Wave Bifurcation in Reaction-Diffusion Systems

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Abstract: For reaction-diffusion systems with unequal diffusion coefficients hypotheses are given concerning the kinetic equations whereas the diffusion coefficients are considered as bifurcation parameters. In two variable systems stability preserving bifurcation is possible only to stationary nonconstant (or layered) solutions. For three or more equations both stationary and nonstationary nonconstant solutions (such as standing or travelling waves) bifurcate from a stable equilibrium. What happens can be judged solely by the linearization of the kinetic system.

1.1 Problem settings

Reaction-diffusion systems are usually studied in the form

$$\frac{\partial \mathbf{u}}{\partial t} = F(\mathbf{u}, t, x, \Lambda) = \nabla \cdot (D \nabla \mathbf{u}(t, x, \Lambda)) + f(\mathbf{u}, t, x, \Lambda) \tag{1}$$

in $\Omega \times (0, \infty)$, where Ω is a bounded domain in $\mathbb{R}^n$ such that $\bar{\Omega}$ is an n-dimensional smooth (i.e. C^∞-) submanifold of $\mathbb{R}^n$, the diffusion coefficients $\bar{d}_i$ are positive, and in the simplest case constant entries on the diagonal matrix D, such that this term simplifies to $-D\Delta\mathbf{u}$. The kinetic system f consists of smooth functions f_i, $i = 1, \cdots, N$, depending on $\mathbf{u} := (u_1, \cdots, u_N)$, possibly also on the time t and on $x \in \Omega$, and a set of parameters Λ. The System (1) has to be complemented by boundary conditions such as for example homogeneous Dirichlet conditions or Neumann, that is 'no flux' conditions.
Let A describe the linearization of the kinetic equations (or ODEs) at the constant zero solution. D_m is the linearization of the diffusive term depending on the mth eigenvalue of the Laplace Operator, and diffusion coefficients are $\bar{d}_i$, $i = 1, \cdots, N$, for an N-variable system. The tilde $\sim$ always denotes the linearization of the PDE and the index m indicates the respect to the appropriate mode.
In order to apply theorems from bifurcation theory that concern stability, a constant stable equilibrium shall be destabilized on varying a critical parameter.

1.2 Wave bifurcation

A wave bifurcation is a supercritical Hopf bifurcation from a stable stationary constant zero solution to a stable nonstationary nonconstant solution. Therefore the real part of a single pair of complex eigenvalue has to cross the imaginary axis.
In two variable systems this means that on varying a single bifurcation parameter, the trace $\mathrm{tr}\tilde{A}_m$ changes sign whereas the determinant $\det\tilde{A}_m$ remains positive (see Figure 1). Since $-\mathrm{tr}A$ is assumed to be positive (the constant solution is stable), the trace of the PDE $\mathrm{tr}\tilde{A}_m$ cannot change sign for any combination of positive $\bar{d}_1$ and $\bar{d}_2$.
It is impossible to destabilize the constant solution to an oscillating nonconstant solution.
Therefore it is not possible to get a wave bifurcation for a two variable system (see in the original paper of Turing [1], and therein the cases e) and f): e) *Oscillatory case with a finite wave-length and* f) *Oscillatory case with extreme short wave-length,* [...] *possibilities* [that] *can only occur with three or more morphogens.* [...] *no attempt was made to develop formulae for these.*).

For N-variable systems general theorems tell about where the eigenvalues are located.

Theorem 1 (Routh-Hurwitz) *The number k of roots of the real polynomial $p(z) = a_0 z^N + b_0 z^{N-1} + a_1 z^{N-2} + b_1 z^{N-3} + \cdots \quad (a_0 \neq 0)$ which lie in the right half plane is given by the formular*

$$k = V\left(a_0, \Delta_1, \frac{\Delta_2}{\Delta_1}, \frac{\Delta_3}{\Delta_2}, \cdots, \frac{\Delta_N}{\Delta_{N-1}}\right)$$

or equivalently

$$k = V(a_0, \Delta_1, \Delta_3, \cdots) + V(1, \Delta_2, \Delta_4, \cdots)$$

with $\Delta_i,\ i = 1, \cdots, N$ *the successive principal minors, or Hurwitz determinants, of a square matrix* H*, the Hurwitz matrix of order* N*, and* V *counts for the number of changes of sign of adjacent members of a finite sequence (see* GANTMACHER [2]*, p.230).*

The Routh-Hurwitz Criterion. In order for all roots of the real polynomial $p(z) = z^N + \cdots \quad (a_0 = 1 > 0)$ to have negative real parts it is necessary and sufficient that the inequalities

$$\Delta_1 > 0,\ \Delta_2 > 0,\ \cdots,\ \Delta_N > 0$$

hold.

Theorem 2 *An odd number* k *of eigenvalues in the right half plane is equivalent to* $(-1)^N \det A < 0$.

Theorem 3 *A constant steady state solution of a reaction-diffusion system that is stable against spatially constant perturbations cannot reveal unstable when perturbed inhomogeneously if diffusion coefficients are equal.*

Proofs are straightforward and left to the reader.
If diffusion destabilizes the zero solution that is stable to spatially homogeneous perturbations, the number k of the Routh-Hurwitz Theorem has to increase when considering $\tilde{A}_m = A - D_m$, instead of A.
A stable equilibrium as starting point, has $-\mathrm{tr}A > 0$ or in other terms $V(a_0, \Delta_1) = 0$. Adding diffusive terms to the trace will only decrease the trace and therefore increase $-\mathrm{tr}\tilde{A}_m$. It yields $-\mathrm{tr}\tilde{A}_m > -\mathrm{tr}A > 0$, and $-\mathrm{tr}\tilde{A}_m$ is always positive.
The case of $N = 3$ variables is the smallest number of equations making it possible to have a bifurcation to a spatially nonconstant and temporally periodic solution.

On notation: For a 3×3 matrix,

$$\tilde{A}_m = A - D_m = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} - \begin{pmatrix} \bar{d}_1 & & \\ & \bar{d}_2 & \\ & & \bar{d}_3 \end{pmatrix} \mu_m^2 = A - \begin{pmatrix} d_1 & & \\ & d_2 & \\ & & d_3 \end{pmatrix}$$

$A\begin{bmatrix} i_1 & i_2 \\ i_1 & i_2 \end{bmatrix}$ denoting the minors with same columns as rows, and therefore will be abbreviated with $A|i_1 i_2|$. The trace of a submatrix of A consisting of the i_1 and i_2 column and row will be denoted as tr$A$ $(i_1 i_2)$.
The eigenvalues of a system of three equations are the roots of

$$\chi_A(\lambda) = \lambda^3 - \mathrm{tr}A\ \lambda^2 + \sum_{1 \le i < j \le 3} A|ij|\ \lambda - \det A = 0\ .$$

The Hurwitz matrix is

$$H = \begin{pmatrix} -\mathrm{tr}A & -\det A & 0 \\ 1 & \sum A|ij| & 0 \\ 0 & -\mathrm{tr}A & -\det A \end{pmatrix} = \begin{pmatrix} -\sigma_1 & -\sigma_3 & 0 \\ 1 & \sigma_2 & 0 \\ 0 & -\sigma_1 & -\sigma_3 \end{pmatrix}$$

with σ_i denoting symmetric functions. The successive Hurwitz determinants are:

$$
\begin{array}{llll}
\Delta_1 & = H\left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right] & = -\sigma_1 & = -\mathrm{tr}A \\
\Delta_2 & = H\left[\begin{smallmatrix} 1 & 2 \\ 1 & 2 \end{smallmatrix}\right] & = -\sigma_1\sigma_2 + \sigma_3 & = -\mathrm{tr}A(\sum A|ij|) + \det A \\
\Delta_3 & = H\left[\begin{smallmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{smallmatrix}\right] & = -\sigma_3(-\sigma_1\sigma_2 + \sigma_3) & = -\det A(-\mathrm{tr}A(\sum A|ij|) + \det A)
\end{array}
$$

All three eigenvalues have negative real parts iff $\Delta_i > 0$ for $i = 1, 2, 3$ (Routh-Hurwitz Criterion). This is equivalent to

$$
\begin{array}{rrcl}
 & \sigma_1 & < & 0 \\
\wedge & \sigma_3 & < & 0 \\
\wedge & \sigma_1\sigma_2 & < & \sigma_3 \, .
\end{array}
$$

Comparing two and three variable systems, the following figures give an impression, where the regions of stable nodes are ($k = 0$, shaded areas), and which lines or surfaces seperate regions for the various numbers of k.

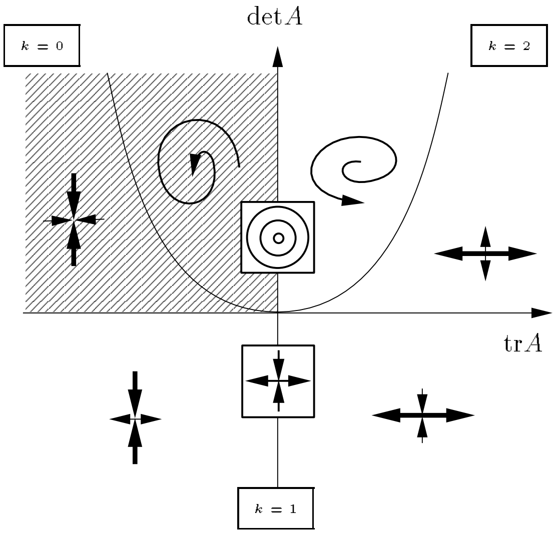

Figure 1: For a two variable system a sign change of the trace results in an increase of k by 2.

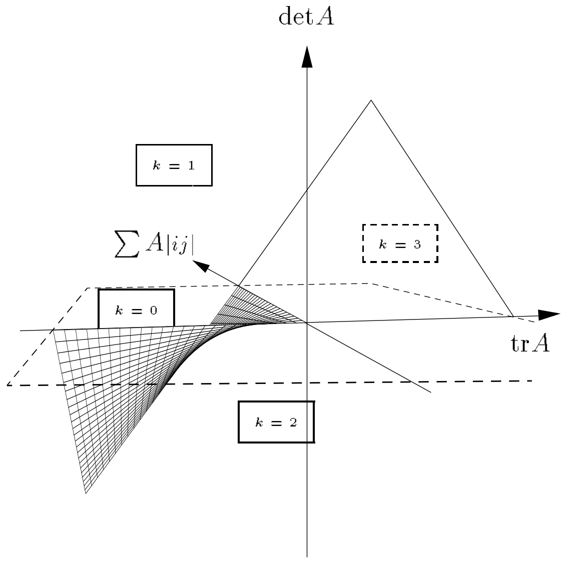

Figure 2: For a three variable system the surface $\sigma_1\sigma_2 = \sigma_3$, $\sigma_2 > 0$, has to be crossed to increase k by 2.

In general k is for a system of three equations

$$
\begin{aligned}
k = V\left(a_0, \Delta_1, \frac{\Delta_2}{\Delta_1}, \frac{\Delta_3}{\Delta_2}\right) &= V(a_0, \Delta_1, \Delta_3) + V(1, \Delta_2) \\
&= V(a_0, \Delta_1) + V(\Delta_1, \Delta_3) + V(1, \Delta_2)
\end{aligned}
$$

with $a_0 = 1$ and Hurwitz determinants as above.
The idea is to compare the symmetric functions σ_i of the kinetic system to those $\tilde{\sigma}_i$, $i = 1, 2, 3$, of the full system.
For infinite dimensional systems the number k of eigenvalues in the right half plane is the sum $k = \sum_{l=0}^{\infty} k_l$. The number k_l belongs to the lth mode. If $\tilde{\Delta}_{l2} > 0$ for all $l \neq m$, and $\tilde{\Delta}_{m2} < 0$ for a single m, the overall sum $k = k_m$ increases by two. This situation can be adjusted with the diffusion coefficients as bifurcation parameters.

This number k is zero, iff the sign conditions are fulfilled for all m. In the case of the Turing instability a single eigenvalue crosses for a single m. In the case of the wave bifurcation two complex conjugate eigenvalues cross the imaginary axis, and again this shall happen for a single m.

$\boxed{k=0}$	Stable nodes	
	$\left.\begin{array}{rrcl} & V(a_0,\Delta_1) & = & 0 \\ \wedge & V(\Delta_1,\Delta_3) & = & 0 \\ \wedge & V(1,\Delta_2) & = & 0 \end{array}\right\} \Leftrightarrow \begin{array}{rrcl} & -\mathrm{tr}\tilde{A}_m & > & 0 \\ \wedge & -\det\tilde{A}_m & > & 0 \\ \wedge & \tilde{\Delta}_{m2} & > & 0 \end{array}$	
$\boxed{k=1}$	Turing instability	$A\|23\| < 0$
	$\left.\begin{array}{rrcl} & V(a_0,\Delta_1) & = & 0 \\ \wedge & V(\Delta_1,\Delta_3) & = & 1 \\ \wedge & V(1,\Delta_2) & = & 0 \end{array}\right\} \Leftrightarrow \begin{array}{rrcl} & -\mathrm{tr}\tilde{A}_m & > & 0 \\ \wedge & -\det\tilde{A}_m & < & 0 \\ \wedge & \tilde{\Delta}_{m2} & > & 0 \end{array}$	
	or	
	$\left.\begin{array}{rrcl} & V(a_0,\Delta_1) & = & 0 \\ \wedge & V(\Delta_1,\Delta_3) & = & 0 \\ \wedge & V(1,\Delta_2) & = & 1 \end{array}\right\} \Leftrightarrow \begin{array}{rrcl} & -\mathrm{tr}\tilde{A}_m & > & 0 \\ \wedge & -\det\tilde{A}_m & < & 0 \\ \wedge & \tilde{\Delta}_{m2} & < & 0 \end{array}$	
$\boxed{k=2}$	Wave instability	$A\|23\| > 0$
	$\left.\begin{array}{rrcl} & V(a_0,\Delta_1) & = & 0 \\ \wedge & V(\Delta_1,\Delta_3) & = & 1 \\ \wedge & V(1,\Delta_2) & = & 1 \end{array}\right\} \Leftrightarrow \begin{array}{rrcl} & -\mathrm{tr}\tilde{A}_m & > & 0 \\ \wedge & -\det\tilde{A}_m & > & 0 \\ \wedge & \tilde{\Delta}_{m2} & < & 0 \end{array}$	

Table 1: Diffusion induced periodic nonconstant solution is possible for $N = 3$.

What can be observed by now is that for $-\mathrm{tr}\tilde{A}_m > 0$ a change to a positive sign of $\det\tilde{A}_m$ gives exactly one positive real eigenvalue same as for the case of two variables (see Theorem 2). In general a Turing bifurcation from a stable constant solution to a stable steady but nonconstant solution can be decided on the sign of the determinant. For the wave bifurcation when k jumps from 0 to 2, k is even and $(-1)^N\det\tilde{A}_m > 0$.
The surface $\sigma_1\sigma_2 = \sigma_3,\ \sigma_2 > 0$ makes it possible to have a wave bifurcation of a three variable system: The trace of the linearization is still negative, the determinant indicates an even number of eigenvalues in the right half plane (see Theorem 2), and k increases when crossing through this surface, while the determinant is still negative.

$$-\tilde{\sigma}_1 = \quad -\mathrm{tr}\tilde{A}_m \quad = -(\mathrm{tr}A - (d_1 + d_2 + d_3)) \tag{2}$$

$$\begin{aligned} \tilde{\sigma}_2 = \quad \sum \tilde{A}_m|ij| \quad &= \sum A|ij| - d_1(a_{22} + a_{33} - d_2) - \\ &d_2(a_{11} + a_{33} - d_3) - d_3(a_{11} + a_{22} - d_1) \end{aligned} \tag{3}$$

$$\begin{aligned} -\tilde{\sigma}_3 = \quad -\det\tilde{A}_m \quad &= -(\det A - d_1 A|23| - d_2 A|13| - d_3 A|12| + \\ &d_1 d_2\ a_{33} + d_1 d_3\ a_{22} + d_2 d_3\ a_{11} - d_1 d_2 d_3) \end{aligned} \tag{4}$$

Now look at Δ_2 and $\tilde{\Delta}_{m2}$ on condition that $-\mathrm{tr}\tilde{A}_m$ and $-\det\tilde{A}_m$ are positive.

$$\Delta_2 = -\mathrm{tr}A\left(\sum A|ij|\right) + \det A > 0$$

$$\begin{aligned}\tilde{\Delta}_{m2} = \Delta_2 \quad & +d_1(A|12| + A|13| + (\mathrm{tr}A(23))^2 + a_{11}\mathrm{tr}A(23)) \\ & +d_2(A|12| + A|23| + (\mathrm{tr}A(13))^2 + a_{22}\mathrm{tr}A(13)) \\ & +d_3(A|13| + A|23| + (\mathrm{tr}A(12))^2 + a_{33}\mathrm{tr}A(12)) \\ & -{d_1}^2(\mathrm{tr}A(23)) - {d_2}^2(\mathrm{tr}A(13)) - {d_3}^2(\mathrm{tr}A(12)) \\ & -2(d_1d_2 + d_1d_3 + d_2d_3)\mathrm{tr}A \\ & +{d_1}^2(d_2+d_3) + {d_2}^2(d_1+d_3) + {d_3}^2(d_1+d_2) \\ & +2d_1d_2d_3\end{aligned} \tag{5}$$

1.3 The limiting case $\mathbf{d} = 0$

In order to derive a short formulation for $N = 3$ it is convenient to look at a limiting case. Consider unequal diffusion coefficients $d_1 \neq \mathbf{d} = d_2 = d_3$. Without loss of generality the first species is considered to diffuse. The second and third equation are refered to as the subsystem $A(23)$ of nondiffusive variables. In the limit for $\mathbf{d} \to 0$ this is

$$\begin{aligned}\lim_{\mathbf{d}\to 0} \tilde{\Delta}_{m2} &= \Delta_2 + d_1(A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A) - {d_1}^2\mathrm{tr}A(23) \\ &= p(d_1)(-\mathrm{tr}A(23))\end{aligned} \tag{6}$$

a quadratic polynomial in d_1, say $p(d_1)$, in which d_1 still hides the dependence on the mth eigenvalue $d_1 = \bar{d}_1\mu_m^2$. The cubic part always contains a factor $\mathbf{d}$.
The trace of the submatrix $\mathrm{tr}A(23)$ has to be negative $(-\mathrm{tr}A(23) > 0)$ such that the parabola is positive for all but a single mode m (see Figure 3).
Note that $p(0) > 0$, so the first eigenvalue $\mu_{0N}^2 = 0$ of the Neumann problem with its positive eigenfunction (that is a constant) remains stable. The bifurcating solution is therefore oscillating in space and time.

$$p(d_1) = {d_1}^2 - d_1\left(\frac{A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A}{\mathrm{tr}A(23)}\right) + \frac{\Delta_2}{-\mathrm{tr}A(23)}$$

$$\Leftrightarrow \qquad \nu^{\pm} = \frac{1}{2}\left(\frac{A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A}{\mathrm{tr}A(23)} \pm \sqrt{(\sim)^2 - 4\frac{\Delta_2}{-\mathrm{tr}A(23)}}\right)$$

On condition that $\mathrm{tr}A(23) < 0$, the roots $\nu^{\pm}$ are both positive real numbers, iff

$$\begin{aligned} & A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A < 0 \\ \wedge \quad & (\mathrm{tr}p(d_1))^2 + 4\mathrm{tr}A(23)\Delta_2 > 0\,. \end{aligned}$$

The following hypotheses give the conditions for a change in sign of $\tilde{\Delta}_{m2}$ by diffusion coefficient $\bar{d}_1$:

Hypotheses: (H1) – (H3) guarantee a stable constant equilibrium of the kinetic system. (H4) is needed for the right opening of the parabola, and (H5) and (H6) are sufficient for the existence of two positive real roots of this parabola.

- (H1) $-\mathrm{tr}A > 0$
- (H2) $-\det A > 0$
- (H3) $\Delta_2 = -\mathrm{tr}A(\sum A|ij|) + \det A > 0$
- (H4) $-\mathrm{tr}A(23) > 0$
- (H5) $-(A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A) > 0$
- (H6) $(A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A)^2 + 4\mathrm{tr}A(23)\Delta_2 > 0$

Note that these hypotheses only concern the kinetic system.

Theorem 4 *Consider a System (7) of a parabolic and two ordinary differential equations that has an asymptotically stable constant equilibrium ((H1) − (H3) are satisfied).*

$$\begin{aligned} u_{1_t} &= B(u_1, \bar{d}_1) + f_1(\mathbf{u}) \\ u_{2_t} &= \qquad\qquad + f_2(\mathbf{u}) \\ u_{3_t} &= \qquad\qquad + f_3(\mathbf{u}) \end{aligned} \tag{7}$$

The spectrum of $-B(u_1, \bar{d}_1)$ is nonnegative, real and discrete. If the linearized kinetic system fulfills (H4) − (H6)*, varying $\bar{d}_1 > 0$ leads generically to the crossing of two complex conjugate eigenvalues through the imaginary axis. That is*

$$\begin{aligned} p(\bar{d}_1 \mu_m^2) &\leq 0 \quad \text{for } m \\ p(\bar{d}_1 \mu_l^2) &> 0 \quad \text{for } l \neq m \end{aligned}$$

for a single m, where μ_m^2 denotes the mth eigenvalue of $-B(u_1, \bar{d}_1)$.
If the solution on the center manifold is centerstable then there exists a periodic nonconstant solution.

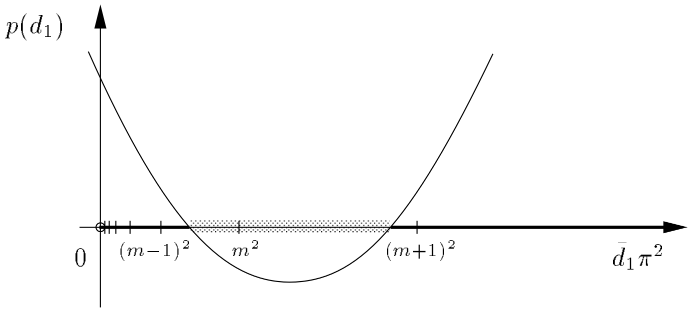

Figure 3: The regular perturbation with d_1 as bifurcation parameter shows the parabola $p(d_1)$ selecting just a single mode of oscillating solutions (here for the Laplace operator on a one dimensional domain).

Proof: For the number k of eigenvalues to really jump from 0 to 2 it must be checked that $-\det\tilde{A}_m > 0$ (see Table 1 and Figure 2). Therefore consider the limit in Equation (4).

$$\lim_{\mathbf{d} \to 0} \left(-\det\tilde{A}_m \right) = -\det A + d_1 A|23| \tag{8}$$

If $A|23|$ is positive, then $-\det\tilde{A}_m > -\det A > 0$ for all $d_1 = \bar{d}_1 \mu_m^2$ and all m, so that there is no change in sign of the determinant. Since the above hypotheses already imply that $A|23|$ is positive, the main thing to proof is the following lemma. □

Lemma 1 *Let A be such that* (H1) − (H5) *are fulfilled. Then $A|23|$ is positive.*

Proof:

$$\begin{aligned} \text{(H5)} \;\Rightarrow\;& A|12| + A|13| + \mathrm{tr}A(23)\mathrm{tr}A < 0 \\ \Leftrightarrow\;& A|12| + A|13| < -\mathrm{tr}A(23)\mathrm{tr}A \overset{\text{(H1)(H4)}}{<} 0 \\ \Rightarrow\;& A|12| + A|13| < 0 \end{aligned}$$

Assume $A|23| \leq 0$. Then $\underbrace{\underbrace{\mathrm{tr}A}_{<0} \; \underbrace{(A|12| + A|13| + A|23|)}_{<0}}_{>0} \overset{\text{(H3)}}{<} \det A \overset{\text{(H2)}}{<} 0$.

This is a contradiction. □

For the wave bifurcation $A|23|$ has to be positive. This therefore can be used as a first check whether wave bifurcation is possible or not. It is only a necessary condition, not sufficient!
FIRST CHECK: tr$A(23) < 0$ and $A|23| > 0$ resembles a stable situation for the subsystem.
The scenario for a 3×3 system that satisfies (H1) $-$ (H3):

- If $A|23| < 0$ this is the necessary (and sufficient) condition to arrange a Turing bifurcation.
- If $A|23| > 0$ this is the necessary (but not sufficient) condition to arrange a wave bifurcation, since (H4) and (H5) imply $A|23| > 0$.

Remark 1 *A simultaneous change of sign of det$\tilde{A}_m$ and $\tilde{\Delta}_{m2}$ would also lead to a Turing instability (see Table 1, $k = 1$). But it is not possible in the limiting case $\mathbf{d} = 0$ (see* FIRST CHECK*). $A|23|$ has to have different signs for the both requirements.*

Further investigations of the wave bifurcation concern the biggest mode m for which there is bifurcation to the left (right). For one dimensional spatial domains Ω this can be estimated by the roots of $p(d_1)$ which were determined only by the linearization of the kinetic system. For all integers less than m, a bifurcation to a wave solution with the appropriate wave number can be arranged either for shrinking or growing $\bar{d}_1$. But for wave numbers greater than m, at least two modes are within the unstable area, contradicting Theorem 4. This doesn't mean that there is no such solution, but it cannot be predicted which solution will survive. This strongly depends on the initial conditions.

Lemma 2 *The biggest m for which only a single mode is destabilized in a one space dimensional system can be estimated by* $\mu^- := \dfrac{2\nu^-}{\nu^+ - \nu^-}$ *with*

$$\mu^- < m < \mu^- + \frac{3}{2} .$$

Proof: Fix the left root ν^- at the $(m-1)$-mode with the scaling factor $\bar{d}_1 \pi^2$.

$$\bar{d}_1 \pi^2 (m-1)^2 = \nu^- \tag{9}$$

Maximizing the scaling factor gives the following inequalities. Equation (10) is for not to get a second mode into the unstable region, Equation (11) is to be greater than the previous spacing between two eigenvalues.

$$\nu^+ - \nu^- < \bar{d}_1 \pi^2 (m^2 - (m-1)^2) = \bar{d}_1 \pi^2 (2m - 1) \tag{10}$$

$$d_1 \pi^2 ((m-1)^2 - (m-2)^2) = \bar{d}_1 \pi^2 (2m - 3) < \nu^+ - \nu^- \tag{11}$$

Estimation from above is done with Equation (9) and Equation (10).

$$\frac{2(m-1)^2}{2\nu^-} = \frac{1}{\bar{d}_1 \pi^2} < \frac{2m-1}{\nu^+ - \nu^-}$$

$$\Rightarrow \quad \frac{2(m-1)^2}{2m-1} = m - \frac{3m-2}{2m-1} < \frac{2\nu^-}{\nu^+ - \nu^-} = \mu^-$$

$$\Rightarrow \quad m - \frac{3}{2} < m - \frac{3m-2}{2m-1} < \mu^- \quad \Rightarrow \quad m < \mu^- + \frac{3}{2}$$

The mode $m = 1$ can always be arranged to lie inbetween $\nu^\pm$. Consider $m > 1$ for the estimation from below with Equation (9) and Equation (11).

$$\frac{2m-3}{\nu^+ - \nu^-} < \frac{1}{\bar{d}_1 \pi^2} = \frac{2(m-1)^2}{2\nu^-}$$

$$\Rightarrow \mu^- < \frac{2(m-1)^2}{2m-3} = \frac{m(2m-3)-m+2}{2m-3} = m + \frac{2-m}{2m-3} \leq m \;\Rightarrow\; \mu^- < m$$

There are at most two integers within the bounds. It has to be checked if p always evaluates negative for both modes (then take the smaller one), or only for one of them. □

Once the maximal m is found, the critical $\bar{d}_{1_{crit_r}}$ for which there is bifurcation to the wave solution for shrinking $\bar{d}_1 < \bar{d}_{1_{crit_r}}$, can be calculated easily. In the same way a critical $\bar{d}_{1_{crit_l}}$ is calculated for $m-1$, and there is a bifurcation to a periodic solution for growing $\bar{d}_1 > \bar{d}_{1_{crit_l}}$. The two possibilities resemble the situation to either touch the square number with the right or left wing of the parabola (see Figure 3). This yields the following sequence

$$\text{(mode } m) \qquad \bar{d}_{1_m} < \bar{d}_{1_{crit_r}} < \bar{d}_{1_{crit_l}} < \bar{d}_{1_{(m-1)}} \qquad \text{(mode } m-1)$$

and there is no mode destabilized within the open interval $(\bar{d}_{1_{crit_r}}, \bar{d}_{1_{crit_l}})$. So the mode destabilization is well seperated up to the mode with the maximal number that can be estimated with Lemma 2.

1.4 Wave bifurcation in case of $d_1 = d_2 \neq d_3 = 0$

Return to equation Equation (5) and now consider the case where $d_1 = d_2 = d$ and $d_3 = \mathbf{d}$. The second Hurwitz determinant is

$$\begin{aligned}
\tilde{\Delta}_{m\,2} = \Delta_2 \quad & + d(A|12| + \textstyle\sum A|ij| + (\mathrm{tr}A)^2 + a_{33}\mathrm{tr}A) \\
& + \mathbf{d}(A|13| + A|23| + (\mathrm{tr}A(12))^2 + a_{33}\mathrm{tr}A(12)) \\
& + d^2(-\mathrm{tr}A - a_{33}) + \mathbf{d}^2(-\mathrm{tr}A(12)) \\
& + 2(d^2 + 2d\mathbf{d})(-\mathrm{tr}A) \\
& + d^2(d+\mathbf{d}) + d^2(d+\mathbf{d}) + 2\mathbf{d}^2 d \\
& + 2d^2\mathbf{d}
\end{aligned}$$

and for $\mathbf{d} \to 0$

$$\begin{aligned}
\lim_{\mathbf{d}\to 0} \tilde{\Delta}_{m\,2} \; = \Delta_2 \quad & + \quad d\big(A|12| + \textstyle\sum A|ij| + (\mathrm{tr}A)^2 + a_{33}\mathrm{tr}A\big) \\
& + \quad d^2(-3\mathrm{tr}A - a_{33}) \\
& + \quad 2d^3 \qquad = 2q(d)
\end{aligned}$$

that is a cubic polynomial q in d. It can be solved by Cardan's formula, and for a negative discriminant there are three real roots. Since the leading coefficient is positive and the value for $d = 0$ is $\Delta_2 > 0$ you know from the general shape of the cubic polynomial, that one of the roots is always real and negative. But the other two might be positive, resulting in the same behavior for wave bifurcation as described in the previous section.

1.5 Example for both limiting cases

To give a simple example for a linearization to fulfill all the hypotheses to get a wave bifurcation for only $d_1 \neq 0$ as well as $d \neq 0$ consider

$$A = \begin{pmatrix} -\varepsilon & \varepsilon & 2\varepsilon \\ 1+2\varepsilon & -(1+\varepsilon) & \varepsilon^2+6\varepsilon+1 \\ 1 & -1 & 1 \end{pmatrix}, \qquad \dot{x} = A\;x + o(|x|^2)\;.$$

All eigenvalues of A have negative real parts as can be easily seen when computing (H1) $-$ (H3):

$$\begin{aligned}
-\mathrm{tr}A &= 2\varepsilon &> 0 \\
\Delta_2 &= \varepsilon^2 &> 0 \\
-\mathrm{det}A &= 3\varepsilon^2 &> 0\;.
\end{aligned}$$

For the limiting case $d_1 \neq 0$ compute these conditions in case of a diffusion term in the first equation.

$$\tilde{A}_m = \begin{pmatrix} -\varepsilon - d_1 & \varepsilon & 2\varepsilon \\ 1+2\varepsilon & -(1+\varepsilon) & \varepsilon^2+6\varepsilon+1 \\ 1 & -1 & 1 \end{pmatrix}$$

The trace and determinant are decreased. It remains to show that $\tilde{\Delta}_{m2}$ may change sign for a single m with $d_1 = \bar{d}_1 \mu_m^2$.

$$\begin{aligned} -\mathrm{tr}\tilde{A}_m &= 2\varepsilon + d_1 & > 0 \\ \tilde{\Delta}_{m2} &= \varepsilon^2 + d_1(\varepsilon^2 - 3\varepsilon) + {d_1}^2\varepsilon & < 0 \\ -\det\tilde{A}_m &= 3\varepsilon^2 + d_1(\varepsilon^2 + 5\varepsilon) & > 0 \end{aligned}$$

This is the case for $0 < \varepsilon < 1$ and $\nu^- < d_1 < \nu^+$ with

$$\nu^\pm = \frac{1}{2}\left(3 - \varepsilon \pm \sqrt{(3-\varepsilon)^2 - 4\varepsilon}\right) .$$

For $\varepsilon = 0.01$ it yields $\nu^\pm = \{0.3348231 \cdot 10^{-2}, 2.9866518\}$.
For the limiting case $d_1 = d_2 \neq 0$ and for the same $\varepsilon = 0.01$ that means for the same kinetics system you can compute three real roots of $q(d) = 0$ to be round about $\{-1.0050631 \cdot 10^{-2}, 1.0597026 \cdot 10^{-2}, 0.4694536\}$. Therefore one can imagine the wave bifurcation for all intermediate parameters of d_2 so that Theorem 4 holds with additional hypotheses as well for two parabolic equations coupled with a single ordinary equation. These hypotheses are quite ugly when extracted from Cardan's formula and should be left to the computer.

2.1 Application to autocatalytic surface reactions

For computation of a system of three equations that has a background as autocatalytic reaction-diffusion system, think of the following model, derived from stoichiometric network analysis (see Eiswirth [3]). It may be interpreted to describe a surface reaction of carbon monoxid on platinum.

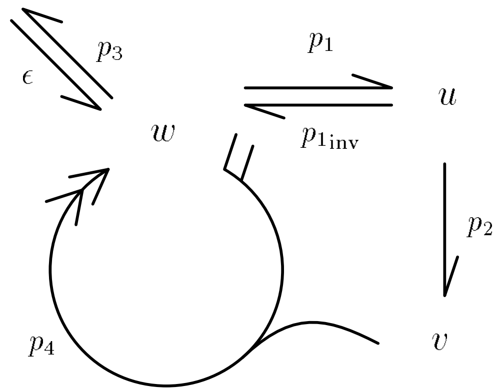

Figure 4: The stoichiometric network scetches the autocatalytic process. Reaction kinetic parameters are written to the according arrows which indicate the stoichiometry by the numbers of flags and feathers.

The Pt(110) well defined surface of a platinum single crystal undergoes a reconstruction process in the absence of adsorbate. This reconstruction is lifted when CO adsorbs at the surface. The resulting nonreconstructed or bulk like surface is able to enhance the slowest process of the reaction that is the dissociation of oxygen. Adsorbed atomic oxygen can now react with the preadsorbed CO to build carbon dioxid that disappears from the surface. This gives rise to the network shown in Figure 4. No flux boundary conditions on the cylinder $\partial\Omega \times (0, T]$ and solutions in the appropriate Hilbert spaces are considered.

$$
\begin{array}{rcll}
[\mathrm{CO_{rec}}] & \dot{u} & = & d_1\Delta u \; - p_{1_{\mathrm{inv}}}u - 2p_2u + 3p_1w \\
[\mathrm{CO}_{[1\times 1]}] & \dot{v} & = & d_2\Delta v \; + p_2u - p_4vw^2 \qquad\qquad\qquad \text{in } \Omega\times(0,\mathrm{T}] \\
[\mathrm{O}_{[1\times 1]}] & \dot{w} & = & d_3\Delta w + p_{1_{\mathrm{inv}}}u - 3p_1w - p_3w + 2p_4vw^2 + \epsilon
\end{array}
$$

$$
\frac{\partial}{\partial n}u = \frac{\partial}{\partial n}v = \frac{\partial}{\partial n}w = 0 \qquad\qquad \text{on } \partial\Omega\times(0,\mathrm{T}]
$$

$$
(u,v,w)^t \in [H^2(\mathring{\Omega}\times(0,T]) \cap H^1(\overline{\Omega}\times(0,T])]^3
$$

A crucial fact is that CO on the reconstructed surface is mobile and can diffuse whereas all the other variables of the system have neglectable mobility. Therefore $d_1 >> d_2 \approx d_3$ and both d_2 and d_3 can be set to zero. The equation for u is considered as a single parabolic equation coupled with ordinary differential equations for v and w. In the sense of stoichiometric networks the parameters p_i are simply set to 1. This yields a linearization A at the stable equilibrium $E_s = (u_s, v_s, w_s)^t$ that fulfills the hypotheses (H1) – (H6). A critical diffusion coefficient $\bar{d}_1$ can be determined and the numerical result of Figure 5 can be predicted.

2.2 Numerical Parameters

The discretisized system of ordinary differential equations is solved with the LSODE package (see Hindmarsh, [4]), using numerical estimates of Jacobian matrix. The error tolerances are 1×10^{-8} relative and 1×10^{-12} absolute. The space discretization is 300 gridpoints on a unit interval. Time discretization is done implicitely.
These results are comparable to those of Zhabotinsky et al. [5] using the same tolerances and discretization schemes. They also show the phenomenon of wave bifurcation in a three variable system modelling cubic autocatalysis but on a more complicated kinetic system.

Conclusion: The advantage of analysing general three variable system lies in the possibility of not only being able to predict what comes out of a straight forward integration but also to construct possible simple networks that already have a special behaviour.

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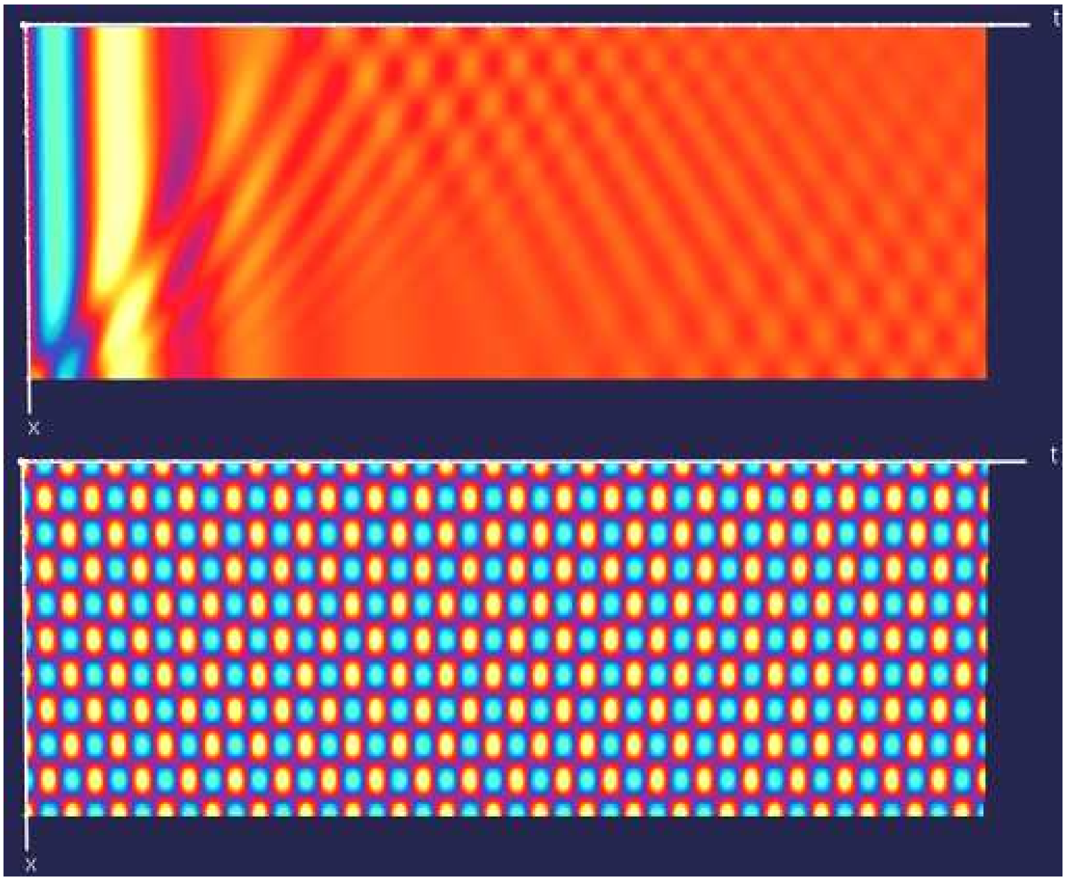

Figure 5: The horizontal axis shows the temporal evolution of a 1-D spatially nonuniform initial data (above, time steps 1-100) to a standing wave pattern (below, time steps 4900-5000).