Permanence of Sparse Autocatalytic Networks

By

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Abstract

Some global dynamical properties of catalytic networks, in particular permanence, are closely related with a directed graph representing the differential equation. It can be shown that for every directed graph with a Hamiltonian circuit there is a choice of rate constants such that the system is permanent. On the other hand one can find properties of the graphs, e.g. reducibility or the presence of end points, which are incompatible with permanence.

1. Replicator Dynamics

In evolutionary game theory, interacting groups within a population play genetically determined, distinguished strategies. To each group i a pay-off f_i is assigned that depends not only on i, but also on the strategies adopted by the other groups, and on the distribution $x = (x_1, x_2, \ldots, x_n)$ of the population over the groups $1, 2, \ldots, n$. The state space is thus the n-simplex

$$S_n = \big\{x \in \mathbb{R} | x_k > 0 \quad \wedge \quad \sum_{j=1}^{n} x_j = 1\big\},$$

and the pay-offs are functions $f_i : S_n \to \mathbb{R}$. The pay-offs relative to the population average,

$$\psi_i(x) = f_i(x) - \sum_{j=1}^{n} x_j f_j(x),$$

are known as *relative fitness functions.* Selection of strategies proportional to their relative fitness, i.e., a dynamics of the form

$$\dot{x}_k = x_k \big[f_k(x) - \sum_{j=1}^{n} x_j f_j(x)\big] \tag{1}$$

has been introduced into game theory by Taylor and Jonker [26]. Recently there has been increasing interest in a more general class of dynamical systems which describe selection consistent with the relative fitness of the strategies, see for example [7, 17].

Equation (1) has been termed *replicator equation* by Schuster and Sigmund [19], after it has become appearent that this equation arises in a variety of different contexts ranging from biochemical replication to theoretical economics. Hofbauer [8] showed that it is topologically equivalent with the Lotka-Volterra equations of theoretical ecology. Following Eigen and Schuster [4] the dynamics of an autocatalytic network of selfreplicating macromolecules can be modeled by a replicator equation. Here x_k stands for the relative concentrations of the macromolecular species I_k and $f_k(x)$ models the catalytic activity for the template induced replication reaction

$$I_k \quad \xrightarrow{I_1, I_2, \dots, I_n} \quad 2I_k,$$

which is mediated by the species I_1 through I_n.

In the simplest case, assuming mass action kinetics for reaction of the type

$$I_k + I_j \;\longrightarrow\; 2I_k + I_j,$$

the growth functions are linear,

$$f_k(x) = \sum_{j=1}^{n} a_{kj} x_j \qquad k = 1, \dots n. \tag{2}$$

In the game dynamical context this means that the payoff received for strategy i in the population is a linear combination of the payoffs a_{ij} obtain against strategy j. Subsequently we shall often make use of vector notation; equ.(1) then reads

$$\dot{x}_k = x_k \left[(Ax)_k - (xAx) \right]; \tag{3}$$

This equation is commonly called *second order replicator equation* since it describes autocatalytic reaction networks consisting of chemical reactions with second order kinetics. We shall refer to A as the *game matrix* or *interaction matrix* of the second order replicator equation.

The dynamics of this rather simple differential equation can be extremely complicated. In the case of two independent variables ($n = 3$, the state space is an equilateral triangle) there are 35 different generic phase portraits [3, 25], in the case case of three independent variables, ($n = 4$ species, the state space is the unit tetrahedron S_4) there are strange attractors and hundreds of different generic phase portraits [18]. A huge body of theory has accumulated on replicator equations in the last two decades. For a review we refer to the book by Hofbauer and Sigmund [13].

In the remaining part of this section we list a few results concerning the second order replicator equation (3) and provide some notation that will be used throughout this contribution.

Lemma 1. [20] The second order replicator equation (3) does not change under the transformation

$$a_{ij} \longrightarrow a_{ij} + c_j$$

with arbitrary $c_j \in \mathbb{R}$.

Thus we may define a *normal form* by

$$a_{ij} \longrightarrow a_{ij} - a_{jj},$$

i.e., by subtracting the diagonal element in each column. The game matrix A in normal form therefore has no non-zero entries in the diagonal.

Notation. The flux term of a replicator equation in normal form will be denoted by

$$\Phi(x) = (xAx). \tag{4}$$

We will often make use of the following important

Theorem 1. [14] *(Exclusion Principle)* If equ.(4) does not admit an interior rest point, then all orbits converge to the boundary ∂S_n.

Notation. The interior of a face on the boundary of the simplex will be denoted by

$$F_K = \{x \in \partial S_n | x_k = 0 \iff k \in K\}.$$

The set-valued index K lists the coordinates vanishing on F_K; by $N \setminus K$ we will denote the list of all non-vanishing coordinates on F_K.

Lemma 2. [10] Let $x^K \in F_K$ be an arbitrary point on the boundary. Then

$$\lambda_k(x^K) = (Ax^K)_k - (x^K Ax^K) \qquad k \in K. \tag{5}$$

is an eigenvalue of the Jacobian of equ.(3) at the point x^K, with the corresponding eigenvector pointing towards the corner $\mathbf{e}_k$ of the simplex.

Definition. Following Hofbauer and Sigmund [10, 13] the eigenvalues (5) are called *transversal.* A rest point $\hat{x} \in \partial S_n$ is called *saturated* if all its transversal eigenvalues are non-positive.

2. Permanence

Often one is not interested in all details of a dynamical system or in the structure of its ω-limit sets, less detailed knowledge may well be sufficient. In this contribution we shall investigate the following question: *Can all species coexist in the system for arbitrarily long time? Or will some species die out in the long run ?* Schuster *et al.* [21] introduced the notion of *permanence* (permanent coexistence) to formalize this question. A variety of different notions of cooperation, the first of which is now called *weak persistence* [6], have been proposed by various authors. For an overview see reference [5]. A recent review of permanence is [15].

A replicator equation (1) is said to be permanent if there is a compact subset $C \subset \operatorname{int} S_n$ of the interior of the state space, such that any trajectory starting in the interior will eventually end up in C. In other words, there is a (possibly very thin but finite) repulsive “skin” on the boundary of the state space. More formally, we have the following

Definition. Equ.(1) is permanent if there is compact set C such that for all initial conditions $x_0 \in \operatorname{int} S_n$ there is a $0 < T(x_0) < \infty$ fulfilling $x(t) \in C$ for all $t > T(x_0)$.

A sufficient (but for $n \geq 5$ not necessary) criterion for permanence of second order replicator equations was derived by Jansen [16]:

Theorem 2. If there is a vector $p \in \text{int}\, S_n$ such that for every isolated rest point $x^K \in F_K$ on the boundary of the simplex holds

$$\sum_{k \in K} p_k \cdot \lambda_k(x^K) > 0 \tag{6}$$

then equ.(3) is permanent.

A number of necessary conditions for permenence are known. We will make use of the following results:

Theorem 3. If equ.(3) is permanent, then there is a unique interior restpoint. Furthermore $(-1)^n \det\, \text{A} < 0$ [2, 14].

Theorem 4. If there is a regular saturated rest point $\hat{x} \in \partial S_n$, then equ.(3) is not permanent [10].

3. Catalytic Networks

Definition. A second order replicator equation in normal form with $a_{ij} \geq 0$ and $A \not\equiv 0$ is a *catalytic network* [20].

The defining property of catalytic networks is that cross-catalysis a_{kj}, $k \neq j$, is larger than self-catalysis, a_{kk}, i.e., for all j and k we have $a_{kj} - a_{kk} \geq 0$. The trivial case $A = 0$, which implies that all $x \in S_n$ are fixed points, is excluded for convenience.

Remark. For any catalytic network holds $\Phi(x) > 0$ for all $x \in \operatorname{int} S_n$.

Definition. For each non-negative matrix A with vanishing diagonal elements we define the directed graph $\Gamma(A)$ by the following rules [12, 11]:

(i) For $A \in \mathbb{R}^{n\times n}$ there a n vertices (1) through (n).

(ii) There is an edge from (i) to (k) if and only if $a_{ki} > 0$.

Because of theorem 1 the existence of an isolated interior equilibrium is a crucial feature for the dynamics of catalytic networks. Any notion of cooperativity, even if it is much weaker than permanence or persistence, will require the existence of an interior equilibrium as a consequence of the exclusion principle.

Definition. A vertex (q) which has no edge incident into it will be called a *source vertex* and a vertex (p) which has no edge incident out from it will be called a *sink vertex.*

Theorem 5. If a catalytic network admits an isolated interior restpoint, then it graph $\Gamma(A)$ contains neither source-vertices nor sink-vertices.

Proof. (i) First we show that if $\Gamma(A)$ contains a source vertex, say (q), then there is no interior rest point of the catalytic network. The differential equation for x_q reads $\dot{x}_q = x_q(-\Phi)$. For an interior rest point we have $\Phi > 0$ and thus $x_q = 0$, a contradiction.

(ii) If (1) is a sink vertex then by definition all entries $a_{k1} = 0$, i.e. the interaction matrix A contains a column of zeros and is therefore singular. Thus $Ax = (1, 1, \ldots, 1)$ has either no or infinitely many solutions, and therefore there is no isolated interior rest point. ∎

One can proof an even stronger result using the following

Technical Lemma. The flux of a second order replicator equation (3) fulfils

$$\Phi(t) \geq \frac{\Phi(0)}{1 + 2\Phi(0)\,t}. \tag{7}$$

Proof. The flux fulfils

$$\dot{\Phi}(x) = \sum_{k=1}^{n} x_k \left[(Ax)_k^2 + (xA)_k^2 \right] - 2\Phi(x)^2 \geq -2\Phi(x)^2$$

The solution of the ODE $\dot{\varphi} = -2\varphi^2$ with $\varphi(0) = \Phi(0)$ is

$$\varphi(t) = \frac{\Phi(0)}{1 + 2\Phi(0) \cdot t}.$$

Clearly, we have $\Phi(t) > \varphi(t)$ for all $t > 0$. ∎

Lemma 3. Let (q) be a source vertex. Then $\lim_{t \to \infty} x_q(t) = 0$.

Proof. $x_q(t) = x_q(0) \cdot \exp - \int_0^t \Phi(\tau) d\tau \;\leq\; x_q(0) \cdot \exp - \frac{1}{2} \int_0^t \varphi(\tau) d\tau =$

$$= x_q(0) \frac{1}{\sqrt{2\Phi(0) \cdot t + 1}}$$

Note that strong connectance of $\Gamma(A)$, i.e., irreducibility of A, implies the absence of source-vertices and sink-vertices. The following result is well known:

Theorem 6. If the catalytic network is permanent, then its graph $\Gamma(A)$ is strongly connected, i.e., A is an irreducible matrix [22].

In the following we will discuss a few conditions on the graph $\Gamma(A)$ that are necessary for permanence. For small networks we have the following result by Amann [1, 13]:

Theorem 7. If the catalytic network is permanent and $n \leq 5$ then $\Gamma(A)$ it contains a Hamiltonian circuit.

For $n \geq 6$ counter-examples are known [1], see figure 1.

Lemma 4. The efforts for applying Jansen's inequalities can be reduced by the following observations:

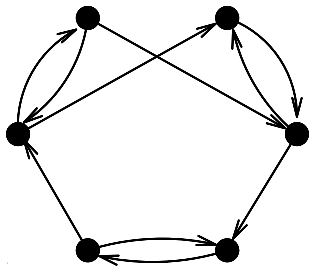

Figure 1: Non-Hamiltonian graphs compatible with permanence for $n \geq 6$ [1].

(i) If A is nonsingular, then for the evaluation of the system of inequalities (6) all equilibria with vanishing flux $\Phi(\hat{x}) = 0$ need not be considered. In particular, one may ignore all corner equilibria.

(ii) Denote by $\Gamma(A) \setminus K$ the subgraph of $\Gamma(A)$ which is obtained by removing the vertices in K. Then we need not check all faces F_K for which $\Gamma(A) \setminus K$ has no edges or contains a source vertex or a sink vertex.

Proof. (ii) Suppose $\Phi(x) = 0$, thus $a_{ij}x_ix_j = 0$ for all i, j. If $a_{ij} > 0$ then $x_i = 0$ or $x_j = 0$. Jansen's inequality now reduces to $\sum_{i,j} p_i a_{ij} x_i > 0$. This can be fulfilled provided there is a positive entry in each row and in each column of A, which is guaranteed by the regularity of A.
(ii) If $\Gamma(A) \setminus K$ contains no edges, then F_K consists entirely of rest points, and hence there is no isolated interior rest point on this face. Theorem 5 finally implies that there is no interior isolated rest point in F_K if $Gamma(A) \setminus K$ contains a source or a sink vertex. ∎

4. Networks without Hamiltonian Circuits

Graphs without Hamiltonian circuits arise for instance from the competition hypercycles [4]. A common motif in such models is a branching of the catalytic cycle into parallel reaction pathways. Formally, we will use the following

Definition. An *isolated* Y is a configuration of 3 vertices (f), (s_1) and (s_2), such that the only arcs incident into (s_1) and (s_2) are incident out from (f).

There is no restriction to the arcs at (f) and the arc incident out from (s_1) and (s_2). The coupling along the arcs $(f \to s_1)$ and $(f \to s_2)$ will be denoted by a and b, respectively

Theorem 8. If Γ contains an *isolated* Y, then the catalytic network is not permanent.

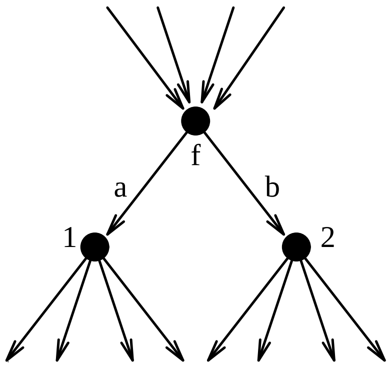

Figure 2: Isolated Y.

Proof. The ODEs for the vertices (a_1) and (s_2) read

$$\begin{aligned} \dot{x}_1 &= x_1\big[ax_f - \Phi\big]\,, \\ \dot{x}_2 &= x_1\big[bx_f - \Phi\big]\,. \end{aligned}$$

From the first two equation we see immediately that the existence of an interior rest point requires therefore $a = b$. The exclusion principle (theorem 1) contradicts permanence in the case $a \neq b$. It remains to show that the system cannot be permanent for $a = b$. We find

$$\frac{\dot{x}_1/x_1}{\dot{x}_2/x_2} = 1 \qquad \Longrightarrow \qquad \ln x_1(t) - \ln x_1(0) = \ln x_2(t) - \ln x_2(0),$$

and hence $x_2(t)/x_3(t) = x_2(0)/x_3(0) = c$ remains constant. Now suppose the system is permanent. Then there is a $\delta > 0$ such that $x_1(t), x_2(t) > \delta$ for some $t > 0$, where δ is independent of the initial condition, and in particular indepent of c. On the other hand we have the inequalities

$$\delta < x_2(t) = x_3(t)\frac{x_2(0)}{x_3(0)} < \frac{x_2(0)}{x_3(0)} = c,$$

which contradict the independence of c and δ. ∎

In fact, we have even stronger consequences for the generic case, which follows immediately from the absence of an interior rest point:

Corollary. If $a \neq b$ then all orbits converge to the boundary ∂S_n.

An interesting type of non-Hamtiltonian Graphs are "*plaits*" consisting of n vertices and the arcs $(k \to k+1)$ and $(k+1 \to k)$. The interaction matrix for such systems are of the form

$$A_{\text{plait}} = \begin{pmatrix} 0 & a_{n-1} & 0 & 0 & \dots & 0 & 0 \\ b_{n-1} & 0 & a_{n-2} & 0 & \dots & 0 & 0 \\ 0 & b_{n-2} & 0 & a_{n-3} & \dots & 0 & 0 \\ 0 & 0 & b_{n-3} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & a_1 \\ 0 & 0 & 0 & 0 & \dots & b_1 & 0 \end{pmatrix} \tag{8}$$

Figure 3: The plait with six vertices.

Lemma 5. For matrices of the form (8) holds

$$\det A = \begin{cases} (-1)^{n/2} a_1 a_3 a_5 \dots a_{n-1} \cdot b_1 b_3 b_5 \dots b_{n-1} & \text{for } n \text{ even,} \\ 0 & \text{for } n \text{ odd.} \end{cases} \tag{9}$$

Proof. By expanding the determinant with respect to the first two columns we find the recursion

$$\det A(n) = (-1) a_{n-1} b_{n-1} \cdot \det A(n-2)$$

where $A(n-k)$ denotes the submatrix of A which is obtained by omitting the first k rows and columns. Iterating this procedure yields the result for even dimensions.

For odd dimensions n the last determinant which has to be evaluated is $\det A(1) = \det[0] = 0$, and hence $\det\ \mathrm{A} = 0$. ∎

A plait can therefore never be permanent if n is odd or if $(-1)^{2n/2} < 0$, i.e., if $n \equiv 0, 1, 3 \bmod n$. The plait with $n = 2$, $\bullet \rightleftharpoons \bullet$, on the other hand is the two-species hypercycle, and thus always permanent. What about the remaining cases, $n = 6, 10, \ldots$?

Theorem 9. A plait is never permanent for $n > 2$.

Proof. We will show that a plait with more then $n = 2$ vertices which has in isolated interior rest point has also a regular saturated equilibrium on the boundary. Theorem 3 then implies that it cannot be permanent.
We will only use the differential equations, counting from left to right in figure 3.

$$\begin{aligned} \dot{x}_1 &= x_1(c_2 x_2 - \Phi) \\ \dot{x}_2 &= x_2(c_3 x_3 + d_1 x_1 - \Phi) \\ \dot{x}_3 &= x_3(c_4 x_4 + d_2 x_2 - \Phi) \end{aligned}$$

Existence of an interior rest point requires $x_2 = \Phi/c_2$ and $x_4 = (\Phi/c_4)(1 - d_2/c_2)$. Since $\Phi > 0$ for an interior equilibrium we can conclude that $c_2 > d_2$ in order to ensure $x_4 > 0$ (For n=3 there is no isolated interior rest point since A is singular). On the boundary there is always a rest point y in the interior of the $(1-2)$ edge, $y_2 = \phi/c_2$ and $y_1 = \phi/d_1$, where $\phi = y_1 y_2 (c_2 + d_1) > 0$ denotes the flux on this rest point. The transversal eigenvalue in (3)-direction is $\lambda_3 = d_2 y_2 - \phi = (d_2/c_2 - 1)\phi$. For $c_2 > d_2$ we have thus $\lambda_3 < 0$. In all other equations neither x_1 nor y_2 occur, thus the transversal eigenvalues are $\lambda_j = -\phi < 0$, with $3 < j \le n$, and hence y is saturated. ∎

Corollary. If a plait with $n > 2$ has an isolated interior rest point then it has at least two hyperbolic sinks on the boundary.

Proof. The rest point in the $(1-2)$ edge is asymptotically stable along this edge (with non-zero eigenvector) and hence it is a hyperbolic sink. Symmetry between the two ends of the plait implies that there are two rest points of this type. ∎

The features of plaits carry over to much more general systems which contain plaits as subgraphs.

Definition. From the directed graph $\Gamma(A)$ with $n > 2$ vertices we obtain the non-directed graph $\Gamma^*(A)$ by drawing an edge between (i) and (j) if there is an arc $(i) \to (j)$ or $(j) \to (i)$. A vertex (k) of $\Gamma^*(A)$ is an *end point* if there is only a single edge at (k). For simplicity we will say that a vertex (k) is an end-point of a directed graph Γ if and only if it is an end-point of the corresponding undirected graph Γ^*.

Theorem 10. If the catalytic network with game matrix A and $n > 2$ is permanent, then $\Gamma(A)$ does not contain an end point.

Proof. As in the proof of the previous theorem we shall show that if there is an isolated interior rest point, then there is also a regular saturated rest point on the boundary. We have to distinguish 2 cases:
(i) The end point is source-vertex or a sink-vertex; then theorem 5 implies that there is no interior restpoint, and hence the network cannot be permanent.
(ii) The endpoint (1) is neither a source nor a sink vertex. It has a unique neighbor (0) which provided the only arc incident into (1) and receives the only arc incident out from (1). The system of differential equations is therefore of the form

$$\begin{aligned}
\dot{x}_1 &= x_1(a_0 x_0 - \Phi) \\
\dot{x}_0 &= x_0(a_1 x_1 + \sum_{i=2}^{n} c_i x_i - \Phi) \\
\dot{x}_j &= x_j(a_j x_0 + \sum_{i=2}^{n} b_{ji} x_i - \Phi)
\end{aligned}$$

where $a_0, a_1 > 0$, and at least some of the constants c_i and d_{ij} are nonzero. The first line yields $\hat{x}_0 = 1/a_0\Phi$ at the interior equilibrium. The third line implies $(a_j/a_0 - 1)\Phi + H_j(x) = 0$ for all $j \geq 2$, where $H_j(x) \geq 0$ is a short hand for the sum term. Suppose first $H_j(x) = 0$; then the existence of an interior rest point implies $b_{ji} = 0$ for all i, j and $a_j = a_0$ and thus A is singular, which contradicts the existence of an isolated interior rest point. Thus $H_j(x) > 0$, and therefore $a_j < a_0$ for all $j \geq 2$. Now consider the rest point $\tilde{s}$ in the interior of the $(0-1)$ edge; it is given by

$$\tilde{x}_1 = \varphi/a_0 \quad \tilde{x}_0 = \varphi/a_1$$

It is stable along the edge. The transversal eigenvalues are given by

$$\lambda_j = \varphi a_j/a_0 - \varphi = (a_j/a_0 - 1)\varphi < 0$$

for all $j \geq 2$ and hence $\tilde{s}$ is a sink. ∎

Corollary. If the undirected graph $\Gamma^*(A)$ is a tree, then equ.(3) is not permanent.

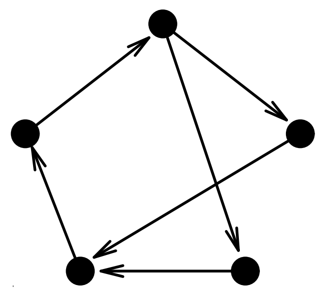

Figure 4: The graph Γ_5 is irreducible and does not contain end points, but it is not Hamiltonian and thus incompatible with permanence.

An irreducible graph without end points contains a Hamiltonian circuit for $n = 3$ and $n = 4$. For $n = 5$, however, Hamiltonicity is a stronger condition. The graph Γ_5 in figure 5, for instance, does not contain a Hamiltonian circuit and is thus not compatible with permanence, but it is irreducible and does not contain an endpoint. Amman's example for $n = 6$ shows that there are permanent networks without a Hamiltonian circuit for $n \geq 6$. On the other hand, irreducibility and the lack of end points does not does not imply that there is a choice of rate constants such that the network becomes permanent as the example in figure 5 shows:

Lemma 6. Let Γ_6 consist of two disjoint circuits $(1 \to 2 \to 3 \to 1)$ and $(4 \to 5 \to 6 \to 4)$ coupled by the arcs $(3 \to 4)$ and $(4 \to 3)$. The graph Γ does not belong to a permanent catalytic network.

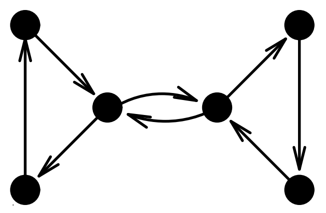

Figure 5: The graph Γ_6 does not contain an end point and still contradicts permanence.

Proof. The system of ODEs for this graph reads

$$\begin{aligned}
\dot{x}_1 &= x_1(a_3x_3 - \Phi) \\
\dot{x}_2 &= x_2(a_1x_1 - \Phi) \\
\dot{x}_3 &= x_3(a_2x_2 + b_4x_4 - \Phi) \\
\dot{x}_4 &= x_4(a_3x_3 + b_6x_6 - \Phi) \\
\dot{x}_5 &= x_5(a_4x_4 - \Phi) \\
\dot{x}_6 &= x_6(a_5x_5 - \Phi)
\end{aligned}$$

A necessary condition for the existence of an interior rest point is $b_4 > a_4$ and $b_6 > a_6$. The subsystem on the $(3,4)$-edge has an interior rest-point $y_3 = 1/b_3 \cdot \varphi$ and $y_4 = 1/b_4 \cdot \varphi$ with transversal eigenvalues $\lambda_1 = (a_3/b_3 - 1)\varphi$, $\lambda_2 = -\varphi$, $\lambda_5 = (a_4/b4 - 1)\varphi$ and $\lambda_6 = -\varphi$, i.e. a sink.

5. Networks with Hamiltonian Circuits

Definition. A catalytic network consisting of a single Hamiltonian circuit is called *hypercycle.*

Theorem 11. A hypercycle is permanent [12, 9].

We have seen in the previous section that the existence of a Hamiltonian circuit is neither necessary nor is it sufficient for permanence. We have, however,

Theorem 12. Let Γ contain an Hamiltionian circuit. Then there is a non-negative matrix A with $\Gamma(A) = \Gamma$ such that the replicator equation (3) is permanent.

Proof. We shall show that all catalytic networks A fulfilling

$$a_{ij} = \begin{cases} 0 & i = j \\ 1 & i = j - 1 \bmod n \\ c_{ij} \leq \epsilon & \text{otherwise} \end{cases} \tag{10}$$

with $\epsilon < 1/n$ are permanent. To this end we show that Jansen's inequalities are satiesfied by $p = \frac{1}{n}(1, 1, \ldots, 1)$. Thus we have to prove that for all isolated rest points $\hat{x}^K \in F_K$ holds

$$\sum_{k \in K} \lambda_k = \sum_{k \in K} \hat{x}^K_{k-1} + \alpha_k(\hat{x}^K) - \varphi(\hat{x}^K) > 0,$$

where $\alpha_k(\hat{x}^K) = \sum_{j \neq k-1} c_{kj} \hat{x}^K_j$. In the following we shall omit the superscript K and the arguments in α_k and φ. We may write the list of all non-vanishing coordinates of $\hat{x}^K$ as follows:

$$N \setminus K = \{r_1, r_1 + 1, r_1 + 2, \ldots, r_1 + s_1, r_2, r_2 + 1, \ldots, r_p + s_p\},$$

with $r_j + s_j + 1 \neq K$. From each component j of the replicator equation we obtain either a linear equation in $\hat{x}_i$ with $i \in N \setminus K$, or an expression for a transversal eigenvalue:

$$
\begin{aligned}
0 &= 0 + \alpha_{r_1} - \varphi \\
0 &= \hat{x}_{r_1} + \alpha_{r_1+1} - \varphi \\
0 &= \hat{x}_{r_1+1} + \alpha_{r_1+2} - \varphi \\
&\vdots \\
0 &= \hat{x}_{r_1+s_1-1} + \alpha_{r_1+s_1} - \varphi \\
\lambda_{r_1+s_1+1} &= \hat{x}_{r_1+s_1} + \alpha r_1 + s_1 + 1 - \varphi \\
\lambda_{r_1+s_1+2} &= 0 + \alpha_{r_1+s_1+2} - \varphi \\
&\vdots \\
\lambda_{r_2-1} &= 0 + \alpha_{r_2-1} - \varphi \\
0 &= 0 + \alpha_{r_2} - \varphi \\
0 &= \hat{x}_{r_2+1} + \alpha_{r_1+2} - \varphi \\
&\vdots \\
0 &= \hat{x}_{r_p+s_p-1} + \alpha_{r_p+s_p} - \varphi \\
\lambda_{r_p+s_p+1} &= \hat{x}_{r_p+s_p} + \alpha r_p + s_p + 1 - \varphi \\
\lambda_{r_p+s_p+2} &= 0 + \alpha_{r_p+s_p+2} - \varphi \\
&\vdots
\end{aligned}
$$

The equations for the coordinates r_i yield the estimates $0 \le \varphi = \alpha_{r_i} \le \epsilon$, from the subsequent equations down to $r_i + s_i$ we find $0 \le \hat{x}_j = \varphi - \alpha_{r_i+1} \le \epsilon$ for all $j \ne r_i + s_i$. Using $\sum_i x_i = 1$ we obtain $\sum_{i=1}^{p} \hat{x}_{r_i+s_i} \ge 1 - \#(N \setminus K)\,\epsilon$. Adding up all transversal eigenvalues yields

$$
\sum_{k\in K} \lambda_k = \sum_i \left(\hat{x}_{r_i+s_i} + \sum_{j=1}^{r_{i+1}-r_i-s_i} (\alpha_{r_i+s_i+j} - \epsilon) \right) \ge 1 - \#(N \setminus K)\epsilon - \#K\epsilon,
$$

where the last term comes from the $\#K$ transversal eigenvalues. Thus Jansen's inequalities become $\sum_{k\in K} \lambda_k(\hat{x}^K) \ge 1 - n \cdot \epsilon > 0$, and we have permanence if $\epsilon < 1/n$. ∎

In the remaining part of this section we will investigate special types of networks with Hamiltonian circuits. All of these will be sparse in the sense that the number of arcs is of the same order as the number of vertices. As a consequence of the above theorem all of them have a range of parameters for which they are permanent.

Definition. A graph Γ will be said to be *pseudo-hypercyclic* if it contains a uniquely defined Hamiltonian arc. An arc which is not contained in this circuit will be called a *short cut*.

Notation. The interaction coefficients along the Hamiltonian arc will be denoted by h_j for the arc $(j) \to (j+1)$. For short cuts we use s_{kj} for $(j) \to (k)$.

Definition. A pseudo-hypercyclic graph is called *easy* if all its short cuts fulfil the following conditions:

(i) Any two short cuts are incident into different vertices.

(ii) If there is a short cut incident into a vertex (x) then there are no short cuts incident out from the precursor $(x-1)$ of (x) along the Hamiltonian circuit.

Lemma 7. An easy network has an isolated interior rest point if and only if for all short cuts $(r \to k)$ holds

$$h_r > s_{kr} \tag{11}$$

Proof. Since any two short cuts incident into different vertices, only two types of equations occur

$$\dot{x}_k = x_k(h_{k-1}x_{k-1} - \Phi)$$
$$\dot{x}_j = x_j(h_{j-1}x_{j-1} + s_{jl}x_l - \Phi)$$

Let (l) be a vertex with a short cut incident out from it. Property (ii) implies that there is no short cut incident into vertex $(l+1)$, and thus

$$\dot{x}_{l+1} = x_{l+1}(h_l x_l - \Phi).$$

The existence of an isolated interior equilibrium is equivalent to a positive solution to $h_l x_l = \Phi$ and $h_j x_j + x_{jl} x_l = \Phi$ for all short cuts $(l \to j)$, i.e.,

$$x_j = \frac{h_l - s_{jl}}{h_j} \cdot x_l > 0.$$

Clearly this equation is equivalent to $h_l > s_{jl}$. ∎

Theorem 13. The pseudo-hypercycle with a single shortcut is permanent if and only if $h_1 > s_{m1}$.

Proof. The system is easy, thus the condition is necessary. By lemma 4 there is only a single isolated restpoint on the boundary which contributes to Jansen's criterion, namely

$$\hat{x}_{bd} = \frac{1}{q}(\frac{1}{s_{m1}}, 0, \ldots, \frac{1}{h_m}, \ldots, \frac{1}{h_n}),$$

where q denotes the sum over all entries in the vector. Substituting into inequality (6) yields

$$\frac{1}{q^2}(\frac{1}{s_{m1}} + \frac{1}{h_m} + \ldots + \frac{1}{h_n}) = \frac{1}{q} < \frac{1}{q}(p_1 + p_m + \ldots + p_n + p_2 \cdot \frac{h_1}{s_{m1}})$$

Using $\sum_j p_j = 1$ and the abbreviation $\xi = p_3 + p4 + \cdot + p_{m-1}$ we find

$$1 < 1 - \xi - p_2 + p_2 \frac{h_1}{s_{m1}} \qquad \Longleftrightarrow \qquad \frac{h_1 - s_{m1}}{s_{m1}} > \frac{\xi}{p_2} > 0$$

Since ξ is independent of p_2 we can choose it arbitrarily small, thus arriving at $h_1 > s_{m1}$ also as sufficient condition for permanence. ∎

Corollary. The hypercycles are the only graphs with a Hamiltonian arc that are permenent irrespective of the choice of the rate constants.

Proof. For any such Γ choose the constants along the Hamiltonian arc $h_i = 1$, choose an arbitrary short cut $(r \rightarrow q)$ with $s_{qr} \gg 1$ sufficiently large and all other connections $b_{ij} < \epsilon$ sufficiently small. Then A is invertible and of the form $A = A_1 + \epsilon B$, where A_1 is a catalytic network with a single short cut. The solution $\hat{x}$ of $Ax = 1$ is arbitratily close to the solution $\hat{x}^*$ of $A_1 x = 1$ if ϵ is chosen sufficiently small. As a consequence of lemma 7 x^* does not have positive components only, otherwise the pseudo-hypercycle with a single short-cut would have an interior rest point for arbitrarily large ratio of s_{qr}/h_r. ∎

For pseudo-hypercycles with two short cuts, $(1 \to m)$ and $(r \to q)$ the situation is more involved. The relations depend crucially on the relative positions of the two short cuts. As shown in figure 6 we may group the various cases into 4 classes depending on the relativ orientation of the two short cuts. Systems A, B, C, D, A', and B' are easy (A' and B' can be considered as degenerate extremal cases of A and B, respectively). The networks B1, D1, and B2, D2 violate condition (ii) in the definition of "easy" once and twice, respectively. The system C1, finally, violates condition (i); it is a special case of the model considered in theorem 14 below. The **proofs** for the conditions in table 1 proceeds case by case and parallels the proof of the theorem 13 above: The necessary condition is the the existence of a unique interior rest point (The sign of det$A$ does not supply more restrictive conditions), and Jansen's inequalities are used to derive sufficient conditions (details of the calculations can be found in [23]).

Table 1. Classification of pseudo-hypercycles with two shortcuts (1,m) and (r,q).

<table>
<tr><th></th><th>Case</th><th>Necessary</th><th>Sufficient</th></tr>
<tr><td>A
B
C
A'
B'</td><td>$1<m<r<q$
$1<r<m<q$
$1<m<q<r$
$1=r,m=q$
$1<q<m=r$</td><td colspan="2">$h_1>s_{m1}, \quad h_r>s_{qr}$</td></tr>
<tr><td>B1
B2</td><td>$1<r=m-1,m<q$
$1<m-1=r,m<n=q$</td><td colspan="2">$h_1>s_{m1}, \quad h_1(h_r-s_{qr})+s_{qr}s_{m1}$</td></tr>
<tr><td>C1</td><td>$1<r<m=q$
$1<m=q<r$</td><td colspan="2">$s_{m1}/h_1+s_{qr}/h_q<1$</td></tr>
<tr><td>D</td><td>$1<q<r<m$</td><td>$h_1>s_{m1}, \quad h_r>s_{qr}$</td><td>$\frac{h_1-s_{m1}}{s_{m1}}>\frac{s_{qr}}{h_r-s_{qr}}>0$</td></tr>
<tr><td>D1</td><td>$q=2<r<m$</td><td>$h_r(h_1-s_{m1})+s_{m1}s_{qr}>0, \quad h_r>s_{qr}$</td><td>$h_1>s_{m1}, \quad h_r>s_{qr}$</td></tr>
<tr><td>D2</td><td>$q=2,r=m-1$</td><td>$(h_1-s_{m1})(h_r-s_{qr})>0$</td><td>$h_1>s_{m1}, \quad h_r>s_{qr}$</td></tr>
</table>

The conditions in table 1 can be simplified considerably by using the dimensionless parameters $\alpha = s_{m1}/h_1$ and $\beta = s_{qr}/h_r$. A graphical representation for the various cases is given in figure 7.

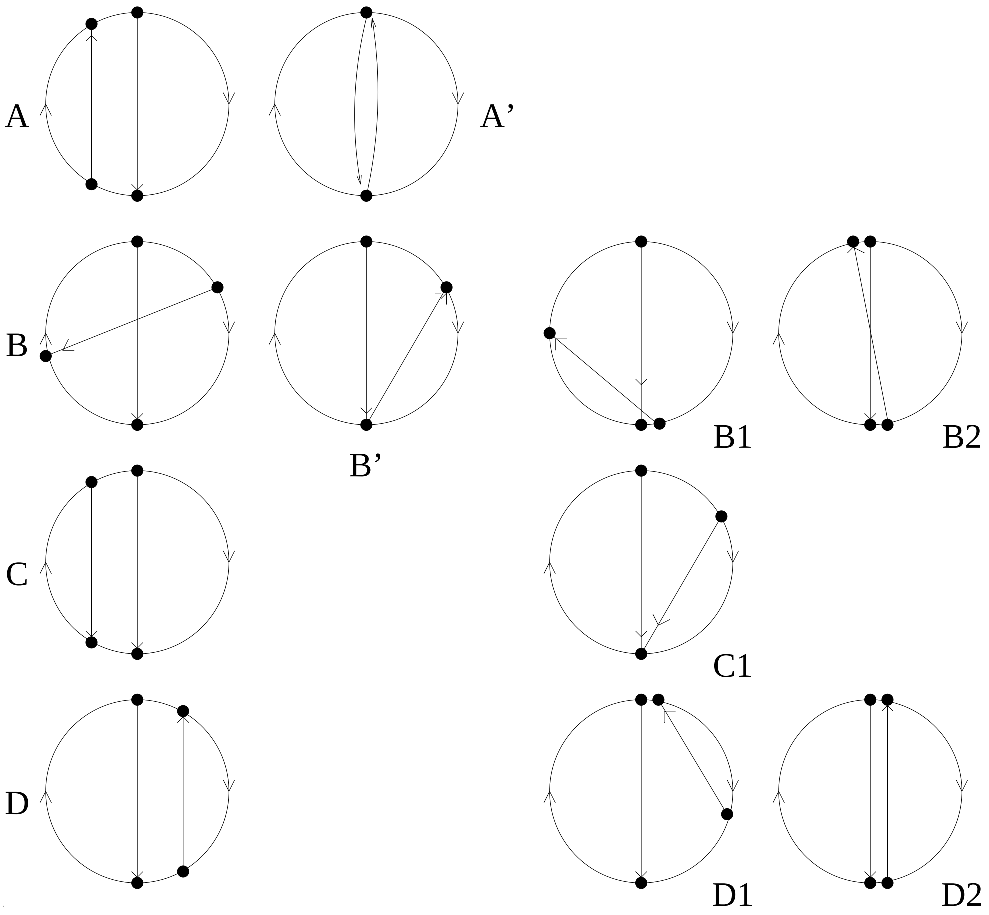

Figure 6: Topologies of pseudo-hypercycles with two short cuts.

Theorem 14. A pseudo-hypercycle with ν shortcuts (k_i, m), $i = 1, \ldots, \nu$ all ending in m is permanent if and only if

$$\sum_{i=1}^{\nu} \frac{h_{k_i}}{s_{mk_i}} < 1.$$

Proof. For an interior rest point one obtains the $x_j = \Phi/h_j$ for $j \neq m-1$ and $x_{m-1} = \frac{1}{h_{m-1}}(1 - \sum_{i=1}^{\nu} s_{mk_i}/h_{k_i})$. Thus the condition is necessary. The relevant rest points on the boundary are by Lemma 3.2

$$\hat{x}_w = \frac{1}{q_w}\left(\frac{1}{h_1}, \ldots, \frac{1}{h_{k_w}}, \frac{(1-\Psi_w)}{s_{mk_w}}, 0, \ldots, 0, \frac{1}{h_m}, \ldots, \frac{1}{h_n}\right)$$

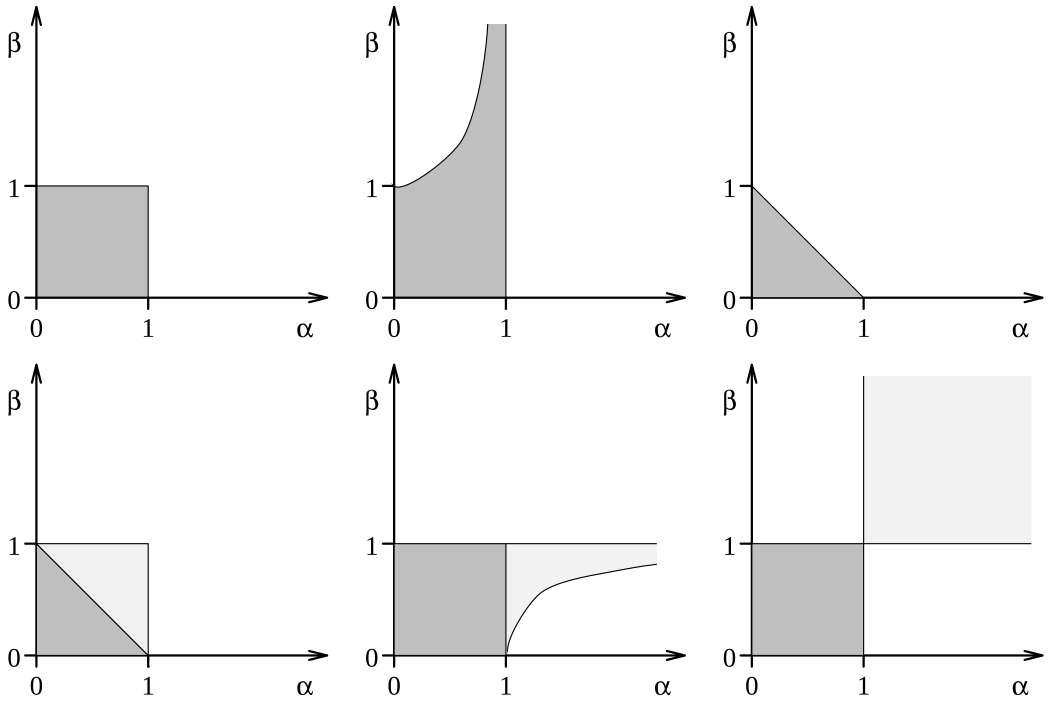

Figure 7: Permanence for pseudo-hypercycles with two shortcuts.
a) Cases A, B, C, A', and B'; **b)** Cases B1 and B2; **c)** Case C1; **d)** Case D; **e)** Case D1; **f)** Case D2.
Permanence can be proven for the dark-shaded regions be means of Jansen's inequalities. Light-gray regions correspond to parameter values which fulfil all necessary conditions for permanence that are discussed in this paper, for which a sufficient condition could not be established, however. In the non-shaded regions permanence is ruled out.

with the abbreviation $\Psi_w = \sum_{i=1}^{w} s_{mk_i}/h_{k_i}$. Jansen's inequalities become

$$p_{k_w}\frac{h_{k_w}}{s_{mk_w}}(1-\Psi_{w-1}) > p_{k_w} + \ldots + p_{m-1} \qquad 1 \le w \le \nu$$

and bringing p_{k_w} to the left side yields

$$p_{k_w}\frac{h_{k_w}}{s_{mk_w}}(1-\Psi_{w}) > p_{k_w+1} + \ldots + p_{m-1} \qquad 1 \le w \le \nu$$

Each of these inequalities can be fulfilled for some $p \in \operatorname{int} S_n$ if and only if $\Psi_w < 1$ for all w, or equivalently, if and only if $\Psi_\nu < 1$. ∎

6. Conclusions

A simple and straight forward representation of autocatalytic networks by directed graphs $\Gamma(A)$ was suggested as a tool for classification [4] and turned out to be useful also for the analysis of their dynamical behaviour [1, 4, 12, 11, 22]. Certain properties of the directed graph $\Gamma(A)$, namely the presence of source or sink vertices, rule out the existence of of regular rest points in the interior of the simplex independent of the particular choice of rate constants A. Thus a large and easily recognized class of autocatalytic networks are ruled out as candidates for permanence. Further properties of the graphs $\Gamma(A)$ are incompatible with permanence. End points in the graph, for example, contradict permanence and this provides a stronger criterion than irreducibility [22]. Such general criteria, however, are rare and a huge class of graphs remains for which a quick inspection does not allow for decisive conclusions on permanence of the corresponding networks.

Clearly we cannot expect a one-to-one relationship between graphs and dynamical properties of the network. For a large class of networks the dynamics changes with a change in the numerical values of the (non-zero) rate constants. For example, there is a choice of rate constants for every Hamiltonian graph such that makes this system permanent. It has been shown, on the other hand, the existence of a Hamiltonian arc is neither a sufficient nor a necessary general condition for permanence. Hypercycles were considered to be special because they are simplest sparse autocatalytic networks showing permanence [4]. What makes hypercycles even more interesting is that they are the only known graphs having this property independent of the choice of the rate constants. We have indeed shown that no other catalytic network with a Hamiltonian arc can have this property, and it is hard to imagine how any other graph could then be permanent for all rate constants.

It is interesting to note that the conditions derived from Jansen's theorem often lead to necessary and sufficient conditions for permanence in sparse networks with certain topologies, whereas in general most networks fulfilling the necessary conditions for permanence (section 2) do not fulfil Jansen's criterion. For an extensive numerical study on this issue see [24].

Our conclusions thus is that a representation of dynamical systems of a particular class, such as autocatalytic networks, in terms of graphs may be helpful but is by no means sufficient to understand and classify the long-time behaviour. This is even true on a rather coarse grained resolution of the dynamics dealing with properties such as permanence, which is far beyond the level of individual attractors.

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