

Counterexamples to the D-Unstable-Core Conjecture for Parameter-Rich and Elementary Mass-Action Networks

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Abstract

Vassena and Stadler conjectured that a reaction network with parameter-rich kinetics cannot have an unstable positive equilibrium without a D-unstable core, a minimal square child-selection submatrix that becomes unstable under positive column scaling. We give two exact counterexamples on four species. The first has five reactions and an admissible rational reactivity matrix whose Jacobian has eigenvalue $\frac{1}{500} + \frac{51}{500}i$ with a Gaussian-integer eigenvector. A positive kernel flux gives an explicit generalized-mass-action equilibrium. The second has six reactions, at most two molecules on each side of every reaction, and no catalysts. Under classical mass action with fixed integer kinetic orders it has a positive rational equilibrium with an integer Jacobian and a strictly unstable complex conjugate pair. The two networks have the same reactant incidence relation and the same 24 nonempty child selections, although their stoichiometric child matrices differ. Exact weighted symmetrizations, triangular blocks and cubic factorizations show that every child matrix is D-nonunstable in both examples. Permanent zero eigenvalues in an exceptional child explain why D-noninstability must be distinguished from strict D-stability. Both counterexample theorems have Lean 4 proofs with Mathlib. For the elementary example, a shifted-quartic intermediate-value argument gives strict instability, and a separate asymptotic calculation explains the circulation and fast-branch mechanism. These results concern linear instability at a positive equilibrium; they do not assert a Hopf bifurcation or a nonlinear periodic orbit.

1 Introduction

A recurring theme in chemical reaction network theory is that dynamical properties which depend on unknown kinetic parameters can sometimes be decided from stoichiometry alone. For the question of whether a network can have an unstable positive equilibrium, Vassena and Stadler [1] gave a remarkably clean sufficient condition in the setting of *parameter-rich* kinetics, a class that contains generalized mass action [4] and Michaelis–Menten kinetics. Their tool is the *child selection*: an injective assignment J of distinct reactions to a subset κ of species such that each species is a reactant of its assigned reaction. The square submatrix $S[\kappa]$ of the stoichiometric matrix S obtained by selecting the columns $J(\kappa)$ in the order of κ is a *child-selection matrix*. A child-selection matrix is *D-unstable* if $S[\kappa]D$ has an eigenvalue with positive real part for some positive diagonal matrix D , and a *D-unstable core* is a D-unstable child-selection matrix none of whose proper principal submatrices is D-unstable. Through a Cauchy–Binet expansion of the characteristic polynomial, Vassena and Stadler prove that a D-unstable core forces the existence of parameters at which the network has a positive equilibrium with a Hurwitz-unstable Jacobian [1, Cor. 12, Cor. 13].

The converse is the natural question, and it was raised explicitly. In the words of [1, Conj. 17]: “Suppose that the network does not possess any D-unstable core. Then $G(r')$ cannot

be Hurwitz-unstable and thus the network Γ does not admit instability.” The conclusion of that paper restates the position: unstable cores “provide a sufficient condition for network instability”, and “we conjecture that the slightly more general D-unstable cores are even necessary”. If true, the conjecture would make instability of parameter-rich networks a purely stoichiometric, finitely checkable property.

Main results

We show that the conjecture is false, already for four species.

Theorem 1.1. *There is a reaction network Γ with four species and five reactions, without catalysts, admitting a strictly positive equilibrium flux, and an admissible reactivity matrix R (positive exactly on reactant incidences), such that*

- (i) *the Jacobian $G = SR$ has the eigenvalue $\lambda = \frac{1}{500} + \frac{51}{500}i$, so G is Hurwitz-unstable;*
- (ii) *every child-selection matrix of Γ is D-nonunstable: for every child selection κ and every positive diagonal D , no eigenvalue of $S[\kappa]D$ has positive real part.*

Consequently Γ possesses no D-unstable core, and Γ endowed with generalized mass-action kinetics admits instability in the sense of [1, Def. 2]. Conjecture 17 of [1] is false.

Classical mass action fixes the kinetic orders to the integer reactant stoichiometries, so its reactivities cannot be chosen independently. Our second result shows that this additional constraint, even with at most two molecules on either side of every reaction, does not restore necessity of a D-unstable core.

Theorem 1.2. *There is a reaction network Γ_{elem} with four species and six reactions, with reactant and product matrices satisfying*

$$\sum_i Y_{ij} \leq 2, \quad \sum_i P_{ij} \leq 2, \quad Y_{ij}P_{ij} = 0 \quad \text{for all } i, j,$$

and positive rational classical mass-action rate constants and a positive rational equilibrium $\bar{x}$, such that

- (i) *its Jacobian G_{elem} has integer entries and a nonreal eigenvalue λ with $0 < \text{Re } \lambda < 5$;*
- (ii) *every child-selection matrix is D-nonunstable, so the network has no D-unstable core.*

Thus the absence of D-unstable cores does not exclude an unstable positive equilibrium even in a two-sided elementary bimolecular network under classical mass action.

In the parameter-rich construction, every number is an explicit rational and the unstable eigenvector has Gaussian-integer entries. For both networks, the child certificates are finite exact identities. The argument is therefore checkable by hand, by exact computer algebra, and by a proof assistant. We took the third route seriously: the complete chain from the literal network data to the negation of the universal necessity statement is verified in Lean 4 [19] on top of Mathlib [20], with warnings treated as errors and no `sorry`. Section 7 describes the formalization and records the toolchain and content hashes needed to reproduce it.

What the counterexample shows

The first example isolates three features of the obstruction. The second shows that the phenomenon persists when kinetic orders are fixed by elementary reactant complexes.

The obstruction is collective. Every square child of S is safe under every positive column scaling, yet a positive combination of whole reaction columns produces a complex eigenvalue in the open right half-plane. The instability is not stored in any single child selection; it is created by cross-terms between independently tunable derivatives that belong to different reactions and cannot be separated by choosing one reaction per species.

Boundary spectra matter. One maximal child of the example is not diagonally dissipative and its scaled characteristic polynomial factors as $X(X + 4d_0)(X + 4d_1 + 2d_2)$: it carries a permanent zero eigenvalue. Under the strict notion of D-stability it would not count as stable; under the boundary-permitting negation of D-instability, which is the notion the conjecture actually uses, it is harmless. Any argument that silently replaces “not D-unstable” by “D-stable” misclassifies this child.

Consistency is not automatic. The first source we found had a nonsingular 4×4 stoichiometric matrix and hence no positive equilibrium flux. It refutes a matrix-level statement but not the conjecture as posed, since parameter-rich models require a positive equilibrium. Appending one reactant-free inflow reaction repairs consistency without changing either the Jacobian or the lattice of child selections. This scope correction was found by a literature audit after the matrix-level result had already been formalized.

Related work

Child selections were introduced by Vassena as the combinatorial carrier of the Cauchy–Binet expansion of characteristic-polynomial coefficients [2, 3]. For instability through a positive *real* eigenvalue the localization to child-selection determinant signs is exact: Vassena’s sign-change results give sufficiency, and the necessity direction is established in the formal development accompanying this paper (Section 6). The failure exhibited here lives entirely in the complex (Hopf-type) branch. D-stability and its relatives have a long history in economics and matrix theory [5, 6, 7, 8, 9]; the gap between diagonal (Volterra–Lyapunov) stability, D-stability, and boundary-permitting D-noninstability is precisely the gap that our exceptional child occupies. Rank-one and non-square variants of D-stability are known to resist general theorems [10, 11]. Graph-theoretic and combinatorial approaches to Hopf bifurcations in reaction networks include [12, 13]; classical stability analysis of networks through Routh–Hurwitz conditions goes back to Clarke [14]. The autocatalytic-core notion of Blokhuis, Lacoste and Nghe [15], shown in [1] to coincide with Metzler unstable-positive feedbacks, is not involved: no child-selection matrix of the network below is Hurwitz-unstable, so by [1, Cor. 26] the network is not autocatalytic, and its Jacobian instability is of complex-pair type with no positive real eigenvalue. Injectivity-type results that exclude multistationarity [16, 17, 18] concern uniqueness of equilibria rather than their stability.

Organization

Section 2 fixes definitions and states the refuted implication precisely. Sections 3–4 prove the parameter-rich counterexample, Theorem 1.1. Section 5 proves the elementary classical mass-action counterexample, Theorem 1.2, and explains its circulation and fast-branch mechanism. Section 6 discusses what fails and what survives. Section 7 records the separate formal-verification histories, Section 8 the discovery of the parameter-rich example, and Section 9 the remaining questions. Appendix A gives the original exact certificates and reproduction information.

2 Setting

2.1 Networks, reactivities, and Jacobians

A reaction network on species $\{X_0, \dots, X_{n-1}\}$ and reactions $\{r_0, \dots, r_{m-1}\}$ is given by reactant and product matrices $Y, P \in \mathbb{N}^{n \times m}$; the stoichiometric matrix is $S = P - Y \in \mathbb{Z}^{n \times m}$. Species X_i is a *reactant* of r_j if $Y_{ij} > 0$. We write $\text{supp}(Y) = \{(i, j) : Y_{ij} > 0\}$ for the reactant incidence relation. Throughout we index species and reactions from 0, matching the formal development.

Following [1, Def. 1, Def. 3], a kinetic model assigns to every reaction a nonnegative rate $r_j(x)$ that depends only on the concentrations of its reactants and increases in each of them. At a positive state $\bar{x}$ the *reactivity matrix* is $R_{ji} = \partial r_j / \partial x_i(\bar{x})$, and the Jacobian of $\dot{x} = Sr(x)$ is $G = SR$. A kinetic model is *parameter-rich* if, for every positive equilibrium $\bar{x}$ and every matrix R with

$$R_{ji} > 0 \iff Y_{ij} > 0, \quad R_{ji} = 0 \iff Y_{ij} = 0, \quad (1)$$

there are parameters realizing $\bar{x}$ as an equilibrium with reactivity R . We call a matrix $R \in \mathbb{R}^{m \times n}$ satisfying (1) an *admissible reactivity* for the network. Generalized mass action (GMA), $r_j(x) = a_j \prod_i x_i^{c_{ji}}$ with $c_{ji} \neq 0$ exactly on reactant incidences, is parameter-rich [1, Lemma 6]: for any $\bar{x} > 0$, any positive flux $\bar{r}$ with $S\bar{r} = 0$, and any admissible R , the choice $c_{ji} = \bar{x}_i R_{ji} / \bar{r}_j$, $a_j = \bar{r}_j \prod_i \bar{x}_i^{-c_{ji}}$ realizes both.

In *classical mass action*, the kinetic orders are fixed to the integer reactant stoichiometries:

$$r_j(x) = k_j \prod_i x_i^{Y_{ij}}, \quad R_{ji} = \frac{r_j(\bar{x}) Y_{ij}}{\bar{x}_i}, \quad R = \text{diag}(r(\bar{x})) Y^\top \text{diag}(\bar{x})^{-1}. \quad (2)$$

For an inflow, the empty product is 1 and its reactivity row is zero. Unlike GMA with freely chosen kinetic orders, classical mass action is not generally parameter-rich on a fixed network.

The existence of a positive equilibrium requires a positive flux vector in the kernel of S . We isolate this standing hypothesis.

Definition 2.1 (Consistency). A network is *consistent* if there exists $f \in \mathbb{R}_{>0}^m$ with $Sf = 0$.

A network with a parameter-rich kinetic model *admits instability* [1, Def. 2] if some choice of parameters gives a positive equilibrium whose Jacobian is Hurwitz-unstable, i.e. has an eigenvalue with strictly positive real part. By [1, Obs. 4], for a consistent network with a parameter-rich model this holds if and only if SR is Hurwitz-unstable for some admissible R .

2.2 Child selections and D-instability

Definition 2.2 (Child selection, [1, Def. 7]). A *child selection* is a pair $\kappa = (\kappa, J)$ with κ a nonempty set of species and $J : \kappa \rightarrow \{r_0, \dots, r_{m-1}\}$ injective such that X_i is a reactant of $J(i)$ for every $i \in \kappa$. Its *child-selection matrix* is the $|\kappa| \times |\kappa|$ matrix

$$S[\kappa]_{il} = S_{i, J(l)}, \quad i, l \in \kappa.$$

A child selection κ' is a *restriction* of κ if $\kappa' \subseteq \kappa$ and $J' = J|_{\kappa'}$; then $S[\kappa']$ is the principal submatrix of $S[\kappa]$ on the rows and columns of κ' [1, Obs. 9].

Note that a child selection chooses a whole column of S for each selected species. It cannot keep a favourable entry of a column while discarding other entries of the same column; this whole-column ownership will matter in Section 6.

Definition 2.3 (Spectral notions). Let $A \in \mathbb{R}^{k \times k}$ and let $\mathcal{D}_k$ denote the set of positive diagonal $k \times k$ matrices.

- (a) A is *Hurwitz-unstable* if it has an eigenvalue λ with $\text{Re } \lambda > 0$.

- (b) A is D -unstable if AD is Hurwitz-unstable for some $D \in \mathcal{D}_k$.
- (c) A is D -nonunstable if it is not D -unstable: for every $D \in \mathcal{D}_k$, every eigenvalue of AD has real part ≤ 0 .
- (d) A is D -stable if for every $D \in \mathcal{D}_k$, every eigenvalue of AD has real part < 0 .

D -stability implies D -noninstability, but not conversely: purely imaginary and zero eigenvalues are permitted by (c) and excluded by (d). The conjecture is a statement about (b) and its negation (c); D -stability plays no role in it. We keep the two notions rigorously apart.

Definition 2.4 (D -unstable core, [1, Def. 16]). A child selection κ is a D -unstable core if $S[\kappa]$ is D -unstable and $S[\kappa']$ is not D -unstable for every proper restriction $\kappa' \subsetneq \kappa$.

Since restrictions of child selections are again child selections, a finite descent shows that every D -unstable child selection contains a D -unstable core. Hence:

Lemma 2.5. *A network has a D -unstable core if and only if it has a D -unstable child-selection matrix. In particular, if every child-selection matrix is D -nonunstable, then the network has no D -unstable core.*

2.3 The refuted statement

We can now state the implication whose negation we prove. Fix $n = 4$ species and $m = 5$ reactions.

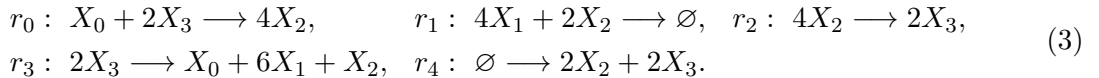
(N) For every consistent network Γ on 4 species and 5 reactions and every admissible reactivity R : if SR is Hurwitz-unstable, then Γ has a D -unstable core.

Statement (N) is the restriction of [1, Conj. 17] to consistent networks of this size, with “admits instability” unfolded through [1, Obs. 4]. Its negation, which is the terminal theorem of the formal development, is exactly what Theorem 1.1 provides. The universal conjecture for arbitrary networks fails a fortiori.

3 The counterexample

3.1 The network

Let Γ be the network on species X_0, X_1, X_2, X_3 with the five reactions



There are no catalysts: no species appears on both sides of a reaction. The reactant and stoichiometric matrices are

$$Y = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 2 & 4 & 0 & 0 \\ 2 & 0 & 0 & 2 & 0 \end{pmatrix}, \quad S = P - Y = \begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ 0 & -4 & 0 & 6 & 0 \\ 4 & -2 & -4 & 1 & 2 \\ -2 & 0 & 2 & -2 & 2 \end{pmatrix}, \quad (4)$$

with rows indexed by species and columns by reactions. Because there are no catalysts, the reactant incidences are exactly the negative entries of S :

$$\text{supp}(Y) = \{(0, 0), (1, 1), (2, 1), (2, 2), (3, 0), (3, 3)\}. \quad (5)$$

In words: X_0 reacts only in r_0 ; X_1 only in r_1 ; X_2 in r_1 and r_2 ; X_3 in r_0 and r_3 . Reaction r_4 is a reactant-free inflow.

Proposition 3.1 (Consistency). Γ is consistent: $f = (2, 3, 2, 2, 2)^\top$ is strictly positive and $Sf = 0$.

Proof. Row by row, $-2 + 2 = 0$; $-12 + 12 = 0$; $8 - 6 - 8 + 2 + 4 = 0$; $-4 + 4 - 4 + 4 = 0$. $\square$

The role of r_4 is only to supply this flux. The first four columns form a nonsingular matrix ($\det S_{[0..3]} = 48$), so without r_4 the network would have no positive equilibrium. Since r_4 has no reactants, the row of every admissible reactivity indexed by r_4 is identically zero, so r_4 contributes nothing to any Jacobian SR and cannot be selected by any child selection. Thus r_4 changes neither the Jacobians nor the lattice of child selections of the four-reaction network; it only moves the example into the scope of the conjecture.

3.2 The reactivity and the Jacobian

Put

$$E = \frac{5187522222797}{46658000000}, \quad F = \frac{28200219703}{46658000000}, \quad (6)$$

and define $R \in \mathbb{Q}^{5 \times 4}$ (rows indexed by reactions, columns by species) by

$$R = \begin{pmatrix} 1 & 0 & 0 & E \\ 0 & \frac{1}{50} & \frac{1}{1000} & 0 \\ 0 & 0 & \frac{5}{11} & 0 \\ 0 & 0 & 0 & F \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (7)$$

Comparing with (5), $R_{ji} > 0$ exactly when $(i, j) \in \text{supp}(Y)$, so R is admissible. The Jacobian is

$$G = SR = \begin{pmatrix} -1 & 0 & 0 & -E + F \\ 0 & -\frac{2}{25} & -\frac{1}{250} & 6F \\ 4 & -\frac{1}{25} & -\frac{1}{500} - \frac{20}{11} & 4E + F \\ -2 & 0 & \frac{10}{11} & -2E - 2F \end{pmatrix}. \quad (8)$$

Proposition 3.2 (Exact unstable eigenpair). Let $\lambda = \frac{1}{500} + \frac{51}{500}i$ and

$$v = \begin{pmatrix} -152886431705 + 15563289455i \\ 23331004034 - 30699360512i \\ 7890610882 + 34396287629i \\ 1399740000 \end{pmatrix} \in \mathbb{Z}[i]^4.$$

Then $Gv = \lambda v$. Hence G is Hurwitz-unstable, with $\text{Re } \lambda = \frac{1}{500} > 0$.

Proof. Direct exact multiplication over $\mathbb{Q}(i)$; each of the four coordinate identities is a rational identity. The characteristic polynomial of G factors over $\mathbb{Q}$ as

$$\chi_G(X) = \frac{(125000X^2 - 500X + 1301)(513238000X^2 + 116236430203X + 13005481800)}{6415475000000},$$

and the first quadratic factor has roots $\frac{1}{500} \pm \frac{51}{500}i$ since $500^2 - 4 \cdot 125000 \cdot 1301 = -25500^2$. The remaining two eigenvalues are real and negative (approximately -226.36 and -0.112). $\square$

Thus the unstable equilibrium is of oscillatory (complex-pair) type: G has no positive real eigenvalue, $\det G > 0$, and every coefficient of χ_G is positive. The instability is detected only by the third Hurwitz determinant of the quartic, which is negative. This is the branch of the problem that child-selection determinant signs cannot see.

3.3 An explicit generalized-mass-action realization

Theorem 1.1 is stated at the level of the symbolic Jacobian, as is Conjecture 17. For concreteness we also give a kinetic model.

Proposition 3.3 (GMA realization). *Endow Γ with the generalized mass-action rates*

$$r_0 = 2x_0^{1/2}x_3^{E/2}, \quad r_1 = 3x_1^{1/150}x_2^{1/3000}, \quad r_2 = 2x_2^{5/22}, \quad r_3 = 2x_3^{F/2}, \quad r_4 = 2.$$

Then $\bar{x} = (1, 1, 1, 1)$ is a positive equilibrium of $\dot{x} = Sr(x)$ with flux $r(\bar{x}) = (2, 3, 2, 2, 2)$, and the Jacobian at $\bar{x}$ is exactly the matrix G of (8). In particular, Γ with GMA kinetics admits instability.

Proof. At $\bar{x} = \mathbf{1}$ the fluxes are the prefactors $(2, 3, 2, 2, 2) = f$, and $Sf = 0$ by Proposition 3.1. For GMA, $\partial r_j / \partial x_i = c_{ji}r_j/x_i$, which at $\bar{x}$ equals $c_{ji}f_j$; the exponents were chosen as $c_{ji} = R_{ji}/f_j$, so the reactivity at $\bar{x}$ is R and the Jacobian is $SR = G$. The exponents are nonzero exactly on reactant incidences, as GMA requires. $\square$

The exponents are rational but not integers, so this realization is generalized rather than classical mass action. Section 5 modifies the stoichiometric coefficients while preserving the reactant incidence relation (5), and obtains an elementary classical mass-action counterexample. Whether the original fixed network Γ itself admits such an equilibrium remains a separate question.

4 Every child-selection matrix is D-nonunstable

4.1 The child-selection lattice

From (5), species X_0 and X_1 have a unique admissible reaction each (r_0 and r_1), while X_2 may choose r_1 or r_2 and X_3 may choose r_0 or r_3 . Call $J(2) = r_1$ and $J(3) = r_0$ the *exceptional edges*; the other choices form the *diagonal* assignment $J(i) = r_i$. Reaction r_4 is never selectable. A direct enumeration gives 24 child selections (6 singletons, 11 pairs, 6 triples, 1 quadruple), and exactly four of them are maximal with respect to restriction:

$$\kappa_{\text{id}} = (\{0, 1, 2, 3\}, i \mapsto r_i), \quad A_{\text{id}} = S[\kappa_{\text{id}}] = \begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & -4 & 0 & 6 \\ 4 & -2 & -4 & 1 \\ -2 & 0 & 2 & -2 \end{pmatrix}, \quad (9)$$

$$\kappa_a = (\{0, 2, 3\}, (0, 2, 3) \mapsto (r_0, r_1, r_3)), \quad A_a = \begin{pmatrix} -1 & 0 & 1 \\ 4 & -2 & 1 \\ -2 & 0 & -2 \end{pmatrix}, \quad (10)$$

$$\kappa_b = (\{1, 2, 3\}, (1, 2, 3) \mapsto (r_1, r_2, r_0)), \quad A_b = \begin{pmatrix} -4 & 0 & 0 \\ -2 & -4 & 4 \\ 0 & 2 & -2 \end{pmatrix}, \quad (11)$$

$$\kappa_2 = (\{2, 3\}, (2, 3) \mapsto (r_1, r_0)), \quad A_2 = \begin{pmatrix} -2 & 4 \\ 0 & -2 \end{pmatrix}. \quad (12)$$

Lemma 4.1 (Classification). *Every child selection of Γ is a restriction of the maximal selection assigned by the following table, according to which exceptional edges it uses:*

<i>uses $J(2) = r_1$</i>	<i>uses $J(3) = r_0$</i>	<i>restriction of</i>
<i>yes</i>	<i>yes</i>	κ_2
<i>yes</i>	<i>no</i>	κ_a
<i>no</i>	<i>yes</i>	κ_b
<i>no</i>	<i>no</i>	κ_{id}

Proof. Let (κ, J) be a child selection. If $J(2) = r_1$ then $1 \notin \kappa$, since X_1 can only select r_1 and J is injective. If $J(3) = r_0$ then $0 \notin \kappa$ for the same reason. In the first row of the table, $\kappa \subseteq \{2, 3\}$ and J agrees with κ_2 . In the second row, $\kappa \subseteq \{0, 2, 3\}$ and $J(3)$, if defined, is r_3 ; so J agrees with κ_a . In the third row, $\kappa \subseteq \{1, 2, 3\}$ and $J(2)$, if defined, is r_2 ; so J agrees with κ_b . In the last row every selected species uses its diagonal reaction, so J agrees with κ_{id} . This assigns a covering maximal selection to each child. A child may also extend to another maximal selection: for example, a singleton that uses neither exceptional edge can be a restriction of several maxima. The argument needs a cover, not a unique maximal extension. $\square$

By Lemma 4.1, it suffices to show that the four maximal child matrices and all their principal submatrices are D-nonunstable. For three of them a single hereditary certificate does this; the fourth needs a separate argument.

4.2 Weighted symmetrization certificates

Definition 4.2. For $A \in \mathbb{R}^{k \times k}$ and a weight vector $p \in \mathbb{R}_{>0}^k$ with $P = \text{diag}(p)$, the *weighted symmetrization* is the symmetric matrix

$$\mathcal{M}(A, p) = -(PA + A^\top P).$$

Lemma 4.3 (Dissipativity bridge). *Let $A \in \mathbb{R}^{k \times k}$ and $p \in \mathbb{R}_{>0}^k$. If $\mathcal{M}(A, p)$ is positive semidefinite, then*

- (a) *A is D-nonunstable;*
- (b) *for every nonempty $I \subseteq \{1, \dots, k\}$, the principal submatrix $A[I]$ is D-nonunstable, with certificate $\mathcal{M}(A[I], p|_I) = \mathcal{M}(A, p)[I]$.*

Proof. (a) Let D be positive diagonal and let $ADz = \lambda z$ with $z \in \mathbb{C}^k \setminus \{0\}$. Put $u = Dz \neq 0$, so that $Au = \lambda D^{-1}u$. Multiplying on the left by u^*P and taking real parts,

$$\text{Re}(u^*PAu) = \frac{1}{2} u^*(PA + A^\top P)u = -\frac{1}{2} u^*\mathcal{M}(A, p)u \leq 0, \quad u^*PD^{-1}u > 0,$$

because PD^{-1} is positive diagonal. Hence $\text{Re } \lambda \leq 0$. (b) The matrix $\mathcal{M}(A, p)[I]$ equals $\mathcal{M}(A[I], p|_I)$ entrywise, and a principal submatrix of a positive semidefinite matrix is positive semidefinite; apply (a). $\square$

We call a matrix with such a certificate *diagonally dissipative*. Note that the certificate only yields $\text{Re } \lambda \leq 0$; it does not, and need not, exclude imaginary-axis eigenvalues.

Proposition 4.4 (Three PSD covers). *The following weighted symmetrizations are positive semidefinite (in fact positive definite):*

$$\begin{aligned}\mathcal{M}(A_2, (1, 2)) &= \begin{pmatrix} 4 & -4 \\ -4 & 8 \end{pmatrix}, \\ \mathcal{M}(A_a, (10, 2, 7)) &= \begin{pmatrix} 20 & -8 & 4 \\ -8 & 8 & -2 \\ 4 & -2 & 28 \end{pmatrix}, \\ \mathcal{M}(A_{\text{id}}, (100, 35, 40, 140)) &= \begin{pmatrix} 200 & 0 & -160 & 180 \\ 0 & 280 & 80 & -210 \\ -160 & 80 & 320 & -320 \\ 180 & -210 & -320 & 560 \end{pmatrix}.\end{aligned}$$

Consequently A_2 , A_a , A_{id} and all their principal submatrices are D -nonunstable.

Proof. The leading principal minors are, respectively,

$$(4, 16), \quad (20, 96, 2608), \quad (200, 56000, 9472000, 1524480000),$$

all positive, so each matrix is positive definite by Sylvester's criterion. Exact $LDL^\top$ factorizations, which are the sum-of-squares form used in the formal proof, are listed in Appendix A. Apply Lemma 4.3. $\square$

4.3 The exceptional child

The maximal child κ_b is different. Its matrix A_b in (11) is singular ($\det A_b = 0$), so no weighted symmetrization of A_b can be positive definite, and a short computation shows that none is positive semidefinite either: the $(2, 3)$ block $\begin{pmatrix} -4 & 4 \\ 2 & -2 \end{pmatrix}$ forces $p_3 = 2p_2$ from the 2×2 minor and then the full 3×3 minor is negative. Thus A_b is not diagonally dissipative and Lemma 4.3 does not apply. Nevertheless:

Proposition 4.5 (Exact cubic factorization). *For every positive diagonal $D = \text{diag}(d_0, d_1, d_2)$,*

$$\det(XI - A_b D) = X(X + 4d_0)(X + 4d_1 + 2d_2).$$

Hence the spectrum of $A_b D$ is $\{0, -4d_0, -(4d_1 + 2d_2)\}$, and A_b is D -nonunstable but not D -stable.

Proof. $A_b D = \begin{pmatrix} -4d_0 & 0 & 0 \\ -2d_0 & -4d_1 & 4d_2 \\ 0 & 2d_1 & -2d_2 \end{pmatrix}$ is block lower triangular with the 1×1 block $-4d_0$ and the 2×2 block $B = \begin{pmatrix} -4d_1 & 4d_2 \\ 2d_1 & -2d_2 \end{pmatrix}$. Since $\det B = 8d_1 d_2 - 8d_1 d_2 = 0$ and $\text{tr } B = -(4d_1 + 2d_2)$, the characteristic polynomial of B is $X(X + 4d_1 + 2d_2)$. $\square$

The zero eigenvalue is permanent: the second and third columns of A_b are proportional, reflecting the fact that reactions r_2 and r_0 act on the pair (X_2, X_3) through the same direction $(-4, 2)$ and $(4, -2)$. This is a genuine boundary case of the conjecture's definitions. The formal proof establishes Proposition 4.5 through the weak cubic Routh–Hurwitz criterion: the coefficients $a_1 = 4d_0 + 4d_1 + 2d_2$, $a_2 = 16d_0 d_1 + 8d_0 d_2$, $a_3 = 0$ are nonnegative and $a_1 a_2 - a_3 \geq 0$, which excludes open-right-half-plane roots of a real monic cubic.

The proper restrictions of κ_b are the three pairs and three singletons of $\{1, 2, 3\}$. The pair $\{1, 2\} \mapsto (r_1, r_2)$ and all singletons use no exceptional edge, so they are restrictions of κ_{id} and are covered by Proposition 4.4. The two remaining faces use the exceptional edge $J(3) = r_0$ and need their own certificates:

$$A_{13} = S[\{1, 3\} \mapsto (r_1, r_0)] = \begin{pmatrix} -4 & 0 \\ 0 & -2 \end{pmatrix}, \quad A_{23} = S[\{2, 3\} \mapsto (r_2, r_0)] = \begin{pmatrix} -4 & 4 \\ 2 & -2 \end{pmatrix}. \quad (13)$$

Proposition 4.6 (Exceptional faces). *The matrices*

$$\mathcal{M}(A_{13}, (1, 2)) = \begin{pmatrix} 8 & 0 \\ 0 & 8 \end{pmatrix}, \quad \mathcal{M}(A_{23}, (1, 2)) = \begin{pmatrix} 8 & -8 \\ -8 & 8 \end{pmatrix}$$

are positive semidefinite. Hence A_{13} and A_{23} are D -nonunstable.

Proof. The first is diagonal with positive entries; the second is $8(1, -1)^\top(1, -1)$, a nonnegative rank-one matrix. Apply Lemma 4.3(a). $\square$

4.4 Proof of Theorem 1.1

Theorem 4.7. *Every child-selection matrix of Γ is D -nonunstable.*

Proof. Let κ be a child selection. By Lemma 4.1 it is a restriction of one of the four maximal selections. If it restricts κ_2 , κ_a or κ_{id} , Proposition 4.4 together with the heredity in Lemma 4.3(b) gives the claim. If it restricts κ_b , then either $\kappa = \kappa_b$ (Proposition 4.5), or κ is one of the faces A_{13} , A_{23} (Proposition 4.6), or κ uses no exceptional edge and is also a restriction of κ_{id} (Proposition 4.4). Since $S[\kappa]$ is determined by κ up to the simultaneous reindexing of rows and columns by the order of κ , and D -noninstability is invariant under such reindexing, the claim follows. $\square$

Proof of Theorem 1.1. Consistency is Proposition 3.1; admissibility of R was checked after (7); (i) is Proposition 3.2; (ii) is Theorem 4.7. By Lemma 2.5, (ii) implies that Γ has no D -unstable core. Proposition 3.3 shows that Γ with GMA kinetics has a positive equilibrium with Jacobian G , so Γ admits instability in the sense of [1, Def. 2]. The hypotheses of [1, Conj. 17] hold and its conclusion fails. $\square$

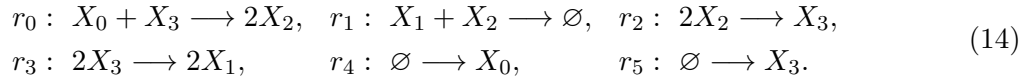
Corollary 4.8. *Statement (N) of Section 2 is false. Equivalently: it is not the case that for every consistent network on 4 species and 5 reactions and every admissible reactivity R , Hurwitz-instability of SR implies the existence of a D -unstable core.*

5 An elementary classical mass-action counterexample

A child selection records reactant incidences and whole stoichiometric columns; it does not record kinetic orders. We preserve the incidence relation (5) while changing the stoichiometric columns. The resulting child-selection lattice is unchanged, but the child matrices must be certified anew. Classical reactivities will now have the constrained form (2).

5.1 The network and its positive equilibrium

Let Γ_{elem} have the six reactions



Here “two-sided elementary bimolecular” means that both reactant and product molecularities are at most two, including the zero molecularity of an empty complex. No species appears on

both sides of any reaction. The matrices are

$$\begin{aligned} Y_{\text{elem}} &= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 0 & 0 \end{pmatrix}, \\ S_{\text{elem}} &= \begin{pmatrix} -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 2 & 0 & 0 \\ 2 & -1 & -2 & 0 & 0 & 0 \\ -1 & 0 & 1 & -2 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{15}$$

The inflows are not selectable. Thus $\text{supp}(Y_{\text{elem}})$ is exactly (5), and Lemma 4.1 applies to the same 24 nonempty selections (6 singletons, 11 pairs, 6 triples and 1 quadruple).

Proposition 5.1 (Classical equilibrium and integer Jacobian). *For the rate constants*

$$k = (9\,000\,000, 320, 999, 9\,000\,000, 1000, 3)^\top,$$

the classical mass-action system has the positive equilibrium

$$\bar{x} = (1/3, 1/160, 1, 1/3000)^\top, \quad v = r(\bar{x}) = (1000, 2, 999, 1, 1000, 3)^\top. \tag{16}$$

Its reactivity and Jacobian are

$$R_{\text{elem}} = \begin{pmatrix} 3000 & 0 & 0 & 3\,000\,000 \\ 0 & 320 & 2 & 0 \\ 0 & 0 & 1998 & 0 \\ 0 & 0 & 0 & 6000 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{17}$$

$$G_{\text{elem}} = \begin{pmatrix} -3000 & 0 & 0 & -3\,000\,000 \\ 0 & -320 & -2 & 12\,000 \\ 6000 & -320 & -3998 & 6\,000\,000 \\ -3000 & 0 & 1998 & -3\,012\,000 \end{pmatrix}. \tag{18}$$

Proof. Substituting $\bar{x}$ into the six monomials gives v in (16). The four entries of $S_{\text{elem}}v$ are

$$-1000 + 1000, \quad -2 + 2, \quad 2000 - 2 - 1998, \quad -1000 + 999 - 2 + 3,$$

all zero. Since $\bar{x}^{-1} = (3, 160, 1, 3000)^\top$, formula (2) gives (17); multiplying by S_{elem} gives (18). $\square$

5.2 Strict instability by a shifted quartic

The characteristic polynomial $p(z) = \det(zI - G_{\text{elem}})$ is

$$\begin{aligned} p(z) &= z^4 + 3\,019\,318z^3 + 1\,068\,048\,720z^2 \\ &\quad + 182\,301\,120\,000z + 69\,050\,880\,000\,000. \end{aligned} \tag{19}$$

Write these positive coefficients as $1, a_1, a_2, a_3, a_4$. The third Hurwitz determinant is strictly negative:

$$\Delta_3 = a_1a_2a_3 - a_1^2a_4 - a_3^2 = -41\,639\,698\,507\,405\,561\,804\,800\,000. \tag{20}$$

The following direct argument obtains an open-right-half-plane eigenvalue without invoking an external quartic stability theorem.

Proposition 5.2 (Shifted-quartic witness). *The matrix G_{elem} has a nonreal eigenvalue λ with $0 < \text{Re } \lambda < 5$.*

Proof. Expand $p(z+t) = z^4 + A(t)z^3 + B(t)z^2 + C(t)z + D(t)$, where

$$\begin{aligned} A(t) &= a_1 + 4t, & B(t) &= a_2 + 3a_1t + 6t^2, \\ C(t) &= a_3 + 2a_2t + 3a_1t^2 + 4t^3, & D(t) &= a_4 + a_3t + a_2t^2 + a_1t^3 + t^4. \end{aligned}$$

Set $H(t) = A(t)B(t)C(t) - A(t)^2D(t) - C(t)^2$. Exact arithmetic gives

$$\begin{aligned} H(0) &= -41\,639\,698\,507\,405\,561\,804\,800\,000 < 0, \\ H(5) &= 11\,388\,286\,332\,249\,931\,520\,000\,000 > 0. \end{aligned}$$

Continuity gives $t \in (0, 5)$ with $H(t) = 0$. All four shifted coefficients are positive there. Put $\omega = \sqrt{C(t)/A(t)} > 0$. Then

$$\text{Im } p(t + i\omega) = \omega(C(t) - A(t)\omega^2) = 0,$$

and

$$\text{Re } p(t + i\omega) = \omega^4 - B(t)\omega^2 + D(t) = -H(t)/A(t)^2 = 0.$$

Thus $p(t + i\omega) = 0$. The complex matrix $(t + i\omega)I - G_{\text{elem}}$ is singular, so it has a nonzero kernel vector and $t + i\omega$ is an eigenvalue. Its conjugate is another eigenvalue because G_{elem} is real. The positivity of the original coefficients also excludes a nonnegative real root of p . $\square$

5.3 All child matrices remain D-nonunstable

Using the maximal selections of Lemma 4.1, the new matrices are

$$A_{\text{id}}^{\text{elem}} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 2 \\ 2 & -1 & -2 & 0 \\ -1 & 0 & 1 & -2 \end{pmatrix}, \quad A_a^{\text{elem}} = \begin{pmatrix} -1 & 0 & 0 \\ 2 & -1 & 0 \\ -1 & 0 & -2 \end{pmatrix}, \quad (21)$$

$$A_b^{\text{elem}} = \begin{pmatrix} -1 & 0 & 0 \\ -1 & -2 & 2 \\ 0 & 1 & -1 \end{pmatrix}, \quad A_2^{\text{elem}} = \begin{pmatrix} -1 & 2 \\ 0 & -1 \end{pmatrix}. \quad (22)$$

In contrast to the parameter-rich example, A_a^{elem} and A_2^{elem} are triangular.

Proposition 5.3. *All 24 nonempty child-selection matrices of Γ_{elem} are D-nonunstable.*

Proof. Positive column scaling preserves triangularity and negative diagonal entries for A_a^{elem} , A_2^{elem} and their principal submatrices, so these matrices are D-stable.

The matrix $A_{\text{id}}^{\text{elem}}$ is block lower triangular with a first block -1 and lower-right block

$$B_{\text{id}} = \begin{pmatrix} -1 & 0 & 2 \\ -1 & -2 & 0 \\ 0 & 1 & -2 \end{pmatrix}.$$

For $p = (1, 2, 4)$,

$$\mathcal{M}(B_{\text{id}}, p) = \begin{pmatrix} 2 & 2 & -2 \\ 2 & 8 & -4 \\ -2 & -4 & 16 \end{pmatrix}. \quad (23)$$

Its leading principal minors are 2, 12 and 160, so it is positive definite. The proof of Lemma 4.3 then gives strict negativity of real parts for every positive scaling of B_{id} and every nonempty principal restriction: its quadratic-form inequality is strict on nonzero vectors. The block structure gives the same conclusion for every principal restriction of $A_{\text{id}}^{\text{elem}}$.

For the exceptional child and $D = \text{diag}(d_0, d_1, d_2) > 0$, direct block factorization gives

$$\det(zI - A_b^{\text{elem}}D) = z(z + d_0)(z + 2d_1 + d_2). \quad (24)$$

Its eigenvalues are zero and two negative numbers. Of its two-dimensional principal restrictions, two are triangular with negative diagonal and the remaining one is $\begin{pmatrix} -2 & 2 \\ 1 & -1 \end{pmatrix}$, whose scaled characteristic polynomial is $z(z + 2d_1 + d_2)$. The one-dimensional restrictions are negative. Thus all these restrictions are D-nonunstable. Applying the covering classification proves the claim for every child. $\square$

The permanent zero eigenvalue in (24) again makes the exceptional child D-nonunstable but not D-stable. No general heredity property of D-noninstability was used; its proper restrictions were checked directly.

Proof of Theorem 1.2. The molecularity and catalyst conditions follow from (14). Proposition 5.1 supplies positive rational rate constants and equilibrium, Proposition 5.2 supplies strict instability, and Proposition 5.3 excludes every D-unstable child. Lemma 2.5 excludes a D-unstable core. $\square$

The theorem concerns strict linear instability. It does not by itself give a Hopf bifurcation or an attracting periodic orbit. The network also has inflows and is not conservative: if $w^\top S_{\text{elem}} = 0$, its inflow columns force $w_0 = w_3 = 0$, so no strictly positive conservation vector exists.

5.4 Circulation and a fast branch explain the mechanism

The finite witness can be understood through a stationary-flux family

$$v(T) = (T, 2, T - 1, 1, T, 3)^\top, \quad T > 1,$$

and reciprocal concentrations $(a, b, c, R_f) > 0$. These determine positive classical rate constants by $k_j = v_j / \prod_i \bar{x}_i^{Y_{ij}}$, with $\bar{x} = (1/a, 1/b, 1/c, 1/R_f)$. The Jacobian is

$$G(T) = \begin{pmatrix} -Ta & 0 & 0 & -TR_f \\ 0 & -2b & -2c & 4R_f \\ 2Ta & -2b & -(4T - 2)c & 2TR_f \\ -Ta & 0 & 2(T - 1)c & -(T + 4)R_f \end{pmatrix}. \quad (25)$$

For fixed T, a, b, c , letting $R_f \rightarrow \infty$ separates one fast negative eigenvalue. The Schur complement of the last coordinate tends to the three-dimensional slow matrix

$$L_T = \begin{pmatrix} -Ta & 0 & 0 \\ 0 & -2b & -2c \\ 2Ta & -2b & -(4T - 2)c \end{pmatrix} + \frac{1}{T + 4} \begin{pmatrix} -T \\ 4 \\ 2T \end{pmatrix} \begin{pmatrix} -Ta & 0 & 2(T - 1)c \end{pmatrix}. \quad (26)$$

Indeed, in the eigenvalue equation the inverse of the last diagonal block is $(z + (T + 4)R_f)^{-1}$, so the relevant factor $R_f/(z + (T + 4)R_f)$ tends to $1/(T + 4)$ on bounded sets of z .

Write $\det(zI - L_T) = z^3 + b_1z^2 + b_2z + b_3$. Exact expansion gives

$$\begin{aligned} b_1 &= \frac{2(2Ta + Tb + 9Tc + 4b - 4c)}{T + 4}, \\ b_2 &= \frac{8(2T^2ac + Tab - Tac + 6Tbc - 6bc)}{T + 4}, \\ b_3 &= \frac{48Tabc(T - 1)}{T + 4}, \end{aligned}$$

and hence

$$\lim_{T \rightarrow \infty} \frac{b_1b_2 - b_3}{T} = 16ac(4a - b + 18c). \quad (27)$$

The coefficients b_i are positive for $T > 1$. When $b > 4a + 18c$, the cubic margin is negative for sufficiently large T , which forces an unstable conjugate pair. One elementary way to see this is to shift the cubic by $t \geq 0$: its margin becomes

$$(b_1 + 3t)(b_2 + 2b_1t + 3t^2) - (b_3 + b_2t + b_1t^2 + t^3).$$

It starts negative and tends to $+\infty$, so at some $t > 0$ the shifted cubic factors as $(z + A)(z^2 + B)$ with $A, B > 0$. Thus the unshifted cubic has roots $t \pm i\sqrt{B}$. Continuity of polynomial roots then preserves strict instability for sufficiently large R_f .

At the displayed finite witness, $(a, b, c) = (3, 160, 1)$ satisfies $160 > 4 \cdot 3 + 18$, with $T = 1000$ and $R_f = 3000$. The exact quartic calculation, rather than an asymptotic estimate, certifies these particular finite values. Large T circulates flux through $X_0 + X_3 \rightarrow 2X_2 \rightarrow X_3$, while X_3 is the fast branching coordinate coupling this circulation to $2X_3 \rightarrow 2X_1$ and $X_1 + X_2 \rightarrow \emptyset$. This subsection is a conventional explanatory calculation; it is not an additional theorem exported by the frozen Lean target.

6 Discussion: what fails and what survives

6.1 The obstruction is collective

Write $G = SR = \sum_j S_{\cdot j} R_j$ as a sum of rank-one contributions of the reactions. The Cauchy–Binet expansion [2, 1] expresses every coefficient of χ_G as a signed sum of terms $\det S[\kappa, E_\kappa] \det R[E_\kappa, \kappa]$ over sets of species and reactions of equal size, and for the *elementary* components, those attached to a single child selection, the reactivity factor is a product of independent positive symbols. This is what makes a D-unstable core sufficient: one can inflate the reactivities of a single child to dominate the polynomial. The converse fails because the Hurwitz conditions for a nonreal eigenvalue are not linear in the coefficients. In our example every coefficient of χ_G is positive and every child-selection determinant has the “safe” sign, so no elementary component is unstable; the negative third Hurwitz determinant $\Delta_3 = a_1a_2a_3 - a_1^2a_4 - a_3^2$ arises from products of contributions of different children. During the search that produced this example (Section 8), 22 of 1297 exactly certified four-species sources whose children were all coefficientwise safe nevertheless had a globally negative Δ_3 for some admissible reactivity. Coefficientwise safety of children does not propagate to the quartic Hurwitz determinant.

6.2 Whole-column semantics

A child selection owns entire reaction columns. In Γ , species X_2 is a reactant of r_1 and r_2 , and species X_3 of r_0 and r_3 ; the full Jacobian uses all four of these derivatives simultaneously, with column r_1 acting on X_1 and X_2 at once and column r_0 on X_0 and X_3 at once. No child can use $R_{1,2}$ and $R_{1,1}$ together with $R_{0,3}$ and $R_{0,0}$: injectivity forbids it. The unstable eigenvector

of Proposition 3.2 has all four coordinates nonzero. The classification in Lemma 4.1 respects this ownership exactly; the counterexample does not exploit any entrywise relaxation of the network.

6.3 Boundary spectra are decisive

The exceptional child A_b has a permanent zero eigenvalue under every positive scaling, so it is D-nonunstable but not D-stable. Conjecture 17 is formulated with D-instability, whose negation permits imaginary-axis spectra; this is the correct formulation, since a child with a zero or purely imaginary eigenvalue cannot by itself produce a strictly unstable elementary component. Any attempt to prove the conjecture by showing that all children are *D-stable* and then concluding stability of G would misclassify A_b and would be attacking a different, stronger statement. Conversely, the reader who wishes to check our claim (ii) should verify D-noninstability, not D-stability, of the exceptional child.

6.4 What survives

Several weaker localization statements remain true and were established, in the same formal development, before the counterexample was found.

- *Positive real eigenvalues localize.* If SR has a positive real eigenvalue for some admissible R , then some child-selection matrix is D-unstable; the argument goes through the sign of a characteristic coefficient, its Cauchy–Binet localization to a single injective supported term, and a block-triangular normalization. This is the direction already implicit in [2], and it is unaffected by our example, whose unstable eigenvalue is nonreal.
- *Coefficient signs localize.* If every child-selection matrix is D-nonunstable, then every coefficient of χ_{SR} is nonnegative for every admissible R . The example shows that this is the most one can extract from the children coefficientwise.
- *At most three species.* For networks with at most three species the necessity statement is true: under the hypothesis that all children are D-nonunstable, the cubic Routh–Hurwitz determinant is preserved under positive column mixtures within each species’ reaction fibre, and the Jacobian is D-nonunstable. Four species is therefore the least possible number for a counterexample.

We do not claim that Γ is minimal in any other sense (number of reactions, size of entries, or uniqueness).

7 Formal verification

7.1 The parameter-rich counterexample

All statements of Sections 3 and 4 are verified in Lean 4 [19] against Mathlib [20]. The proof file `proofs/DUnstableCores/ParameterRichCounterexample.lean` is self-contained at the level of the counterexample and imports frozen interfaces for source networks, child selections, D-scaling, diagonal dissipativity, reindexing, and the cubic Routh–Hurwitz criterion from the same development. Its structure mirrors the mathematical argument (Table 1).

The terminal declaration reads (in ASCII notation for the logical symbols),

```
theorem parameterRich_consistent_core_necessity_fin4_fin5_false :
  Not (forall (Q : SourceNetwork (Fin 4) (Fin 5)), Q.Consistent ->
    forall R : Reactivity Q, HurwitzUnstable (Q.jacobian R) ->
      exists core : ChildSelection Q, IsDUnstableCore core)
```

where `IsDUnstableCore` is Definition 2.4 (D-instability of the child matrix and D-noninstability of every proper restriction) and `DNonUnstable A` unfolds to

$$\forall d > 0 : \neg \text{HurwitzUnstable } (A \text{ diag } d),$$

the boundary-permitting notion of Definition 2.3(c). The formal definitions of `HurwitzUnstable`, `DUnstable`, `DStable` and `DNonUnstable` are kept distinct, and the file proves explicitly that `DNonUnstable A` is equivalent to $\neg \text{DUnstable } A$.

Layer	Lean content
Source contract	<code>SourceNetwork</code> (Fin 4) (Fin 5) with the literal matrices Y , P of (4); reactant relation <code>Reactant s r</code> $:= Y_{sr} > 0$; catalyst matrix 0.
Consistency	<code>Consistent</code> : existence of a strictly positive flux in $\ker S$; witness <code>! [2,3,2,2,2]</code> and the four exact row identities.
Reactivity contract	<code>Reactivity</code> : nonnegative matrix, positive exactly on reactant incidences; the six rationals of (7).
Spectral witness	<code>HasEigenpair</code> over $\mathbb{C}$ for λ and v of Proposition 3.2; <code>HurwitzUnstable (Q.jacobian R)</code> .
Dissipativity bridge	<code>weightedSymmetrization</code> ; <code>PosSemidef $\Rightarrow$ WeightedDissipative $\Rightarrow$ DNonUnstable</code> ; heredity under <code>submatrix</code> ; transport along <code>reindex</code> .
Cover certificates	Exact sum-of-squares proofs of positive semidefiniteness for the five matrices of Propositions 4.4 and 4.6.
Exceptional child	Cubic coefficients of <code>rightScale A_b d</code> ; weak Routh–Hurwitz theorem <code>hurwitzNonpositive_of_cubic_coeff_nonneg_delta_nonneg</code> .
Finite classification	Predicates <code>Uses21</code> , <code>Uses30</code> ; case split into the four regimes of Lemma 4.1; each child restricts an indexed matching.
Terminal refutation	<code>parameterRich_consistent_core_necessity_fin4_fin5_false</code> .

Table 1: Architecture of the Lean proof.

Verification protocol. The file was compiled with the Lean toolchain `leanprover/lean4: v4.30.0` against the pinned Mathlib revision `v4.30.0`, with warnings promoted to errors (`-DwarningAsError=true`), no `sorry`, and exit code 0; elaboration took about 503 seconds including dependencies. The SHA-256 of the proof source is

387eabbde3ffba639cda9a573ff9f3043554dfb5028a294ad466616efce3d87f

and the hash of the elaborated declaration interface is

c7f8cf2c2fa5941ad02f0dcbaeddabaa5deb3aff7c958c01f9bbc192d75c48dc

Every matrix entry, eigenvector coordinate and case split in the proof is checked against the single definition of the source network; no numerical spectral computation enters the terminal theorem.

Verification history. The preceding hashes identify the original Lean 4.30.0 development. Its historical terminal-declaration receipt records seven native-evaluation axioms for finite computations in addition to the three standard classical axioms. The later Palomar registration v1 checks the stated counterexample at a separate pinned Lean 4.35.0-rc2 source commit, with only `propext`, `Classical.choice` and `Quot.sound` permitted. The complete registered source and its registry evidence are supplied in the formalization archive. These are historical checks; no Lean compilation or independent native-checker replay was performed when preparing this edition. The original frozen root and full raw verification receipt are retained alongside the complete later registered source. The older root’s dependency closure is not reconstructed by mixing it with later dependency revisions.

Original receipt. The SHA-256 of the full original verification receipt is

```
09d0383990178a8264087edf2052aea459ec6192770d8aa0becd5deff129dafb
```

This is the hash of the receipt file bytes, distinct from the declaration-interface hash above.

A correction forced by the proof assistant. A preliminary hand-made certificate table for the exceptional child contained the entry 1 where the source matrix has 4. With the erroneous entry the child appeared diagonally dissipative; with the correct entry the proposed PSD certificate is invalid, and Lean rejected it. The exact cubic factorization of Proposition 4.5 and the two independently certified faces of Proposition 4.6 replaced it. We record this because it shows that the final all-children theorem is not a transcription of a numerical certificate list; it was reconstructed from the exact source definition under the discipline of the type checker.

7.2 The elementary classical mass-action counterexample

The frozen root `proofs/BimolecularTypeII3/Target1.lean` proves

```
BimolecularTypeII3.two_sided_bimolecular_counterexample.
```

Its statement provides a source network on `Fin 4` and `Fin 6`, both molecularity bounds and the catalyst-free condition, a stationary classical mass-action instance with a Hurwitz-unstable Jacobian, D-noninstability of every child matrix, and absence of a D-unstable core. The proof constructs the shifted-quartic witness of Proposition 5.2, including conversion of a complex characteristic root into an eigenvector. The bound $0 < \operatorname{Re} \lambda < 5$ follows from that construction; it is not a separately exported bound theorem. The formal enumeration also permits the empty selection, whose safety is vacuous; the manuscript counts the 24 nonempty selections.

The historical terminal receipt records Lean 4.30.0, warnings as errors, exit code 0, about 252.657 seconds, and only `propext`, `Classical.choice` and `Quot.sound`. The root SHA-256 is

```
44fb7395b75155072b4d0f1149f0a9346afeea5dba43e9801f10864aced863e7
```

the full raw receipt-file SHA-256 is

```
ed0a8d2da831d11173cd3cfc747aba85dc1f35d5a53a80f138f5cb94efc2156b
```

and the declaration-interface hash is

```
645435f92e160ed3f4104196e7e348237fa542050b9287fc577b6392dc6227c2
```

The supplied frozen closure contains the root and 21 dependencies, all matched to the receipt's source hashes. Its Mathlib commit is

```
c5ea00351c28e24afc9f0f84379aa41082b1188f
```

and the preserved manifest SHA-256 is

```
a8df0b606ec258561c226df89856884be433c19b49fb0a27335d69bb2b6e9fac
```

The proof sources, module paths, toolchain and manifest bytes are unchanged. A packaging-only Lake wrapper accompanies them; it has not been compiled for this edition.

This elementary result is locally verified and is not covered by the existing Palomar registration, which concerns only the original parameter-rich theorem. No fresh Lean run was performed. A bounded exact SymPy audit for this edition independently rederived the equilibrium, Jacobian, quartic and shifted endpoint signs, the 24 nonempty child certificates, the symmetrization minors (2, 12, 160), and the slow cubic limit. That arithmetic audit and its report are supplied separately from the historical Lean receipts. The asymptotic mechanism in Section 5 is not claimed as formally verified by `Target1.lean`.

8 How the parameter-rich example was found

The search that produced Γ was theory-directed rather than random. An extended attempt to *prove* the conjecture had already established the positive-real, coefficient-sign and three-species results of Section 6 and had isolated the complex-pair branch as the only remaining obstruction. This suggested looking for small sources whose children all carry easy exact certificates while the global quartic has a negative Δ_3 .

1. *Screen.* Among 20,000 random four-species integer sources with reactant support equal to the negative stoichiometric entries, 5,205 passed a coefficientwise safety screen for all children. Random admissible reactivities (416,400 trials) produced no unstable Jacobian; random search alone was too weak.
2. *Exact audit.* An exact expansion of the quartic for 5,000 sources certified 1,297 of them childwise, and found 22 with a negative global Δ_3 coefficient for some admissible reactivity. This refuted the working hypothesis that child safety implies safety of the global Hurwitz determinant.
3. *Witness optimization.* Optimizing the reactivity on the first obstructed source, restricted to the region where the exact coefficient geometry predicts a crossing, turned the negative Δ_3 into a genuine positive-real-part eigenpair. A symbolic implementation of this step exceeded its time budget; a lambdaified numerical implementation succeeded.
4. *Rational reconstruction.* A nearby integer simplification and exact rational reconstruction produced the four-reaction source (columns $r_0, \dots, r_3$ of (4)) and the reactivity (7), with the eigenpair of Proposition 3.2.
5. *Consistency lift.* A scope audit against [1] noted that the four-reaction source has $\det = 48$ and hence no positive equilibrium flux. The reactant-free inflow r_4 was added; an exact preflight confirmed $Sf = 0$ with $f = (2, 3, 2, 2, 2)$, the zero fifth reactivity row, and equality of the old and new Jacobians.

The lesson we draw is methodological: the cheap numerical stages identified the right invariant (Δ_3 of the full quartic) and the smallest obstruction, and exact and formal work was spent only on the resulting stable statements.

9 Open problems

Question 9.1. Characterize the parameter-rich networks for which the necessity direction of Conjecture 17 holds. Natural candidate classes are networks in which every species has a unique admissible reaction (then the child lattice is trivial and the conjecture reduces to the D-stability of a single matrix), networks with at most three species (true, Section 6), and networks whose support graph excludes the two-exceptional-edge pattern of Lemma 4.1.

Question 9.2. Is there a corrected localization theorem for the complex branch? Both examples indicate that such a theorem must control cross-terms between children, rather than only the individual child spectra. Can a compatibility condition on dissipativity certificates across reaction fibres give a useful sufficient criterion? Lemma 4.3 applies to square matrices; applying it to separate children does not by itself provide a certificate for the full Jacobian.

Question 9.3. Can a counterexample be realized by a conservative network without inflows, under classical mass action? Here conservative means that there is a strictly positive vector w with $w^\top S = 0$; this is an additional condition, not a synonym for absence of inflows. Theorem 1.2 resolves the classical mass-action question for a related network, but uses inflows.

Separately, can one exhibit a Hopf bifurcation or an attracting periodic orbit in a core-free elementary network? Strict linear instability alone does not settle either nonlinear question.

Question 9.4. Find simpler counterexamples. The original example has five reactions and an exact prescribed eigenpair; the elementary example has six reactions, stoichiometric entries of absolute value at most two, and an integer Jacobian, at the cost of disparate rate constants. Is there a five-reaction elementary classical mass-action example, or a witness with smaller rate ratios? No minimality in total reaction count is established here. It also remains open whether the original fixed stoichiometry Γ , rather than a related network, admits an unstable classical mass-action equilibrium.

A Exact certificates

A.1 Exact Jacobian

With E, F as in (6), the entries of G in (8) evaluate to

$$G = \begin{pmatrix} -1 & 0 & 0 & -\frac{2579661001547}{23329000000} \\ 0 & -\frac{2}{25} & -\frac{1}{250} & \frac{84600659109}{23329000000} \\ 4 & -\frac{1}{25} & -\frac{10011}{5500} & \frac{20778289110891}{46658000000} \\ -2 & 0 & \frac{10}{11} & -\frac{50885097}{227600} \end{pmatrix}.$$

The reader may verify $Gv = \lambda v$ coordinate by coordinate; for instance the last coordinate reads $-2v_0 + \frac{10}{11}v_2 - \frac{50885097}{227600} \cdot 1399740000 = (\frac{1}{500} + \frac{51}{500}i) \cdot 1399740000$.

A.2 $LDL^\top$ factorizations of the PSD certificates

Each certificate $\mathcal{M} = LDL^\top$ with L unit lower triangular and D diagonal with nonnegative entries exhibits $x^\top \mathcal{M} x = \sum_i D_{ii} (L^\top x)_i^2$ as an explicit sum of squares.

$$\mathcal{M}(A_2, (1, 2)) : \quad L = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}, \quad D = \text{diag}(4, 4).$$

$$\mathcal{M}(A_a, (10, 2, 7)) : \quad L = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{2}{5} & 1 & 0 \\ \frac{1}{5} & -\frac{1}{12} & 1 \end{pmatrix}, \quad D = \text{diag}(20, \frac{24}{5}, \frac{163}{6}).$$

$$\mathcal{M}(A_{\text{id}}, (100, 35, 40, 140)) : \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -\frac{4}{5} & \frac{2}{7} & 1 & 0 \\ \frac{9}{10} & -\frac{3}{4} & -\frac{203}{296} & 1 \end{pmatrix}, \quad D = \text{diag}(200, 280, \frac{1184}{7}, \frac{5955}{37}).$$

$$\mathcal{M}(A_{13}, (1, 2)) : \quad L = I_2, \quad D = \text{diag}(8, 8).$$

$$\mathcal{M}(A_{23}, (1, 2)) : \quad L = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}, \quad D = \text{diag}(8, 0).$$

A.3 Why A_b has no PSD certificate

For $p = (p_1, p_2, p_3) > 0$,

$$\mathcal{M}(A_b, p) = \begin{pmatrix} 8p_1 & 2p_2 & 0 \\ 2p_2 & 8p_2 & -4p_2 - 2p_3 \\ 0 & -4p_2 - 2p_3 & 4p_3 \end{pmatrix}.$$

Positive semidefiniteness of the lower-right 2×2 block requires $32p_2p_3 \geq (4p_2 + 2p_3)^2$, i.e. $(4p_2 - 2p_3)^2 \leq 0$, forcing $p_3 = 2p_2$; then the block is singular with kernel $(1, 1)^\top$ and the full determinant equals $-4p_2^2 \cdot 8p_2 < 0$. Hence A_b is not diagonally dissipative for any weight, and the cubic argument of Proposition 4.5 is necessary.

A.4 Reproduction

Availability. The manuscript and source are published as doi:10.5281/zenodo.23456690; the formalization and computational archives accompany that record.

From the repository root, the strict verification command is

```
python scripts/verify_proof.py \
  proofs/DUnstableCores/ParameterRichCounterexample.lean \
  --declaration \
  DUnstableCores.parameterRich_consistent_core_necessity_fin4_fin5_false
```

It runs Lean from the pinned `mathlib4_project/` directory with the checked-in toolchain and manifest, materializes imports, and treats warnings as errors. An independent exact re-verification of Propositions 3.1–4.6 and of the count of 24 child selections was performed in SymPy over $\mathbb{Q}(i)$ while preparing the original article. The supplied computational archive contains `verify_witness.py`; this historical computation was not rerun for the present edition.

For the elementary result, the formalization archive contains its separate frozen 22-file closure, toolchain, manifest and full historical receipt. The two proof roots have different verification histories and must not be combined into one dependency tree. The computational archive contains `verify_elementary.py`, its frozen certificate and source inputs, and `EXACT-CHECKS.json`. Running that Python script with SymPy rederives the bounded exact checks described in Section 7; it does not compile Lean or rerun the exploratory searches. The original `verify_witness.py` is retained byte-for-byte. No new research search or original-witness computation was replayed for this edition.

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