad i = a, b, c, d \tag{2.3}$$

All spaces X_i for $i = a, b, c, d$ have a *zeroth homology group* of $\mathbf{Z}$ since there is a single connected component. In Figure 2.2(b)-(c), the connected component forms

an enclosed area (e.g. the squares). The square in (b) forms a "hole". The shading indicates that the hole is filled and is thus no longer a "hole". Figure 2.3(b), (d) both contain one hole while (a), (c) contain zero holes. Just as the *zeroth homology group* is concerned with connected segments, the *first homology group* is concerned with "holes".

The terms "piece" and "hole" are informal. Formally, we could say that the k^{th} homology group, $H_k(X)$, represents the group of k-dimensional *holes* of X where a 0-dimensional *hole* is merely the gap between two components (e.g. Y in figure 2.1). As I alluded to earlier, the the rank of the homology group (e.g. the rank 2 of $\mathbf{Z}^2$ in (2.1)) represents the number of k dimensional holes. This is called the *Betti number* β_k. Indeed, Betti numbers are non-zero for all $k < d$ where d is the dimension of the topological space. The Betti numbers are the most important feature of the homology in this thesis since it nicely provides a mathematical quantity to an otherwise visual characteristic of a topological space. Later on I will describe how this information has been used to elucidate information about the dynamics of a system.

2.2 Cubical Homology

In cubical homology, topological spaces are represented as a collection of cubes. This thesis is concerned with digital images as topological spaces. Digital images are quite literally a collection of two-dimensional cubes, *pixels*, thus a homology that examines these objects is a natural environment for examining the output of a computer simulation. In this section I present a brief mathematical description of cubical homology which closely follows that of [4] and [6]. We'll start by defining elementary cubes which make up the building blocks for the theory. It is important to keep in mind here that one of the fundamental ideas in homology theory is to connect topological objects (e.g. connected pieces and holes) to algebraic objects.

Definition 2.2.1. An *elementary interval* is an interval $I \subset \mathbb{R}$ of the form

$$I = [l, l+1] \quad \text{or} \quad I = [l, l]$$

for some $l \in \mathbb{R}$. To simplify notation, say

$$[l] = [l, l]$$

is an interval containing a single point, a *degenerate* interval. Intervals of the form $[l, l+1]$ are called *nondegenerate*.

Definition 2.2.2. An *elementary cube* Q is a finite product of elementary intervals,

$$Q = I_1 \times I_2 \times \ldots \times I_d \subset \mathbb{R}^d$$

where each I_i is an elementary interval. We denote the set of all elementary cubes in $\mathbb{R}^d$ as $\mathcal{K}^d$.
The set of all elementary cubes, $\mathcal{K}$,

$$\mathcal{K} := \bigcup_{d=1}^{\infty} \mathcal{K}^d.$$

Definition 2.2.3. Let $Q = I_1 \times I_2 \times \ldots \times I_d \subset \mathbb{R}^d$ be an elementary cube. The *embedding number* of Q is defined to be d which we denote by $\text{emb}(Q)$. Interval I_i is the i^{th} *component* of Q and is written $I_i(Q)$. The *dimension* of Q is defined as the number of nondegenerate components in Q and denoted $\dim Q$. We refer to an elementary cube Q with $\dim Q = k$ as a *k-cube* and denote

$$\mathcal{K}_k := \{Q \in \mathcal{K} | \dim Q = k\},$$

and

$$\mathcal{K}_k^d := \mathcal{K}_k \cap \mathcal{K}^d.$$

The relationship between the embedding number and dimension might be a little muddy since it seems that they would always be the same. Observe that for elementary cube Q, if $\text{emb}(Q) = d$, then $Q \in \mathcal{K}^d$. The only general relation between the embedding number and dimension of Q is that

$$0 \leq \dim Q \leq \text{emb}(Q).$$

To illustrate this, imagine a Rubik's cube on a desk. The Rubik's cube itself has both emb, dim $= 3$ while any one square *face* has emb $= 3$ but dim $= 2$ (also see Example (2.2.1)).

Example 2.2.1. Given elementary cube $Q := [1,2] \times [1,2] \times [-1] \subset \mathbb{R}^3$, we have $I_1(Q) = [1,2]$, $I_2(Q) = [1,2]$, and $I_3(Q) = [-1]$(*degenerate*). Therefore, $\text{emb}(Q) = 3$ and $\dim Q = 2$.

some examples should be added here later

Now we must define the class of topological spaces for which we define the homology.

Definition 2.2.4. A set $X \subset \mathbb{R}^d$ is *cubical* if X can be written as a finite union of elementary cubes.

Given cubical complex $X \subset \mathbb{R}^d$, we define

$$\mathcal{K}(X) := \{Q \in \mathcal{K} \mid Q \subset X\}$$

and

$$\mathcal{K}_k(X) := \{Q \in \mathcal{K}(X) \mid \dim Q = k\}.$$

We can write $\mathcal{K}^d(X)$ to remind us that $X \subset \mathbb{R}^d$ as well as $\mathcal{K}_k^d := \mathcal{K}^d(X) \cap K_k(X)$. For example, elements of $\mathcal{K}_0(X)$ are *vertices* of X, elements of $\mathcal{K}_1(X)$ are *edges* and so forth. Then $\mathcal{K}_k(X)$ are the *k-cubes* of X.

As previously mentioned, our goal is to have a relationship between algebraic objects and topological spaces. The first step, then, is to associate some algebraic object with the elementary cubes we just defined.

Definition 2.2.5. For each elementary *k-cube* $Q \in \mathcal{K}_k^d$, we associate an algebraic object $\widehat{Q}$ which we call an *elementary k-chain* of $\mathbb{R}^d$ where $\widehat{Q} : \mathcal{K}_k^d \to \mathbb{Z}$ is the function defined by

$$\widehat{Q}(P) = \begin{cases} 1 & \text{if } P = Q, \\ 0 & \text{otherwise.} \end{cases}$$

We also define $0 : \mathcal{K}_k^d \to \mathbb{Z}$ to be the zero function, i.e.$\widehat{0}(Q) = 0$ for all $Q \in \mathcal{K}_k^d$. The set of all *elementary k-chains* of $\mathbb{R}^d$ is given by

$$\widehat{\mathcal{K}_k^d} := \left\{\widehat{Q} \mid Q \in \mathcal{K}_k^d\right\}$$

and the set of all *elementary chains* of $\mathbb{R}^d$ is given by

$$\widehat{\mathcal{K}^d} := \bigcup_{k=0}^{\infty} \widehat{\mathcal{K}_k^d}.$$

For an elementary cube Q, we refer to $\widehat{Q}$ as its *dual elementary chain*. Conversely, given elementary chain $\widehat{Q}$, we call Q is its *dual elementary cube*. What we want is that there is a one-to-one relationship between the elementary *k-cubes* (topological objects) and *elementary k-chains* (algebraic objects). In other words, the map of *k-cubes* ($\mathcal{K}_k^d$) to *k-chains* ($\widehat{\mathcal{K}_k^d}$) is a *bijection*.

Proposition 2.2.1. *The map $\phi : \mathcal{K}_k^d \to \widehat{\mathcal{K}_k^d}$ given by $\phi(Q) = \widehat{Q}$ is a bijection.*

Proof. See [6]. □

Proposition 2.2.1 allows us invoke the inverse of ϕ to go from an algebraic object, the elementary chain $\widehat{Q}$, to a topological set, Q. The following definition uses the algebra we've built up to give the elementary *k-chains* algebraic structure.

Definition 2.2.6. The group C_k^d of *k-dimensional chains* (or *k-chains*) of $\mathbb{R}^d$ is the free abelian group generated by the elementary chains of $\mathcal{K}_k^d$. Thus the elements of C_k^d are functions $c : \mathcal{K}_k^d \to \mathbb{Z}$ such that $c(Q) = 0$ for all but a finite number of $Q \in \mathcal{K}_k^d$.

I really want to make this section very readable with nice figures and stuff. Figure 2.3 illustrates how we can use information about the boundary to exact information about the k-cubes, but we are again using topological information (the existence of a boundary) to derive more topological information (the existence of loops). What we would really like to do is use algebra to get at this information, so we start by defining the algebraic boundary of a k-chain.

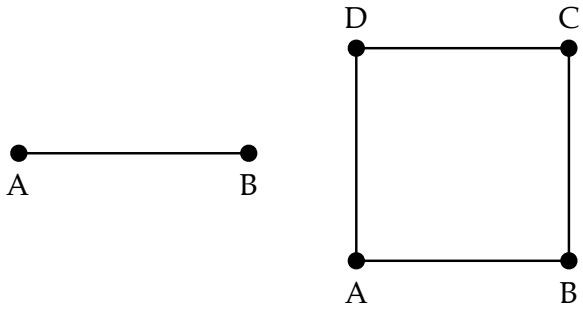


Figure 2.3: The left picture has a boundary given by $\{A\} \cup \{B\}$ and therefore does not form a loop (a 0-cube). The picture on the right, however, does not have a boundary and therefore forms a loop (a 1-cube).

Appendix A

The First Appendix

A.1 Extra definitions, theorems, etc.

Definition A.1.1. The *free abelian group generated by a finite set*

$$S = \{s_1, s_2, \ldots, s_n\}$$

is the set of all functions $f : S \to \mathbb{Z}$, with the pointwise addition

$$(f + g)(s_i) := f(s_i) + g(s_i), \quad i = 1, 2, \ldots, n.$$

Definition A.1.2. The *free abelian group generated by a possibly infinite set* S is the subgroup of $\mathbb{Z}^S$, consisting of all functions $f : S \to Z$ satisfying

$$f(s) = 0 \quad \text{for all but finitely many } s \in S.$$

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