Bifurcations in planar quadratic mass action networks with few reactions and low molecularity

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Credits

Joint work with **Balázs Boros** and **Josef Hofbauer**, mainly in the paper:

> (B.–Boros–Hofbauer) *Bifurcations in planar, quadratic mass-action networks with few reactions and low molecularity*, Nonlinear Dynamics, 2024
> `https:doi.org/10.1007/s11071-024-10068-1`

Connects with work in several previous papers.

Many slides and all nice pictures and tables courtesy of Balázs!

Bifurcations in small mass action networks

Main goal:

To fully describe generic local bifurcations of equilibria in **PQT4** mass action networks

1. Two species (**P**lanar)
2. Bimolecular sources (**Q**uadratic)
3. Product molecularity no more than three (**T**rimolecular).
4. No more than **4** reactions

Along the way we prove a number of results which go beyond PQT4 networks.

Bifurcations

- Qualitative changes in behaviour as some parameters are varied (here: rate constants).
- They organise the interesting behaviours in parameterised families of dynamical systems. (E.g., easier to look for Hopf bifurcations than directly search for periodic orbits.)
- Local bifurcations of equilibria:
  - Generic codimension one: *fold*, *Andronov–Hopf*.
  - Generic codimension two: *cusp*, *Bautin*, *Bogdanov–Takens*, *fold–Hopf*, *Hopf–Hopf*.
  - Bifurcations of higher codimension, non-generic bifurcations, etc...

Genericity, transversality and all that

We confirm a local bifurcation of equilibria by checking various conditions on the Taylor coefficients of a family of vector fields:

- **Main bifurcation conditions**: often relatively easy to check.
- **Nondegeneracy conditions**: often hard to check.
- **Transversality conditions**: may be relatively straightforward to check. These tell us if the parameters "unfold" the bifurcation.

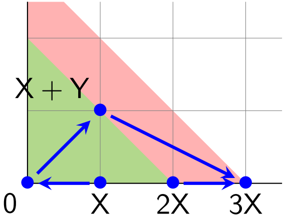
Remark. Mass action networks throw up *lots* of examples where the main bifurcation conditions are fulfilled, but genericity and/or transversality fails. I.e., we have degenerate and/or incompletely unfolded bifurcations.

Why study bifurcations in small networks?

- Helps us make sense of larger networks via **inheritance results**: these tell us how behaviours in a subnetwork can be "lifted" to results about a network. See: (B.–Boros–Hofbauer) *The inheritance of local bifurcations in mass action networks*, `https://arxiv.org/abs/2312.12897`, 2023.
- We sometimes discover patterns in the data, leading to new general theorems. (I'll give some examples.)
- The work often inspires new questions and conjectures.

Mass action by example (a PQT4 network)

$$\mathsf{X} \xrightarrow{\kappa_1} 0$$
$$0 \xrightarrow{\kappa_2} \mathsf{X}+\mathsf{Y}$$
$$\mathsf{X}+\mathsf{Y} \xrightarrow{\kappa_3} 3\mathsf{X}$$
$$2\mathsf{X} \xrightarrow{\kappa_4} 3\mathsf{X}$$



$$\dot{\boldsymbol{x}} = \Gamma(\kappa \circ \boldsymbol{x}^A)$$

$$\underbrace{\begin{pmatrix} -1 & 1 & 2 & 1 \\ 0 & 1 & -1 & 0 \end{pmatrix}}_{\Gamma} \qquad \underbrace{\begin{pmatrix} \kappa_1 \\ \kappa_2 \\ \kappa_3 \\ \kappa_4 \end{pmatrix}}_{\kappa} \qquad \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 1 & 1 \\ 2 & 0 \end{pmatrix}}_{A} \qquad \underbrace{\begin{pmatrix} x \\ 1 \\ xy \\ x^2 \end{pmatrix}}_{\boldsymbol{x}^A}$$

stoichiometric matrix — rate constants — exponent matrix — monomials

Mass action networks

An n-species, m-reaction mass action network gives rise to a system of ODEs which can be written:

$$\dot{x} = \Gamma(\kappa \circ x^A)\,.$$

- $x \in \mathbb{R}^n_+$ is the vector of **species concentrations**,
- $\Gamma \in \mathbb{Z}^{n \times m}$ is the **stoichiometric matrix**,
- $\kappa \in \mathbb{R}^m_+$ is the vector of **rate constants**, and
- $A \in \mathbb{Z}^{m \times n}_{\geq 0}$ is the **exponent matrix**.
- "$\circ$" is the entrywise product.

The **rank** of the network is the rank of Γ. We refer to an n-species, m-reaction, rank-r mass action network as an (n, m, r)-network.

Classifying networks up to equivalence

Understanding equivalences is useful for classifying MA networks.

Two networks are **dynamically equivalent** if they give rise to the same family of differential equations.

For example, the pair of networks

$$\frac{0 \to X, \quad 2X \to 2Y, \quad Y \to 0}{0 \to X, \quad 2X \to X + Y, \quad Y \to 0}$$

are easily seen to be dynamically equivalent.

(Numbers below are up to dynamical equivalence.)

Diagonal equivalence (a remark)

There are other equivalences amongst MA networks.

Definition. Two networks with the same sources and stoichiometric matrices $\Gamma, \widehat{\Gamma}$ are *diagonally equivalent* if, perhaps after permuting columns of Γ corresponding to the same source, $\widehat{\Gamma} = D_1 \Gamma D_2$, where D_1 and D_2 are positive diagonal matrices.

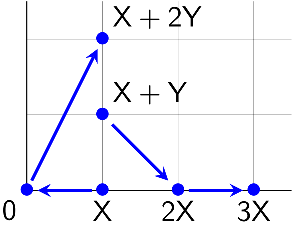
Claim. Diagonally equivalent mass action networks have equivalent dynamics.

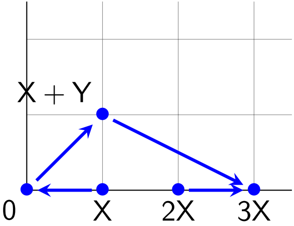
Pf. [Almost trivial!] Given $\dot{x} = \Gamma(\kappa \circ x^A)$, and $d_1 \in \mathbb{R}^n_+, d_2 \in \mathbb{R}^m_+$. Define $y = d_1 \circ x$, $\hat{\kappa} = d_2^{-1} \circ \kappa \circ d_1^{-A}$, $\widehat{\Gamma} = \mathrm{diag}(d_1)\, \Gamma\, \mathrm{diag}(d_2)$. Then

$$\dot{y} = d_1 \circ \dot{x} = d_1 \circ \Gamma(\kappa \circ d_1^{-A} \circ y^A) = d_1 \circ \Gamma(d_2 \circ \hat{\kappa} \circ y^A) = \widehat{\Gamma}(\hat{\kappa} \circ y^A).$$

Diagonally equivalent networks: example

Here are two diagonally equivalent PQT4 networks.





A simple linear change of coordinates and parameters takes trajectories of one to the other.

Remark. Sometimes a network of higher molecularity can be equivalent to one of lower molecularity.

Natural coordinates/ parameters for full rank networks

Given an (n, m, n) network $(m \geq n+1)$ giving rise to the ODE

$$\dot{x} = \Gamma(\kappa \circ x^A),$$

we can write down an equivalent system:

$$\dot{y} = \beta \circ \Gamma(\gamma^U \circ y^A)\,,$$

where $\beta \in \mathbb{R}^n_+$, $\gamma \in \mathbb{R}^{m-n-1}_+$ and U is some constant matrix. Rescaling time we have a system with $m-2$ positive parameters. Moreover, the equilibrium set depends only on the $m-n-1$ "inner parameters" γ.

Remark. The inner parameters are κ^W appearing in the Fredholm solvability condition for the network in convex coordinates.

Natural coordinates/ parameters: example

Consider the PQT4 mass-action network

$$2\mathsf{X} \xrightarrow{\kappa_1} 3\mathsf{X} \qquad \mathsf{X}+\mathsf{Y} \xrightarrow{\kappa_2} 2\mathsf{Y} \qquad \mathsf{Y} \xrightarrow{\kappa_3} 0 \qquad 0 \xrightarrow{\kappa_4} \mathsf{Y}\,.$$

giving rise to the ODE system

$$\begin{aligned} \dot{x} &= \kappa_1 x^2 - \kappa_2 xy\,, \\ \dot{y} &= \kappa_2 xy - \kappa_3 y + \kappa_4\,, \end{aligned}$$

In natural coordinates (X, Y), this takes the form

$$\begin{aligned} \dot{X} &= X^2 - XY\,, \\ \dot{Y} &= \beta(\gamma XY - Y + 1)\,, \end{aligned}$$

namely, we have only a two-parameter family of ODEs, with only one parameter affecting the equilibrium set.

Natural coordinates/ parameters: some corollaries

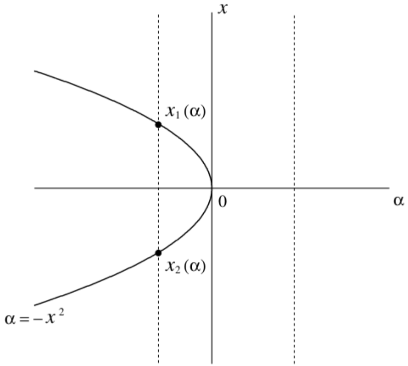
We have the following consequences for bifurcations:

- (n, m, n) networks have, effectively, only $m-2$ parameters. Therefore they forbid (fully unfolded) bifurcations of codimension $> m-2$.
- $(n, n+1, n)$ networks have 0 inner parameters: therefore they forbid (nondegenerate, fully unfolded) fold bifurcations. Note, however, even bimolecular $(3, 4, 3)$ networks allow Hopf and Bautin bifurcations (B.–Boros, Nonlinearity, 2023).
- $(n, n+2, n)$ networks have only one inner parameter: they forbid (nondegenerate, fully unfolded) cusp bifurcations.

Remark. the claims are only for full-rank networks. E.g., $(3, 3, 2)$ networks admit fold bifurcations.

Fold bifurcation

The birth/destruction of equilibria in a fold bifurcation. Picture from Kuznetsov:



Fold bifurcation in quadratic rank one networks

We found a complete – and surprisingly simple – characterisation of fold bifurcations and multiple positive nondegenerate equilibria in quadratic, rank one networks.

Theorem (B.–Boros–Hofbauer 2024)

For a quadratic, rank-one mass-action network the following are equivalent.

(i) *It admits multiple positive nondegenerate equilibria.*

(ii) *It admits a nondegenerate fold bifurcation of a positive equilibrium.*

(iii) *It includes one of the (equivalent) networks* $0 \to a\mathsf{X}$, $\mathsf{X} \to 0$, $2\mathsf{X} \to b\mathsf{X}$ *(*$a \geq 1$, $b \geq 3$*) as an induced subnetwork.*

(Corollary: No bimolecular rank one networks admit fold bifurcation.)

Fold bifurcation in planar bimolecular networks

By the previous result, bimolecular networks admitting fold bifurcation must have rank at least 2. Moreover

Lemma Bimolecular $(2, m, 2)$ with fold bifurcation $\Longrightarrow m \geq 4$.
Pf. Follows from our observations on natural coordinates/ parameters.

Theorem (B–Boros–Hofbauer 2024)

30 bimolecular $(2, 4, 2)$ *networks admit nondegenerate fold bifurcation.*

(up to diagonal equivalence)

Planar bimolecular 4-reaction networks: fold bifurcation

Group 1

$X \to 2X$, $X+Y \to 0$	$2X \to 0$	$2X \to Y$	$2X \to 2Y$	$Y \to X$	$Y \to 2X$	$Y \to X+Y$	$2Y \to X$	$2Y \to 2X$
$0 \to Y$	•	•	•	•	•	•	•	•
$Y \to 2Y$							•	•

Group 2

$Y \to 2X$, $X+Y \to 2Y$	$0 \to Y$	$0 \to X+Y$	$X \to Y$	$X \to X+Y$	$X \to 2Y$	$2Y \to 0$	$2Y \to X$	$2Y \to 2X$
$X \to 0$	•	•				•	•	
$2X \to 0$	•	•	•	•	•	•	•	•

Group 3

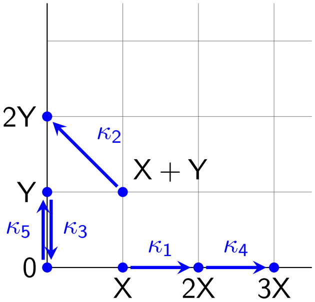
$Y \to 2X$, $2X \to 2Y$	$0 \to X$	$0 \to Y$	$0 \to X+Y$	$2Y \to 0$	$2Y \to X$	$X+Y \to 0$	$X+Y \to X$	$X+Y \to Y$
$X \to 0$	•	•	•	•	•	•	•	•

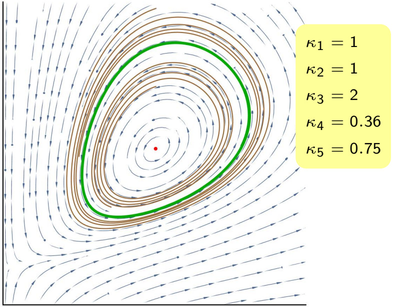
$(2,4,2)$ networks with fold

- ➔ 30 (30) bimolecular (listed on the left)
- ➔ 831 (639) quadratic, trimolecular

Bifurcations leading to periodic orbits

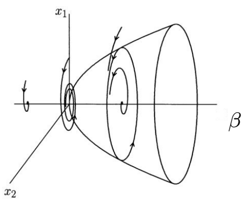
Our interest started with trying to understand which small networks admit periodic orbits, following on from work on *bimolecular* networks.

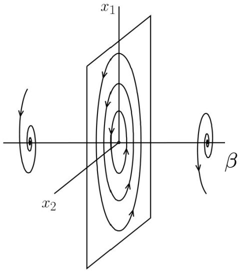


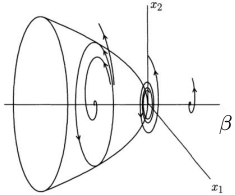


PQT5: Frank-Kamenetsky–Salnikov 1943

Andronov–Hopf bifurcations [Kuznetsov, Section 3.4]



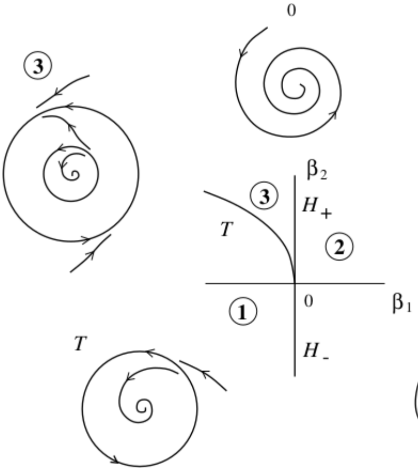




supercritical A–H	vertical A–H	subcritical A–H
$L_1 < 0$	$L_k = 0$ for all $k \geq 1$	$L_1 > 0$
stable limit cycle when $\beta > 0$	continuum of periodic orbits at $\beta = 0$	unstable limit cycle when $\beta < 0$

Bautin bifurcation (co-dimension 2, supercritical case)

Again, from Kuznetsov:



Andronov–Hopf and Bautin bifurcation

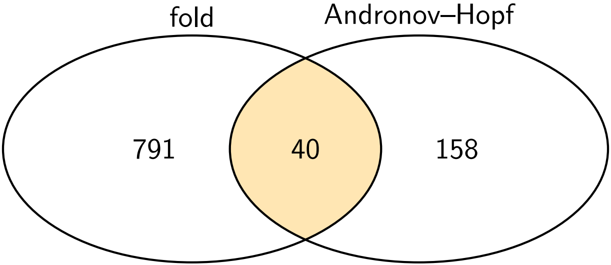
Theorem (B.–Boros–Hofbauer 2024)

198 (157) PQT4 networks admit Andronov–Hopf bifurcation. Some of these bifurcations are vertical. One network admits a (subcritical) Bautin bifurcation.

#	Andronov–Hopf bifurcation	periodic solution
135	supercritical	stable LC
17	vertical	center
42	subcritical	unstable LC
3	supercritical vertical subcritical	stable LC center unstable LC
1	subcritical Bautin	stable LC & unstable LC

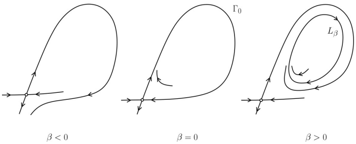
Fold and Andronov–Hopf

Which PQT4 networks admit both fold and Andronov–Hopf bifurcations?

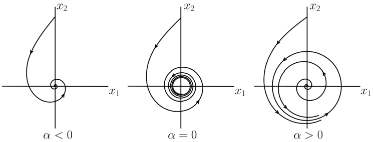


40 PQT4 networks admit both fold and Andronov–Hopf bifurcations... but do these bifurcations "meet"? And do they lead to interesting bifurcations of higher codimension?

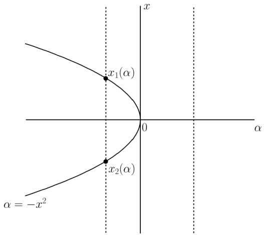
Bogdanov–Takens bifurcation [Kuznetsov, Chapters 3, 6, 8]



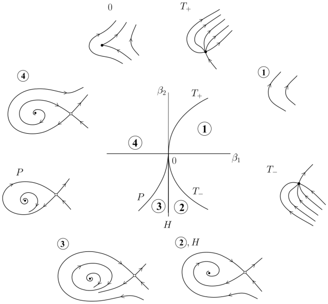
homoclinic



Andronov–Hopf



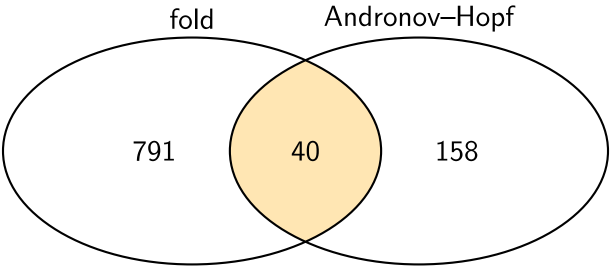
fold (a.k.a. saddle-node)



Bogdanov–Takens

Fold and Andronov–Hopf

Which PQT4 networks admit both fold and Andronov–Hopf bifurcations?

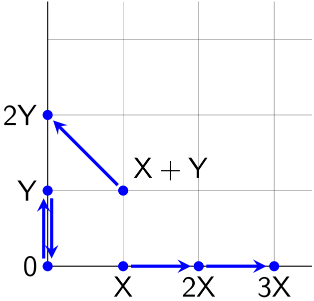


- ➔ 33 (28) admit $\sigma(J) = \{0, 0\}$ with $J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$
- ➔ 7 don't admit $\sigma(J) = \{0, 0\}$

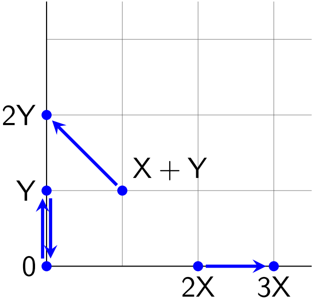
PQT4 networks admitting B–T bifurcation

supercritical B–T	1	$2X \to 3X$	$X+Y \to 2Y$	$Y \to 0$	$0 \to Y$
	2	$2X \to 3X$	$X+Y \to 3Y$	$Y \to 0$	$0 \to Y$
	3	$2X \to 3X$	$X+Y \to 2Y$	$Y \to 0$	$X \to Y$
	4	$2X \to 3X$	$X+Y \to 3Y$	$Y \to 0$	$X \to Y$
	5	$2X \to 3X$	$X+Y \to 2Y$	$Y \to 0$	$X \to 2Y$
	6	$2X \to 3X$	$X+Y \to 3Y$	$Y \to 0$	$X \to 2Y$
	7	$2X \to 3X$	$X+Y \to 2Y$	$Y \to 0$	$X \to 3Y$
	8	$2X \to 3X$	$X+Y \to 3Y$	$Y \to 0$	$X \to 3Y$
vertical B–T	9	$2X \to 3X$	$X+Y \to 2X$	$0 \to Y$	$X \to 0$
	10	$2X \to 3X$	$X+Y \to 3X$	$0 \to Y$	$X \to 0$
subcritical B–T	11	$2X \to 3X$	$X+Y \to 2X$	$0 \to X+2Y$	$X \to 0$
	12	$2X \to 3X$	$X+Y \to 3X$	$0 \to X+2Y$	$X \to 0$
	13	$2X \to 3X$	$X+Y \to 2X$	$0 \to X+Y$	$X \to 0$
	14	$2X \to 3X$	$X+Y \to 3X$	$0 \to X+Y$	$X \to 0$
	15	$2X \to 3X$	$X+Y \to 2X$	$0 \to 2X+Y$	$X \to 0$
	16	$2X \to 3X$	$X+Y \to 3X$	$0 \to 2X+Y$	$X \to 0$
	17	$2X \to 3X$	$X+Y \to X$	$Y \to X+2Y$	$X \to Y$
	18	$2X \to 3X$	$X+Y \to X$	$Y \to X+2Y$	$X \to 2Y$
	19	$2X \to 3X$	$X+Y \to X$	$Y \to X+2Y$	$X \to 3Y$
	20	$2X \to 3X$	$X+Y \to 0$	$Y \to 2X$	$X \to 2Y$
	21	$2X \to 3X$	$X+Y \to 0$	$Y \to 3X$	$X \to 2Y$
	22	$2X \to 3X$	$X+Y \to 0$	$Y \to X$	$X \to 3Y$
	23	$2X \to 3X$	$X+Y \to 0$	$Y \to 2X$	$X \to 3Y$
	24	$2X \to 3X$	$X+Y \to 0$	$Y \to 3X$	$X \to 3Y$
	25	$2X \to 3X$	$X+Y \to 0$	$Y \to X$	$X \to X+Y$
	26	$2X \to 3X$	$X+Y \to 0$	$Y \to 2X$	$X \to X+Y$
	27	$2X \to 3X$	$X+Y \to 0$	$Y \to 3X$	$X \to X+Y$
	28	$2X \to 3X$	$X+Y \to Y$	$2Y \to 0$	$X \to 2X+Y$
	29	$2X \to 3X$	$X+Y \to Y$	$2Y \to X$	$X \to 2X+Y$
	30	$2X \to 3X$	$X+Y \to Y$	$2Y \to 2X$	$X \to 2X+Y$
	31	$2X \to 3X$	$X+Y \to Y$	$2Y \to 3X$	$X \to 2X+Y$
	32	$2X \to 3X$	$X+Y \to Y$	$2Y \to 2X+Y$	$X \to 2X+Y$
	33	$2X \to 3X$	$X+Y \to 2Y$	$2Y \to 0$	$0 \to X+2Y$

Frank-Kamenetsky–Salnikov (1943) revisited



supercritical Andronov–Hopf



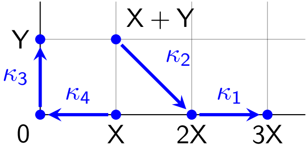
supercritical Bogdanov–Takens

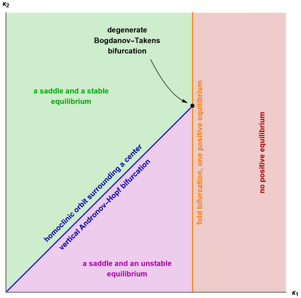
- supercritical Andronov–Hopf
- supercritical homoclinic
- fold

The F-K–S network *inherits* the Bogdanov–Takens bifurcation!

B.–Boros–Hofbauer (2023): The inheritance of local bifurcations in mass action networks

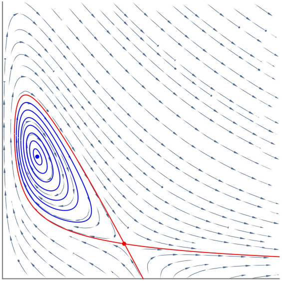
Vertical Bogdanov–Takens bifurcation (remark)





bifurcation diagram

(κ_1, κ_2 varied; κ_3, κ_4 fixed)



phase portrait

($4\kappa_1\kappa_4 < \kappa_3^2$ and $\kappa_1 = \kappa_2$)

Remarks

1. Small networks display a surprisingly rich variety of bifurcations.
2. Studying bifurcations in small networks opens up new avenues in CRNT, and suggests new questions and conjectures.
3. There is more in the paper: e.g.,
   - some necessary conditions for various bifurcations;
   - an exploration of small networks admitting two *stable* equilibria, one positive, and one at the origin (we found an error in the previous literature).
   - more on nongeneric bifurcations.
4. The symbolic algebra behind the paper is nontrivial and can be found in Balázs' Mathematica Notebook:

   https://github.com/balazsboros/reaction_networks

References... and thank you for listening!

*(B.–Boros–Hofbauer) *Bifurcations in planar, quadratic mass-action networks with few reactions and low molecularity*, Nonlinear Dynamics, 2024
https:doi.org/10.1007/s11071-024-10068-1

(B.–Boros–Hofbauer) *Oscillations in three-reaction quadratic mass-action systems*
Studies in Applied Mathematics, 2024.

(B.–Boros) *The smallest bimolecular mass action reaction networks admitting Andronov–Hopf bifurcation*, Nonlinearity 36(2) (2023) 1398–1433.

(B.–Boros–Hofbauer) *The inheritance of local bifurcations in mass action networks*, https://arxiv.org/abs/2312.12897, 2023.