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Destabilization of uniform steady states in linear diffusion systems with nonlinear boundary conditions

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Abstract.

Systems of linear diffusion equations are considered in smooth bounded domains under nonlinear boundary conditions of Neumann type. We show that the interaction between the difference in diffusion rates and the nonlinear boundary conditions destabilizes uniform steady states, resulting in time periodic spatial patterns.

§1. Introduction and main results

Let $\Omega \subset \mathbb{R}^m$ $(m \geq 1)$ be a bounded domain whose boundary $\partial\Omega$ is smooth. We consider the following system of diffusion equations with the nonlinear boundary conditions for $\boldsymbol{u}(t,x) = (u_1(t,x), \ldots, u_N(t,x))$;

$$\partial_t \boldsymbol{u} = \boldsymbol{D} \triangle \boldsymbol{u} \quad \text{in } \Omega, \qquad \boldsymbol{D} \partial_{\boldsymbol{n}} \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{u}) \quad \text{on } \partial\Omega, \tag{1}$$

where $\partial_t = \partial/\partial t$, $\triangle$ the Laplace operator, $\boldsymbol{D} = \mathrm{diag}(d_1, \ldots, d_N)$ the diffusion matrix, $\partial_{\boldsymbol{n}} = \partial/\partial \boldsymbol{n}$ with $\boldsymbol{n}$ being the unit outward normal vector on $\partial\Omega$, and $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^N$ is a nonlinear mapping.

The first source of motivation to study (1) comes from application. In chemical engineering, the dynamics of inert materials diffusing in a container Ω whose boundary $\partial\Omega$ is the site of catalytic reactions is modeled by (1), see [3] and references therein. In this model, experimentalists are interested in permanent concentration profiles of the materials and their stability.

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The second source of motivation is our desire to study more general systems of reaction-diffusion equations

$$\partial_t \boldsymbol{u} = \boldsymbol{r}(\boldsymbol{u}) + \boldsymbol{D}\triangle \boldsymbol{u} \quad \text{in } \Omega, \qquad \boldsymbol{D}\partial_{\boldsymbol{n}} \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{u}) \quad \text{on } \partial\Omega \tag{2}$$

under nonlinear boundary conditions, see [5], [1], [2]. We would like to find out how the reaction, diffusion and nonlinear boundary conditions, separately or as a whole, influence the dynamics of (2). As a first step, we concentrate on the specific class of (2) in which the reactions are absent inside the domain; $\boldsymbol{r} \equiv 0$. Under suitable conditions, the wellposedness of (2) and the existence of the global compact attractor for the dynamics of (2) have been established by various authors [1], [2] (see also [5]).

The purpose of this article is to study the stability of uniform steady states of (1) and their destabilization due to the interaction between the nonlinear flux $\boldsymbol{f}$ on $\partial\Omega$ and the linear diffusion process $\partial_t \boldsymbol{u} = \boldsymbol{D}\triangle \boldsymbol{u}$ in Ω.

If $\boldsymbol{u}^*$ is a zero of $\boldsymbol{f}$, then $\boldsymbol{u}(x) \equiv \boldsymbol{u}^*$ is a uniform steady solution of (1) for any possible choice of diffusion rates $d_k > 0$ ($k = 1, \dots, N$). For $\lambda \in \mathbb{C}$, we pose the linearized problem:

$$\lambda \boldsymbol{\phi}(x) = \boldsymbol{D}\triangle \boldsymbol{\phi}(x) \quad x \in \Omega, \qquad \boldsymbol{D}\partial_{\boldsymbol{n}} \boldsymbol{\phi}(x) = J\boldsymbol{\phi} \quad x \in \partial\Omega, \tag{3}$$

where J is the Jacobian matrix of $\boldsymbol{f}(\boldsymbol{u})$ at $\boldsymbol{u} = \boldsymbol{u}^*$, and $\lambda \in \mathbb{C}$ is called an *eigenvalue* when (3) has a nontrivial solution $\boldsymbol{\phi}(x) \not\equiv 0$. It is known ([1], [2]) that if all of the eigenvalues satisfy $\operatorname{Re}\lambda < 0$ then $\boldsymbol{u}^*$ is *asymptotically stable* and that if there is an eigenvalue with $\operatorname{Re}\lambda > 0$ then $\boldsymbol{u}^*$ is *unstable.* Applying these criteria, we obtain our first result.

Theorem 1. *Let $\boldsymbol{u}^*$ be a zero of $\boldsymbol{f}$.*

(i) *Assume that J is symmetric. For any choice of diffusion rates $d_k > 0$ ($k = 1, \dots, N$), all eigenvalues of (3) are real. If, moreover, the eigenvalues of J are negative, then $\boldsymbol{u}^*$ is asymptotically stable. If J has a positive eigenvalue, then $\boldsymbol{u}^*$ is unstable.*

(ii) *Assume that J is not symmetric. If the diffusion rates are of the same value $d_1 = d_2 = \dots = d_N$ and all eigenvalues of J have negative real part, then $\boldsymbol{u}^*$ is asymptotically stable.*

Theorem 1 (i) says that when the linearization of $\boldsymbol{f}$ at $\boldsymbol{u}^*$ is symmetric then the stability of $\boldsymbol{u}^*$ is completely determined by the eigenvalues of J. In this case, the eigenvalues of (3) have variational characterizations. On the other hand, if J is not symmetric, it is not so easy to determine the sign of $\operatorname{Re}\lambda$. If the diffusion rates are equal $d_1 = d_2 = \dots = d_N$, then the eigenvalue problem (3) in some sense decouples, and the problem reduces to the scalar case ($N = 1$), leading to Theorem 1 (ii).

To investigate how the asymmetry of J affects the eigenvalues, we now concentrate on the special case of (1) in which $N = 2, m = 1$.

Theorem 2. *Suppose that* $N = 2, \Omega = (-1, +1) \subset \mathbb{R}$. *If the linearization* J *of* $\boldsymbol{f}$ *at its zero* $\boldsymbol{u}^*$ *satisfies*

$$J = \begin{pmatrix} p & q \\ r & s \end{pmatrix}, \quad p < 0, \;\; s > 0, \;\; p + s < 0, \;\; ps - qr > 0, \tag{4}$$

then we have:

(i) *For each fixed* $d_1 < (ps - qr)/s$, *a Hopf bifurcation from* $\boldsymbol{u}^*$ *with a nontrivial spatial mode occurs as* $d_2 \to 0$.

(ii) *For each fixed* $d_1 > (ps - qr)/s$, *a Hopf bifurcation or a steady bifurcation from* $\boldsymbol{u}^*$ *with a nontrivial spatial mode occurs as* $d_2 \to 0$.

Theorem 2 says that interaction between the difference in the diffusion rates and the boundary flux cause Turing type instabilities. If J plays the role of a linear reaction matrix, as in

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} p & q \\ r & s \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

then the conditions in (4) indicate that u_1 is an *inhibitor* and u_2 an *activator*. The statements of Theorem 2 now look similar to those of *diffusion-induced instability* in 2-component systems of reaction-diffusion equations. In the present case (1), however, notice that time-periodic solutions with nontrivial spatial modes bifurcate from the uniform steady state $\boldsymbol{u}^*$ as the pair of diffusion rates (d_1, d_2) crosses the critical curve.

§2. Proofs

2.1. Proof of Theorem 1

Let $\lambda \in \mathbb{C}$ be an eigenvalue of (3) and $\boldsymbol{\phi}$ a corresponding eigenfunction. Multiplying the both sides of (3) by $\overline{\boldsymbol{\phi}}$ (the complex conjugate of $\boldsymbol{\phi}$), integrating on Ω by parts, and using the boundary conditions in (3), we have, after splitting into the real and imaginary parts,

$$\begin{aligned} \mathrm{Re}\,\lambda \int_\Omega |\boldsymbol{\phi}|^2 \mathrm{d}x &= \frac{1}{2}\int_{\partial\Omega} \overline{\boldsymbol{\phi}} \cdot (J + J^{\mathrm{T}})\boldsymbol{\phi}\,\mathrm{d}S_x - \int_\Omega \sum_{k=1}^N d_k |\nabla \phi_k|^2 \mathrm{d}x, \\ \mathrm{Im}\,\lambda \int_\Omega |\boldsymbol{\phi}|^2 \mathrm{d}x &= \frac{1}{2\mathrm{i}}\int_{\partial\Omega} \overline{\boldsymbol{\phi}} \cdot (J - J^{\mathrm{T}})\boldsymbol{\phi}\,\mathrm{d}S_x, \end{aligned}$$

where J^{T} is the transpose of J. If J is symmetric, then $J - J^{\mathrm{T}} = 0$, and hence $\operatorname{Im} \lambda = 0$. This proves that the eigenvalues are real and that the eigenfunctions are real-valued. We therefore have

$$\lambda \int_{\Omega} |\phi|^2 \mathrm{d}x = \int_{\partial\Omega} \phi \cdot J\phi \, \mathrm{d}S_x - \int_{\Omega} \sum_{k=1}^{N} d_k |\nabla \phi_k|^2 \mathrm{d}x. \tag{5}$$

If all eigenvalues of J are negative, then $\phi \cdot J\phi \leq -C|\phi|^2$ for some $C > 0$, and hence (5) implies that

$$\lambda \int_{\Omega} |\phi|^2 \mathrm{d}x \leq -C \int_{\partial\Omega} |\phi|^2 \, \mathrm{d}S_x - \int_{\Omega} \sum_{k=1}^{N} d_k |\nabla \phi_k|^2 \mathrm{d}x < 0,$$

proving the second part of (i). The identity (5) also allows us (see, [4]) to characterize the largest eigenvalue λ_1 by

$$\lambda_1 = \max \left\{ \int_{\partial\Omega} \phi \cdot J\phi \, \mathrm{d}S_x - \int_{\Omega} \sum_{k=1}^{N} d_k |\nabla \phi_k|^2 \mathrm{d}x \;\middle|\; \int_{\Omega} |\phi|^2 \mathrm{d}x = 1 \right\}.$$

If J has a positive eigenvalue $\alpha > 0$, by choosing the corresponding eigenvector ϕ with $|\phi|^2 = |\Omega|^{-1}$ as a test function, we then find that $\lambda_1 \geq \alpha |\partial\Omega| |\Omega|^{-1} > 0$. This completes the proof of Theorem 1 (i).

To prove Theorem 1 (ii), let us define a map called the Dirichlet-to-Neumann map. For a given function $p(x)$ ($x \in \partial\Omega$), the Dirichlet boundary value problem for a scalar valued function $v(x)$, $x \in \Omega$

$$\lambda v(x) = \Delta v(x) \quad x \in \Omega, \qquad v(x) = p(x) \quad x \in \partial\Omega \tag{6}$$

has a unique solution, if $\lambda \in \mathbb{C} \backslash \{\mu_j \mid j = 1, 2, \ldots\}$ where $0 > \mu_1 \geq \mu_2 \geq \ldots \geq \mu_j \to -\infty$ are the eigenvalues of the Laplacian on Ω with the homogeneous Dirichlet boundary conditions. The Dirichlet-to-Neumann map $\mathcal{T}(\lambda) : p \mapsto \mathcal{T}(\lambda)p$ is defined by

$$\left(\mathcal{T}(\lambda)p\right)(x) := \partial_{\boldsymbol{n}} v(x) \quad x \in \partial\Omega. \tag{7}$$

From the definition of $\mathcal{T}$, it is easy to see that (3) is equivalent to

$$\operatorname{diag}[d_1 \mathcal{T}(\lambda/d_1), \ldots, d_N \mathcal{T}(\lambda/d_N)] \phi(x) = J\phi(x) \quad x \in \partial\Omega. \tag{8}$$

When $d_k = d$ for $k = 1, 2, \ldots, N$, we find, by using the eigenfunction expansion associated with the operator $\mathcal{T}(\lambda/d)$ (cf. [4]), that (8) has nontrivial solutions ϕ if and only if the problem

$$d\mathcal{T}(\lambda/d)p(x) = \alpha p(x) \quad x \in \partial\Omega \tag{9}$$

has nontrivial solutions, where α is one of the eigenvalues of the matrix J. If $\operatorname{Re}\alpha < 0$ and (9) has a nontrivial solution, then we obtain

$$\operatorname{Re}\lambda \int_\Omega |v|^2 \, dx = \operatorname{Re}\alpha \int_{\partial\Omega} |v|^2 \, dS_x - d \int_\Omega |\nabla v|^2 \, dx < 0,$$

proving (ii), where v satisfies $\lambda v = d\triangle v$ in Ω and $v = p$ on $\partial\Omega$.

2.2. Proof of Theorem 2

Our proof depends on explicit computations. Let us consider the problem (6) for $N = 2, m = 1, \Omega = (-1, +1)$. This problem has a unique solution for $\lambda \in \mathbb{C}\backslash\{-\pi^2 n^2/4 \mid n = 1, 2, \ldots\}$. By using the solution, the Dirichlet-to-Neumann map $\mathcal{T}(\lambda)$ is explicitly given by the 2×2 matrix:

$$\mathcal{T}(\lambda) \begin{pmatrix} v(-1) \\ v(+1) \end{pmatrix} := \sqrt{\lambda} \begin{pmatrix} \coth 2\sqrt{\lambda} & -\operatorname{cosech} 2\sqrt{\lambda} \\ -\operatorname{cosech} 2\sqrt{\lambda} & \coth 2\sqrt{\lambda} \end{pmatrix} \begin{pmatrix} v(-1) \\ v(+1) \end{pmatrix}.$$

In terms of the matrix $\mathcal{T}(\lambda)$, the problem (8) with J being given by (4) has nontrivial solution if and only if the 4×4 matrix is singular;

$$\det \begin{pmatrix} d_1\mathcal{T}(\lambda/d_1) - pI_2 & -qI_2 \\ -rI_2 & d_2\mathcal{T}(\lambda/d_2) - sI_2 \end{pmatrix} = 0,$$

where I_2 is the 2×2 identity matrix. Applying elementary row (or column) operations on the 4×4 matrix, this condition is further recast as the singularity condition of the 2×2 matrix

$$\det\big[d_1 d_2 \mathcal{T}(\lambda/d_1)\mathcal{T}(\lambda/d_2) - \{p d_2 \mathcal{T}(\lambda/d_2) + s d_1 \mathcal{T}(\lambda/d_1)\} \\ + (ps - qr)I_2\big] = 0.$$

This is equivalent to

$$\text{(10)} \qquad \big[(\mathrm{t}_1^+ - p)(\mathrm{t}_2^+ - s) - qr\big]\big[(\mathrm{t}_1^- - p)(\mathrm{t}_2^- - s) - qr\big] = 0,$$

where $\mathrm{t}_j^\pm = \sqrt{d_j \lambda}(\pm 1 + \cosh 2\sqrt{\lambda/d_j})/\sinh 2\sqrt{\lambda/d_j}$, and we easily find

$$\lim_{d_j \to 0} \mathrm{t}_j^\pm = 0, \quad \lim_{\lambda \to 0} \mathrm{t}_j^- = 0 \text{ and } \lim_{\lambda \to 0} \mathrm{t}_j^+ = d_j \text{ for } j = 1, 2.$$

To determine the steady destabilization curve in the first quadrant of the d_1-d_2 plane, we let $\lambda \to 0$ in (10) and then obtain $(d_1 - p)(d_2 - s) - qr = 0$. This curve intersects d_1-axis at $d_1 = (ps - qr)/s$ and is meaningful for $d_1 > (ps - qr)/s$ where d_2 ranges in $0 < d_2 < s$ and $d_2 \to s$ as $d_1 \to \infty$. If we let $d_2 \to 0$ in (10), then $[\mathrm{t}_1^- - (ps - qr)/s][\mathrm{t}_1^+ - (ps - qr)/s] = 0$. This equation in λ has infinitely many negative solutions, and moreover, one positive solution if $d_1 > (ps - qr)/s$ and two positive solutions if $d_1 < (ps - qr)/s$.

The eigenvalues of the 2×2 matrix J have negative real part under the conditions in (4), and hence, Theorem 1 (ii) implies that all eigenvalues λ of (10) satisfy $\operatorname{Re}\lambda < 0$ for $d_2 = d_1 > 0$. Therefore, as d_2 decreases from $d_2 = d_1$ to $d_2 = 0$, some eigenvalues cross the imaginary axis in $\mathbb{C}$ from $\operatorname{Re}\lambda < 0$ to $\operatorname{Re}\lambda > 0$.

If $d_1 > (ps - qr)/s$, this crossing is either through $\lambda = 0$ or a pair of complex conjugate eigenvalues cross the imaginary axis, possibly several times back and forth, and eventually one pair of complex conjugate eigenvalues remain in the right half plane, which finally collide on the positive real axis and one of them return to the negative real axis through $\lambda = 0$ while the other remain on the positive real axis. Under the conditions in (4), the uniform steady state $\boldsymbol{u}_*$ is isolated and uniform steady states are locally unique. Therefore, if the bifurcation is steady, the spatial mode of the bifurcated solution must be non trivial, and in fact, the eigenfunction is of the form $\phi(x) = (x, \gamma x)$ where $\gamma \neq 0$ is an appropriate constant. If the bifurcation is of Hopf type, then, by elementary computations, the eigenfunction is of the form

$$\phi(t,x) = \mathrm{e}^{\lambda t} \begin{pmatrix} \dfrac{\sinh \sqrt{\lambda/d_1}\, x}{\sinh \sqrt{\lambda/d_1}} \\ \gamma \dfrac{\sinh \sqrt{\lambda/d_2}\, x}{\sinh \sqrt{\lambda/d_2}} \end{pmatrix},$$

where $\lambda = \mathrm{i}\tau$ with $\tau > 0$ is the eigenvalue and $\gamma \neq 0$ is a constant. This proves Theorem 2 (ii).

On the other hand, if $d_1 < (ps - qr)/s$, eigenvalues λ cannot cross the origin, and hence a pair of non-zero complex conjugate eigenvalues have to cross the imaginary axis at least once. The non-triviality of the bifurcated spatial mode is the same as above. This proves Theorem 2 (i).

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