

An Exact Counterexample to the D-Unstable-Core Conjecture for Parameter-Rich Reaction Networks

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Abstract

Vassena and Stadler introduced *unstable cores*, minimal square child-selection submatrices of the stoichiometric matrix, and proved that a D-unstable core is sufficient for a reaction network with parameter-rich kinetics to admit an unstable positive equilibrium. They conjectured the converse: a network without D-unstable cores cannot have a Hurwitz-unstable Jacobian. We show that this conjecture is false. We exhibit a reaction network with four species and five reactions, no catalysts, and a strictly positive equilibrium flux, together with an admissible reactivity matrix for which the Jacobian $G = SR$ has the eigenvalue $\frac{1}{500} + \frac{51}{500}i$, while every one of its 24 child-selection matrices is D-nonunstable, so that no D-unstable core exists. All data are rational, the eigenvector is a Gaussian-integer vector, and the child certificates are exact: three positive-semidefinite weighted symmetrizations, one exact cubic factorization $X(X + 4d_0)(X + 4d_1 + 2d_2)$, and two two-dimensional faces. An explicit generalized-mass-action realization of the unstable equilibrium is given. The complete argument, from the source network to the negation of the universal necessity statement, is verified in Lean 4 with Mathlib, with warnings treated as errors and no unproved placeholders. We also explain why the obstruction is genuinely collective, why the boundary-permitting definition of D-noninstability is essential, and which weaker localization statements survive.

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 result

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.

Every number in the construction is an explicit rational, the unstable eigenvector has Gaussian-integer entries, and every child certificate is a finite exact identity. 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 6 describes the formalization and records the toolchain and content hashes needed to reproduce it.

What the counterexample shows

Three features of the example are, in our view, more informative than the bare refutation.

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 5). 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. A companion manuscript [21] treats the classical fixed-exponent mass-action setting, where the same forgetting of kinetic order in child-selection data produces a separate counterexample.

Organization

Section 2 fixes definitions and states the refuted implication precisely. Section 3 presents the network, the reactivity, the unstable eigenpair, and the equilibrium realization. Section 4 proves that every child-selection matrix is D-nonunstable and completes the proof of Theorem 1.1. Section 5 discusses what fails and what survives. Section 6 documents the formal verification, Section 7 the discovery process, and Section 8 open problems. Appendix A lists all exact certificates.

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 $\dot{x} = S r(x)$ 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.

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 5.

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 $\operatorname{Re} \lambda > 0$.
- (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.

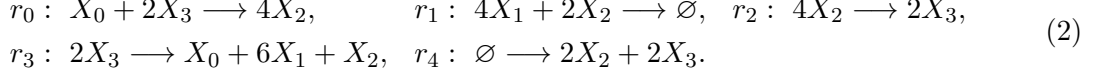
(N) For every consistent network Γ on 4 species and 5 reactions and every admissible reactivity R : if SR is Hurwitz-unstable, then Γ has a D-unstable core.

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

$$Y = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 2 & 4 & 0 & 0 \\ 2 & 0 & 0 & 2 & 0 \end{pmatrix}, \quad S = P - Y = \begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ 0 & -4 & 0 & 6 & 0 \\ 4 & -2 & -4 & 1 & 2 \\ -2 & 0 & 2 & -2 & 2 \end{pmatrix}, \quad (3)$$

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

$$\text{supp}(Y) = \{(0, 0), (1, 1), (2, 1), (2, 2), (3, 0), (3, 3)\}. \quad (4)$$

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

$$E = \frac{5187522222797}{46658000000}, \quad F = \frac{28200219703}{46658000000}, \quad (5)$$

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

$$R = \begin{pmatrix} 1 & 0 & 0 & E \\ 0 & \frac{1}{50} & \frac{1}{1000} & 0 \\ 0 & 0 & \frac{5}{11} & 0 \\ 0 & 0 & 0 & F \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (6)$$

Comparing with (4), $R_{ji} > 0$ exactly when $(i, j) \in \text{supp}(Y)$, so R is admissible. The Jacobian is

$$G = SR = \begin{pmatrix} -1 & 0 & 0 & -E + F \\ 0 & -\frac{2}{25} & -\frac{1}{250} & 6F \\ 4 & -\frac{1}{25} & -\frac{1}{500} - \frac{20}{11} & 4E + F \\ -2 & 0 & \frac{10}{11} & -2E - 2F \end{pmatrix}. \quad (7)$$

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 $\operatorname{Re} \lambda = \frac{1}{500} > 0$.

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

$$\chi_G(X) = \frac{(125000X^2 - 500X + 1301)(513238000X^2 + 116236430203X + 13005481800)}{64154750000000},$$

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 (7). 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 is not classical mass action. Whether the same network admits an unstable equilibrium under fixed integer exponents is a different question, discussed in [21]; the conjecture under refutation is about parameter-rich kinetics.

4 Every child-selection matrix is D-nonunstable

4.1 The child-selection lattice

From (4), 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:

$$\kappa_{\text{id}} = (\{0, 1, 2, 3\}, i \mapsto r_i), \quad A_{\text{id}} = S[\kappa_{\text{id}}] = \begin{pmatrix} -1 & 0 & 0 & 1 \\ 0 & -4 & 0 & 6 \\ 4 & -2 & -4 & 1 \\ -2 & 0 & 2 & -2 \end{pmatrix}, \quad (8)$$

$$\kappa_a = (\{0, 2, 3\}, (0, 2, 3) \mapsto (r_0, r_1, r_3)), \quad A_a = \begin{pmatrix} -1 & 0 & 1 \\ 4 & -2 & 1 \\ -2 & 0 & -2 \end{pmatrix}, \quad (9)$$

$$\kappa_b = (\{1, 2, 3\}, (1, 2, 3) \mapsto (r_1, r_2, r_0)), \quad A_b = \begin{pmatrix} -4 & 0 & 0 \\ -2 & -4 & 4 \\ 0 & 2 & -2 \end{pmatrix}, \quad (10)$$

$$\kappa_2 = (\{2, 3\}, (2, 3) \mapsto (r_1, r_0)), \quad A_2 = \begin{pmatrix} -2 & 4 \\ 0 & -2 \end{pmatrix}. \quad (11)$$

Lemma 4.1 (Classification). *Every child selection of Γ is a restriction of exactly one of $\kappa_{\text{id}}, \kappa_a, \kappa_b, \kappa_2$, according to which exceptional edges it uses:*

uses $J(2) = r_1$	uses $J(3) = r_0$	restriction of
yes	yes	κ_2
yes	no	κ_a
no	yes	κ_b
no	no	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} . Uniqueness is clear because the four maximal selections disagree on the two exceptional edges. $\square$

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,

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

because PD^{-1} is positive diagonal. Hence $\operatorname{Re} \lambda \leq 0$. (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 $\operatorname{Re} \lambda \leq 0$; 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 (10) 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 $D = \operatorname{diag}(d_0, d_1, d_2)$,*

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

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 $\det B = 8d_1d_2 - 8d_1d_2 = 0$ and $\operatorname{tr} B = -(4d_1 + 2d_2)$, 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 $a_1 = 4d_0 + 4d_1 + 2d_2$, $a_2 = 16d_0d_1 + 8d_0d_2$, $a_3 = 0$ are nonnegative and $a_1a_2 - a_3 \geq 0$, 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:

$$A_{13} = S[\{1, 3\} \mapsto (r_1, r_0)] = \begin{pmatrix} -4 & 0 \\ 0 & -2 \end{pmatrix}, \quad A_{23} = S[\{2, 3\} \mapsto (r_2, r_0)] = \begin{pmatrix} -4 & 4 \\ 2 & -2 \end{pmatrix}. \quad (12)$$

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 (6); (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 Discussion: what fails and what survives

5.1 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 7), 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.

5.2 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.

5.3 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.

5.4 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).

6 Formal verification

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).

Layer	Lean content
Source contract	<code>SourceNetwork</code> (Fin 4) (Fin 5) with the literal matrices Y , P of (3); reactant relation <code>Reactant s r := $Y_{sr} > 0$</code> ; 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 (6).
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.

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 `$\neg$ DUnstable A`.

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

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.

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 How the 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 5 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 lambdified 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 (3)) and the reactivity (6), 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.

8 Open problems

Question 8.1. 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 5), and networks whose support graph excludes the two-exceptional-edge pattern of Lemma 4.1.

Question 8.2. Is there a corrected localization theorem for the complex branch? The example indicates that any such theorem must control cross-terms between children, for instance through a common-weight dissipativity certificate that all children share, or through a face-closed family of certificates on the reaction fibres. A statement of the form “if all children admit a common diagonal weight, then the network is stable” is true (Lemma 4.3 applied to S), but it is far from a characterization.

Question 8.3. Does Γ , or a related network, admit an unstable positive equilibrium under classical mass action with fixed integer exponents? Child-selection data do not record reactant multiplicities, and the companion manuscript [21] shows that this lost coordinate can decide stability; whether it does so for Γ itself is open.

Question 8.4. Find the simplest counterexample. The example has four species, four active reactions, entries of absolute value at most 6, and reactivity numerators with thirteen digits. Simpler witnesses with the same qualitative structure (two exceptional edges, one non-dissipative singular child) very likely exist; the all-children theorem gives an exact regression oracle for such a search.

A Exact certificates

A.1 Exact Jacobian

With E, F as in (5), the entries of G in (7) 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

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 this article.

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