A Database Schema for the Analysis of Global Dynamics[1]

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Abstract. A generally applicable, automatic method for the efficient computation of a database of global dynamics of a multiparameter dynamical system is introduced. An outer approximation of the dynamics for each subset of the parameter range is computed using rigorous numerical methods and is represented by means of a directed graph. The dynamics is then decomposed into the recurrent and gradient-like parts by fast combinatorial algorithms and is classified via Morse decompositions. These Morse decompositions are compared at adjacent parameter sets via continuation to detect possible changes in the dynamics. The Conley index is used to study the structure of isolated invariant sets associated with the computed Morse decompositions and to detect the existence of certain types of dynamics. The power of the developed method is illustrated with an application to the two-dimensional density-dependent Leslie population model. Large parts of this article is based on our paper published in [1], which contains more detailed description of the method.

Keywords: database, dynamical system, Conley index, Morse decomposition, Leslie population models, multiparameter system
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INTRODUCTION

Given a nonlinear dynamical system, identifying and classifying the qualitative properties of the system over wide ranges of parameter values is of fundamental importance in many disciplines. In particular, it is of primary interest to many computational biologists. The fact that most topics of interest in systems biology are dynamic in nature suggests the need for a comprehensive, yet efficient method for cataloging the global dynamics of nonlinear systems. In other words, a method is desired which computationally constructs a database of global dynamical behavior of a specific system over a range of parameters.

We restrict our attention to the setting of a multiparameter family of dynamical systems given by a continuous function

$$f\colon X \times \Lambda \ni (x,\lambda) \mapsto f(x,\lambda) = f_\lambda(x) \in X$$

where X is the phase space and Λ is the parameter space. A set $Z \subset X$ is *invariant at* $\lambda \in \Lambda$ if $f_\lambda(Z) = Z$. We use the notation $F\colon X \times \Lambda \to X \times \Lambda$ for the extension of the system to include the parameters as explicit variables defined by $F(x,\lambda) = \big(f_\lambda(x),\lambda\big) = \big(f(x,\lambda),\lambda\big)$. For $\Lambda_0 \subset \Lambda$ we denote the restriction of F to $X \times \Lambda_0$ by $F_{\Lambda_0}\colon X \times \Lambda_0 \to X \times \Lambda_0$. Given a set $S \subset X \times \Lambda$ we denote its restriction to Λ_0 by $S_{\Lambda_0} := S \cap (X \times \Lambda_0)$. We often identify $S_\lambda \subset X$ with $S_{\{\lambda\}} = S_\lambda \times \{\lambda\}$. In this language, a set $S \subset X \times \Lambda$ is *invariant over* Λ_0 if $F_{\Lambda_0}(S_{\Lambda_0}) = S_{\Lambda_0}$.

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To provide perspective on the practicality and utility of our approach, we consider the two-dimensional version of an over-compensatory Leslie population model $g\colon \mathbb{R}^2 \to \mathbb{R}^2$ given by

$$(x_1, x_2) \mapsto ((\theta_1 x_1 + \theta_2 x_2)\, e^{-\phi(x_1+x_2)}, p x_1)$$

where θ_1, θ_2, ϕ and p are parameters. This model and its biological relevance is discussed in considerable detail in work of Ugarcovici and Weiss [3]. As indicated there, the constant ϕ may be scaled arbitrarily, and thus we will assume $\phi = 0.1$ in this paper.

REVIEW OF CONLEY THEORY

Recall that a compact set $N \subset X \times \Lambda_0$ is an *isolating neighborhood* for F_{Λ_0} if $\mathrm{Inv}\,(N, F_{\Lambda_0}) \subset \mathrm{int}_{X\times\Lambda_0}(N)$ where $\mathrm{Inv}\,(N, F_{\Lambda_0})$ denotes the maximal invariant set in N under F_{Λ_0}, and $\mathrm{int}_{X\times\Lambda_0}(N)$ denotes the interior of N. An invariant set $S_{\Lambda_0} \subset X \times \Lambda_0$ is an *isolated invariant set* if $S_{\Lambda_0} = \mathrm{Inv}\,(N, F_{\Lambda_0})$ for some isolating neighborhood N. To simplify the presentation and analysis, throughout this paper we make use of the following assumption: *there exists a compact set $B \subset X \times \Lambda$ which is an isolating neighborhood for F. Its maximal invariant set is denoted by $S := \mathrm{Inv}\,(B, F)$.*

A *Morse decomposition* of S_{Λ_0} is a finite collection $\mathbf{M}(S_{\Lambda_0}) = \left\{M_{\Lambda_0}(p) \subset S_{\Lambda_0} \mid p \in \mathscr{P}_{\Lambda_0}\right\}$ of disjoint isolated invariant sets of F_{Λ_0}, called *Morse sets*, which are indexed by the set $\mathscr{P}_{\Lambda_0}$ on which there exists a strict partial order $>_{\Lambda_0}$, called an *admissible order*, such that for every $(x,\lambda) \in S_{\Lambda_0} \setminus \bigcup_{p\in\mathscr{P}} M_{\Lambda_0}(p)$ and any complete orbit γ of F_{Λ_0} through (x,λ) in S_{Λ_0} there exist indices $p >_{\Lambda_0} q$ such that under F_{Λ_0} $\omega(\gamma) \subset M_{\Lambda_0}(q)$ and $\alpha(\gamma) \subset M_{\Lambda_0}(p)$.

Observe that since $\mathscr{P}_{\Lambda_0}$ is a strict partially ordered set, a Morse decomposition can be represented as an acyclic directed graph $\mathrm{MG}(\Lambda_0)$ called the *Morse graph over* Λ_0. The elements of the index set $\mathscr{P}_{\Lambda_0}$, which naturally correspond to the Morse sets, are the vertices of the Morse graph over Λ_0, and the edges of the Morse graph over Λ_0 are the minimal order relations which through transitivity generate $>_{\Lambda_0}$.

The Conley index, which is an algebraic topological invariant of isolated invariant sets, is used to understand the structure of the dynamics within a Morse set [2].

To explain the index we begin by considering an arbitrary continuous map g and a pair of compact sets $N = (N_1, N_0)$ such that $N_0 \subset N_1$. Consider the pointed quotient space $\left(N_1/N_0, [N_0]\right)$ obtained by collapsing N_0 to a single point $[N_0]$. Define $g_N\colon \left(N_1/N_0, [N_0]\right) \to \left(N_1/N_0, [N_0]\right)$ by $g_N(x) = g(x)$ if $x, g(x) \in N_1 \setminus N_0$ and $g_N(x) = [N_0]$ otherwise. The pair $N = (N_1, N_0)$ is an *index pair* if the map g_N is continuous and $\mathrm{cl}\,(N_1 \setminus N_0)$ is an isolating neighborhood.

For any Morse set $M_{\Lambda_0}(p)$ there exists an index pair $N = (N_1, N_0)$ such that the induced map $F_{\Lambda_0,N}\colon \left(N_1/N_0, [N_0]\right) \to \left(N_1/N_0, [N_0]\right)$ is a continuous function and $M_{\Lambda_0}(p) = \mathrm{Inv}\left(\mathrm{cl}\,(N_1 \setminus N_0), F_{\Lambda_0}\right)$. Passing to homology leads to a family of group endomorphisms $F_{\Lambda_0,N*}\colon H_*\left(N_1/N_0, [N_0]\right) \to H_*\left(N_1/N_0, [N_0]\right)$.

There may exist different choices of index pairs which can lead to different group endomorphisms, therefore, to define the Conley index of an isolated invariant set, one must consider equivalence classes of these group endomorphisms. In constructing our database, we do not utilize the full Conley index; instead, we store a weaker invariant, namely the nonzero eigenvalues of $F_{\Lambda_0,N*}$ restricted to the torsion-free part of $H_*\left(N_1/N_0, [N_0]\right)$.

Let $\Lambda_0 \subset \Lambda$ and $\mathbf{M}(S_{\Lambda_0}) = \left\{M_{\Lambda_0}(p) \subset S_{\Lambda_0} \mid p \in \mathscr{P}_{\Lambda_0}\right\}$ be a Morse decomposition of S_{Λ_0} with admissible order $>_{\Lambda_0}$. The *Conley-Morse graph over* Λ_0 of $\mathbf{M}(S_{\Lambda_0})$ is denoted by $\mathrm{CMG}(\Lambda_0)$ and consists of $\mathrm{MG}(\Lambda_0)$, the Morse graph over Λ_0 with the additional information of the nonzero eigenvalues of the torsion-free part of the index map of each Morse set assigned to the associated node.

We will compute the Conley-Morse graphs over distinct fixed subregions of parameter space. This raises the question of how to relate the resulting Conley-Morse graphs. One answer is provided in the following definition.

Definition 1 Let $\Lambda_0, \Lambda_1 \subset \Lambda$ be such that $\Lambda_{0,1} := \Lambda_0 \cap \Lambda_1$ is a nonempty, contractible set. Let $\mathbf{M}(S_{\Lambda_i}) = \left\{M_{\Lambda_i}(p) \subset S_{\Lambda_i} \mid p \in \mathscr{P}_{\Lambda_i}\right\}$ for $i = 0, 1$ be Morse decompositions with admissible orders $>_i$. The associated Morse graphs $\mathrm{MG}(\Lambda_0)$ over Λ_0 and $\mathrm{MG}(\Lambda_1)$ over Λ_1 are *equivalent* if there is an order preserving bijection $\iota\colon (\mathscr{P}_{\Lambda_0}, >_0) \to (\mathscr{P}_{\Lambda_1}, >_1)$ such that $M_{\Lambda_0}(p) \cap (X \times \Lambda_{0,1}) = M_{\Lambda_1}\left(\iota(p)\right) \cap (X \times \Lambda_{0,1})$.

COMBINATORIAL REPRESENTATION OF DYNAMICS

Let $\mathscr{X}$ and $\mathscr{Q}$ denote grids on X and Λ, respectively. Observe that $\mathscr{X} \times \mathscr{Q}$ is a grid for $X \times \Lambda$. Given $\delta > 0$, we can choose grids such that $\mathrm{diam}\,(\mathscr{X}) < \delta$ and $\mathrm{diam}\,(\mathscr{Q}) < \delta$. A *combinatorial multivalued map* $\mathscr{F}\colon \mathscr{X} \rightrightarrows \mathscr{X}$ assigns to each element $G \in \mathscr{X}$ a finite subset $\mathscr{F}(G)$ of $\mathscr{X}$. Important for efficient computation is the observation that a combinatorial multivalued map $\mathscr{F}\colon \mathscr{X} \rightrightarrows \mathscr{X}$ is equivalent to a directed graph with vertices $\mathscr{X}$ and directed edges (G,H) whenever $H \in \mathscr{F}(G)$.

Fix $\lambda \in \Lambda$ and a compact set $B_\lambda \subset X$. We relate $f_\lambda|_{B_\lambda}\colon B_\lambda \to X$ to the combinatorial multivalued map $\mathscr{F}_\lambda\colon \mathscr{X}(B_\lambda) \rightrightarrows \mathscr{X}$ by requiring that $\mathscr{F}_\lambda$ outer approximates f_λ. A multivalued map $\mathscr{F}_\lambda\colon \mathscr{X}(B_\lambda) \rightrightarrows \mathscr{X}$ is called an *outer approximation* of f_λ restricted to $|\mathscr{X}(B_\lambda)|$ if $f_\lambda(G) \subset \operatorname{int}\left(|\mathscr{F}_\lambda(G)|\right)$ for all $G \in \mathscr{X}(B_\lambda)$.

Since we can only perform a finite number of computations, we cannot compute $\mathscr{F}_\lambda$ individually for each $\lambda \in \Lambda$. By our assumption, the compact set $B \subset X \times \Lambda$ is an isolating neighborhood for F, and $S = \operatorname{Inv}(B,F)$. From the point of view of the computational algorithms it is more convenient to additionally assume the following condition:

For each grid element $Q \in \mathscr{Q}$ the set $\mathscr{B}_Q := \mathscr{X}\left(\bigcup_{\lambda\in Q} B_\lambda\right)$ has the property that $S_Q = \operatorname{Inv}\left(|\mathscr{B}_Q| \times Q, F_Q\right)$.

Now for each $Q \in \mathscr{Q}$ we consider a multivalued map $\mathscr{F}_Q\colon \mathscr{B}_Q \rightrightarrows \mathscr{X}$ with the property that $f(G,Q) \subset \operatorname{int}\left(|\mathscr{F}_Q(G)|\right)$ for all $G \in \mathscr{B}_Q$. Observe that if $\lambda \in Q$, then $\mathscr{F}_Q$ is an outer approximation of f_λ restricted to $|\mathscr{B}_Q|$. We organize the collection of $\mathscr{F}_Q$ via the following definition. Set $\mathscr{B} := \bigcup_{Q\in\mathscr{Q}} \left(\mathscr{B}_Q \times \{Q\}\right) \subset \mathscr{X} \times \mathscr{Q}$. A *combinatorialization* of F on $|\mathscr{B}|$ is the combinatorial multivalued map $\mathscr{F}\colon \mathscr{B} \rightrightarrows \mathscr{X} \times \mathscr{Q}$ defined by $\mathscr{F}(G,Q) = \mathscr{F}_Q(G) \times \{Q\}$. The following proposition indicates how outer approximations are used to capture invariant sets.

Proposition 2 *Suppose $\mathscr{F}$ is a combinatorialization of F on $|\mathscr{B}|$. Let $Q \in \mathscr{Q}$, and suppose $\mathscr{Y} \subset \mathscr{B}_Q$. If $\mathscr{N}$ is the maximal subset of $\mathscr{Y}$ such that the restriction $\mathscr{F}_Q\colon \mathscr{N} \rightrightarrows \mathscr{N}$ is closed, then* $\operatorname{Inv}(|\mathscr{Y}| \times Q, F_Q) = \operatorname{Inv}(|\mathscr{N}| \times Q, F_Q)$.

A natural starting point for examining the global structure of both a dynamical system and a directed graph is to look for recurrence. The *recurrent set of $\mathscr{F}_Q\colon \mathscr{S}_Q \rightrightarrows \mathscr{X}$* is defined by

$$\mathscr{R}_Q := \{G \in \mathscr{S}_Q \mid \text{there exists a nontrivial path from } G \text{ to } G \text{ in } \mathscr{S}_Q\}.$$

The recurrent set $\mathscr{R}_Q$ is naturally partitioned into equivalence classes $\{\mathscr{M}_Q(p) \mid p \in \mathscr{P}_Q\}$ called *combinatorial Morse sets* according to the following equivalence relation: $G \simeq H$ *if and only if there exists a path in $\mathscr{F}_Q$ from G to H and a path in $\mathscr{F}_Q$ from H to G.*

Since every node in $\mathscr{S}_Q$ that lies on a cycle is an element of $\mathscr{R}_Q$, we can define a strict partial order on the indexing set $\mathscr{P}_Q$ by setting $p >_Q q$ if there exist $G \in \mathscr{M}_Q(p)$, $H \in \mathscr{M}_Q(q)$, and a path from G to H in $\mathscr{F}_Q$.

Observe that this construction implies that a combinatorial Morse decomposition can be represented as a directed graph. Let $\mathrm{MG}(\mathscr{F}_Q)$ denote the acyclic directed graph with vertices consisting of the elements of $\mathscr{P}_Q$ and the minimal set of directed edges $p \to q$ which generate $p >_Q q$ under transitivity. The following proposition states that given a combinatorial Morse decomposition for an outer approximation $\mathscr{F}_Q$, there is a Morse decomposition of F_Q such that $\mathrm{MG}(\mathscr{F}_Q)$ is the Morse graph over Q for the Morse decomposition.

Proposition 3 *Let $Q \in \mathscr{Q}$ and let $\{\mathscr{M}_Q(p) \mid p \in \mathscr{P}_Q\}$ be the set of combinatorial Morse sets for $\mathscr{F}_Q$. If $\mathscr{F}_Q\left(\mathscr{M}_Q(p)\right) \subset \mathscr{B}_Q$ for all $p \in \mathscr{P}_Q$, then the acyclic directed graph* $\mathrm{MG}(\mathscr{F}_Q)$ *which represents the combinatorial Morse sets is a Morse graph over Q for the Morse decomposition of S_Q defined by*

$$\mathbf{M}(S_Q) := \{\operatorname{Inv}\left(|\mathscr{M}_Q(p)| \times Q, F_Q\right) \mid p \in \mathscr{P}_Q\}.$$

Moreover, each $|\mathscr{M}_Q(p)|$ is an isolating neighborhood for $\operatorname{Inv}|\mathscr{M}_Q(p)|$.

We now turn to the question of comparing the dynamical information over different parameter regions.

Definition 4 To each $Q \in \mathscr{Q}$, there is an associated $\mathrm{CMG}(\mathscr{F}_Q)$. Consider $Q_0, Q_1 \in \mathscr{Q}$ such that $Q_0 \cap Q_1 \neq \emptyset$. The *clutching graph* $\mathscr{J}(Q_0,Q_1)$ is defined to be the bipartite graph with vertices $\mathscr{P}_{Q_0} \cup \mathscr{P}_{Q_1}$ (the union of the vertices from $\mathrm{MG}(\mathscr{F}_{Q_0})$ and $\mathrm{MG}(\mathscr{F}_{Q_1})$) and with an edge $(p,q) \in \mathscr{P}_{Q_0} \times \mathscr{P}_{Q_1}$ if $\mathscr{M}_{Q_0}(p) \cap \mathscr{M}_{Q_1}(q) \neq \emptyset$.

Observe that if every vertex in $\mathscr{P}_{Q_0}$ in the clutching graph $\mathscr{J}(Q_0,Q_1)$ has a unique edge, then we can define the *clutching function* $\iota_{Q_1,Q_0}\colon \mathscr{P}_{Q_0} \to \mathscr{P}_{Q_1}$ by $\iota_{Q_1,Q_0}(p) := q$ for each edge (p,q) of $\mathscr{J}(Q_0,Q_1)$.

Definition 5 Consider the set of Conley-Morse graphs over the grid elements of the parameter space, i.e. $\{\mathrm{CMG}(\mathscr{F}_Q) \mid Q \in \mathscr{Q}\}$. Let $Q_0, Q_1 \in \mathscr{Q}$ such that $Q_0 \cap Q_1 \neq \emptyset$. If the clutching function $\iota_{Q_1,Q_0}\colon \mathscr{P}_{Q_0} \to \mathscr{P}_{Q_1}$ is defined and gives a directed graph isomorphism from $\mathrm{MG}(\mathscr{F}_{Q_0})$ to $\mathrm{MG}(\mathscr{F}_{Q_1})$, then we say that the Conley-Morse graphs over Q_0 and Q_1, $\mathrm{CMG}(\mathscr{F}_{Q_0})$ and $\mathrm{CMG}(\mathscr{F}_{Q_1})$, are *equivalent*. The equivalence classes of $\{\mathrm{CMG}(\mathscr{F}_Q) \mid Q \in \mathscr{Q}\}$ with respect to the transitive closure of this relation are called *continuation classes*.

Proposition 6 *Let* $Q_0, Q_1 \in \mathcal{Q}$ *such that* $Q_0 \cap Q_1 \neq \emptyset$. *If the clutching function* $\iota_{Q_1,Q_0}\colon \mathcal{P}_{Q_0} \to \mathcal{P}_{Q_1}$ *is a directed graph isomorphism then there exists a Morse decomposition* $\mathbf{M}(S_{Q_0\cup Q_1}) = \{M_{Q_0\cup Q_1}(r) \mid r \in \mathcal{P}_{Q_0\cup Q_1}\}$ *with admissible order* $>_{Q_0\cup Q_1}$ *such that its restriction is the same as the Morse decomposition* $\mathbf{M}(S_{Q_i})$ *over* Q_i *for each* $i = 0,1$. *Specifically, there is a natural correspondence* $\pi_i\colon \mathcal{P}_{Q_0\cup Q_1} \to \mathcal{P}_{Q_i}$ *such that* $M_{Q_i}(\pi_i(r)) = M_{Q_0\cup Q_1}(r) \cap (X \times Q_i)$ *for any* $r \in \mathcal{P}_{Q_0\cup Q_1}$, *and* $>_{Q_0\cup Q_1}$ *agrees with* $>_{Q_i}$ *through the identification. Furthermore, the nonzero eigenvalues associated to the index maps for pairs of corresponding Morse sets* $M_{Q_0}(\pi_0(r))$ *and* $M_{Q_1}(\pi_1(r))$ *are the same.*

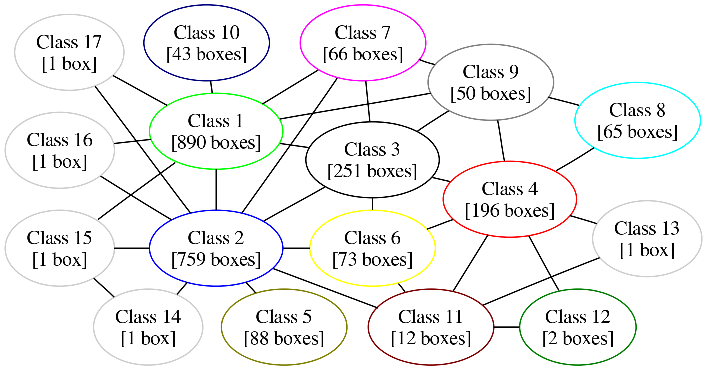
Definition 7 The associated *continuation graph* $\mathrm{CG}(\mathcal{F})$ is a graph whose vertices are the continuation classes $\{(\mathrm{CMG}(j), \mathcal{Q}(j)) \mid j = 1,\ldots,J\}$ where $\mathcal{Q}(k) \subset \mathcal{Q}$ is the set of parameter boxes associated with the k-th continuation class and $\mathrm{CMG}(k) = \mathrm{CMG}(\mathcal{F}_Q)$ for some $Q \in \mathcal{Q}(k)$.

The continuation graph is our database. Of course, additional, problem specific information can also be stored. However, as will be indicated in the context of the density dependent Leslie model, this database provides an extremely compressed yet useful means of describing the global dynamics over a broad range of parameter values.

DATABASE FOR THE LESLIE MODEL

Here we present the results of the computational procedure applied to the density dependent Leslie model when $p = 0.7$. An interactive presentation of the results can be found at `http://chomp.rutgers.edu/database/`, and the C++ source code of the software used to compute this database has also been made freely available.

We compute the continuation graph over the parameter space $\Lambda := \{(\theta_1,\theta_2) \in [8,37]\times[3,50]\}$. We choose an equipartitioned 50×50 grid for this parameter space with $m = 2$, $b_1 = 8$, $b_2 = 3$, $\zeta_1 = 29$, $\zeta_2 = 47$, and $K_1 = K_2 = 50$. The output is indicated in Figure 1. Since there is no natural order on the continuation classes, we have labeled them from "Class 1" to "Class 17", according to their volume in parameter space, beginning with the largest region.



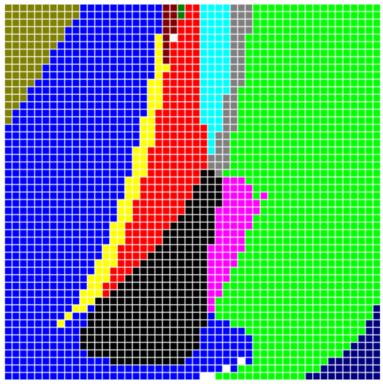


FIGURE 1. Left: The continuation graph computed for the density dependent Leslie population model with $\Lambda = \{\theta = (\theta_1,\theta_2) \in [8,37]\times[3,50]\}$, and $p = 0.7$. The label of each node indicates the class number and the number of boxes in $\mathcal{Q}(j)$. Right: Continuation diagram for the same parameter region.

The purpose of the database is to shed light on the possible dynamics exhibited over a wide range of parameter values. To be effective it must be able to be queried. Recall that the database consists of the continuation graph as indicated in Figure 1. Thus, we have the following information at our disposal:

(1) Associated with each node in the continuation graph we have the Conley-Morse graph and the set of parameter values $\mathcal{Q}(k)$ associated with the continuation class.
(2) The edges of the continuation graph indicating which continuation classes intersect in parameter space.

A fundamental question for any dynamical system is whether there exist multiple basins of attraction. We will demonstrate how the database can be used to answer this question. Our ability to detect basins of attraction is based on the following proposition which follows from the fact that $\mathcal{F}_Q$ is an outer approximation.

Proposition 8 *Assume that* S *is a global attractor for* F. *Let* $\{\mathcal{M}_Q(p) \mid p \in \mathcal{P}_Q\}$ *be the set of combinatorial Morse sets for* $\mathcal{F}_Q$. *If* q *is minimal with respect to the order* $>_Q$, *then* $\mathcal{M}(q)$ *is a trapping region for* F_Q.

With regard to the density dependent Leslie model, the set S is the global attractor for the dynamics restricted to $(\mathbb{R}^+)^2$. Therefore, the existence of multiple disjoint trapping regions in $(\mathbb{R}^+)^2$ implies the existence of multiple distinct basins of attraction. Thus the following query identifies regions in parameter space which support multiple basins of attraction: *"Which continuation classes have a Conley-Morse graph with more than one minimal element?"*

The result of this query is $\{\mathscr{Q}(k) : k = 4, 12, 13\}$, and each of the graphs has two minimal elements. Thus $\widehat{\mathscr{Q}} := \bigcup_{k=4,12,13} \mathscr{Q}(k)$ is a region in parameter space for which there exist at least two basins of attraction. From the edges of the connection graph we see that this defines a connected region.

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