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Diffusion and reaction-diffusion equations on discrete domains

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Summary

Numerous real-world phenomena have been traditionally modeled using partial differential equations. However, there are situations where it is more natural to consider models on discrete spatial domains, which are formulated in terms of semidiscrete or purely discrete evolution equations. For instance, this is common in mathematical biology when modeling populations living in fragmented habitats (islands, ponds, etc.), signal propagation between neurons, etc. Discrete-space evolution equations are also interesting from the viewpoint of numerical mathematics, since they often correspond to discretizations (or semidiscretizations) of PDEs.

The dissertation represents a collection of articles on various phenomena related to discrete-space equations, with a particular emphasis on linear diffusion equations and nonlinear reaction-diffusion equations. We deal with various topics such as well-posedness, asymptotic behavior of solutions, explicit formulas for fundamental solutions of linear equations, or the validity of maximum principles. We pay special attention to the existence of heterogenous equilibrium states, which is a characteristic feature of discrete-space models that has no analogue in the corresponding PDE models. As an illustration, we provide a detailed overview of the Lotka-Volterra competition model on graphs.

The goal of the present theses is to explain the basic ideas and results contained in the dissertation in an accessible and reader-friendly way. The proofs of all results as well as additional technical details are available in the dissertation itself, which consists of the following twelve journal articles:

[AS1] A. Slavík, P. Stehlík: *Dynamic diffusion-type equations on discrete-space domains.* J. Math. Anal. Appl. 427 (2015), 525–545.

[AS2] A. Slavík, P. Stehlík: *Explicit solutions to dynamic diffusion-type equations and their time integrals.* Appl. Math. Comput. 234 (2014), 486–505.

[AS3] M. Friesl, A. Slavík, P. Stehlík: *Discrete-space partial dynamic equations on time scales and applications to stochastic processes.* Appl. Math. Lett. 37 (2014), 86–90.

[AS4] A. Slavík: *Discrete-space systems of partial dynamic equations and discrete-space wave equation.* Qual. Theory Dyn. Syst. 16 (2017), 299–315.

[AS5] A. Slavík: *Invariant regions for systems of lattice reaction-diffusion equations.* J. Differential Equations 263 (2017), 7601–7626.

[AS6] A. Slavík: *Discrete Bessel functions and partial difference equations.* J. Difference Equ. Appl. 24 (2018), 425–437.

[AS7] A. Slavík, P. Stehlík, J. Volek: *Well-posedness and maximum principles for lattice reaction-diffusion equations.* Adv. Nonlinear Anal. 8 (2019), 303–322.

[AS8] A. Slavík: *Lotka-Volterra competition model on graphs.* SIAM J. Appl. Dyn. Syst. 19 (2020), 725–762.

[AS9] A. Slavík: *Asymptotic behavior of solutions to the semidiscrete diffusion equation.* Appl. Math. Lett. 106 (2020), 106392.

[AS10] A. Slavík: *Reaction-diffusion equations on graphs: stationary states and Lyapunov functions.* Nonlinearity 34 (2021), 1854–1879.

[AS11] A. Slavík: *Spatial maxima, unimodality, and asymptotic behaviour of solutions to discrete diffusion-type equations.* J. Difference Equ. Appl. 28 (2022), 126–140.

[AS12] A. Slavík: *Asymptotic behavior of solutions to the multidimensional semidiscrete diffusion equation.* Electron. J. Qual. Theory Differ. Equ. (2022), no. 9, 1–9.

In the cases of coauthored papers, all authors have contributed equally to the manuscript. I am grateful to my coauthors Petr Stehlík, Jonáš Volek, and Michal Friesl from the University of West Bohemia for a fruitful collaboration.

Contents

Chapter 1

Linear diffusion equations on $\mathbb{Z}$ and $\mathbb{Z}^N$

The present chapter is based on the papers [AS1], [AS2], [AS3], [AS4], [AS6], [AS9], [AS11], [AS12].

1.1 Introduction

The classical diffusion (heat) equation $\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$ and its generalizations serve as models for many real-world phenomena. In this chapter, we consider a class of diffusion-type equations with discrete space and arbitrary (continuous, discrete or mixed) time, namely

$$u^\Delta(x,t) = au(x+1,t) + bu(x,t) + cu(x-1,t), \quad x \in \mathbb{Z},\ t \in \mathbb{T}, \tag{1.1.1}$$

where $\mathbb{T}$ is a time scale (arbitrary closed subset of $\mathbb{R}$). The symbol u^Δ denotes the partial Δ-derivative with respect to t, which becomes the usual partial derivative $\frac{\partial u}{\partial t}$ when $\mathbb{T} = \mathbb{R}$, and the forward partial difference $u(x,t+1) - u(x,t)$ when $\mathbb{T} = \mathbb{Z}$. In this way, we are able to study equations with continuous, discrete or mixed time domains in a unified way. Readers who are not familiar with the time scales calculus might consult [4] or [14].

Equations of the form (1.1.1) include the following special cases:

- When $a = c$ and $b = -2a$, Eq. (1.1.1) represents a discretized version of the classical diffusion equation. Depending on the time scale, we can obtain the semidiscrete diffusion equation ($\mathbb{T} = \mathbb{R}$), or the purely discrete diffusion equation ($\mathbb{T} = \mathbb{Z}$).

- The case $a = 0$ and $0 < c = -b$ corresponds to the discrete-space transport equation.

- For $\mathbb{T} = \mathbb{Z}$, $a = c = 1/2$ and $b = -1$, Eq. (1.1.1) reduces to

$$u(x, t+1) = \frac{1}{2}u(x+1, t) + \frac{1}{2}u(x-1, t), \tag{1.1.2}$$

  which (together with the conditions $u(0, 0) = 1$ and $u(x, 0) = 0$ for $x \neq 0$) describes the one-dimensional symmetric random walk on $\mathbb{Z}$ starting from the origin; the value $u(x, t)$ is the probability that the random walk visits point x at time t. More generally, consider a nonsymmetric random walk on $\mathbb{Z}$, where the probabilities of going left, standing still, or going right are $p, q, r \in [0, 1]$, with $p+q+r = 1$. This random walk is described by Eq. (1.1.1), where $\mathbb{T} = \mathbb{Z}$, $a = p$, $b = q - 1$ and $c = r$. For $\mathbb{T} = \mathbb{R}$, we obtain a continuous-time random walk. Finally, for a general time scale $\mathbb{T}$, solutions of (1.1.1) can be regarded as heterogeneous stochastic processes.

Applications of (1.1.1) go far beyond stochastic processes. For example, the semidiscrete diffusion equation appears in signal and image processing [21], while the discrete diffusion equation has been used to model mutations in biology [5]. From a theoretical point of view, our work could be perceived as a contribution to the study of partial dynamic equations (see, e.g., [1, 15, 17, 22]), as well as infinite systems of ordinary dynamic equations (see, e.g., [24]).

1.2 Basic results

A natural starting point is to investigate existence and uniqueness of solutions to initial-value problems for the equation (1.1.1). For the classical diffusion equation with continuous time and space, initial-value problems on the whole real line do not have unique solutions (this was shown by Tychonoff [33]; see also [18]). Also, note that (1.1.1) represents a countable system of dynamic equations; the fact that initial-value problems for countable systems of differential equations need not have unique solutions was also observed by Tychonoff [32].

The following construction shows that solutions of Eq. (1.1.1) with a given initial condition need not be unique. Consider the time scale $\mathbb{T} = \mathbb{R}$. Take a pair of infinitely differentiable functions $f, g : \mathbb{R} \to \mathbb{R}$ such that $f^{(i)}(0) = 0$ and $g^{(i)}(0) = 0$ for every $i \in \mathbb{N}_0$. Let $u(0,t) = f(t)$ and $u(1,t) = g(t)$ for every $t \in \mathbb{R}$. It remains to define $u(x,t)$ for $x \in \mathbb{Z} \setminus \{0,1\}$ so that

$$\frac{\partial u}{\partial t}(x,t) = au(x+1,t) + bu(x,t) + cu(x-1,t) \tag{1.2.1}$$

for all $x \in \mathbb{Z}$ and $t \in \mathbb{R}$. Assuming that $a, c \neq 0$, the formulas

$$u(x+1,t) = \frac{1}{a}\left(\frac{\partial u}{\partial t}(x,t) - bu(x,t) - cu(x-1,t)\right), \quad x \geq 1,\ t \in \mathbb{R},$$

$$u(x-1,t) = \frac{1}{c}\left(\frac{\partial u}{\partial t}(x,t) - au(x+1,t) - bu(x,t)\right), \quad x \leq 0,\ t \in \mathbb{R},$$

determine the remaining values $u(x,t)$ uniquely. By the properties of f and g, we have $u(x,0) = 0$ for every $x \in \mathbb{Z}$. Since there are infinitely many possibilities of choosing f and g, it follows that (1.2.1) has infinitely many solutions corresponding to the zero initial condition at $t = 0$. Obviously, one solution is the zero solution, which corresponds to $f = g = 0$. It can be shown (cf. Theorem 1.2.1 below) that all nonzero solutions display a curious behavior: they are unbounded on all sets of the form $\mathbb{Z} \times [0, \varepsilon]$, where $\varepsilon > 0$ can be arbitrarily small. Conversely, it turns out that if we restrict our attention to solutions which are bounded on all sets of the form $\mathbb{Z} \times [a,b]$, where $[a,b] \subset \mathbb{R}$, then all initial-value problems with bounded initial conditions have a unique solution; this is the content of Theorem 1.2.1 below.

There are other reasons why unbounded solutions are pathological. For example, consider the previous construction with f identically zero and $g(t) = -e^{-1/t^2}$. Then the initial condition at $t = 0$ is symmetric with respect to the origin, but the solution does not maintain this property and is odd in x. Also, the solution violates the maximum and minimum principles.

Let $\ell^\infty(\mathbb{Z})$ denote the space of all bounded real sequences $\{u_n\}_{n \in \mathbb{Z}}$ equipped with the supremum norm $\|u\|_\infty = \sup_{n \in \mathbb{Z}} |u_n|$. The next result guarantess the existence and uniqueness of forward and backward bounded solutions. Its statement involves the graininess operator μ, which measures the sizes of gaps between time scale points, and is defined as follows:

$$\mu(t) = \inf\{s \in \mathbb{T} : s > t\} - t, \quad t \in \mathbb{T}.$$

Also, we use the notation $[a,b]_{\mathbb{T}}$ to denote the time scale interval $[a,b]\cap\mathbb{T}$ with endpoints $a,b\in\mathbb{T}$, $a\le b$. Open and half-open time scale intervals are denoted in a similar way.

Theorem 1.2.1. *Consider an interval $[T_1,T_2]_{\mathbb{T}}$ and $t_0\in[T_1,T_2]_{\mathbb{T}}$. Let $u^0\in\ell^\infty(\mathbb{Z})$. Assume that $\mu(t)<\frac{1}{|a|+|b|+|c|}$ for every $t\in[T_1,t_0)_{\mathbb{T}}$.*

Then, there exists a unique bounded solution $u:\mathbb{Z}\times[T_1,T_2]_{\mathbb{T}}\to\mathbb{R}$ of Eq. (1.1.1) such that $u(x,t_0)=u^0_x$ for every $x\in\mathbb{Z}$.

The proof of existence is easy: Instead of Eq. (1.1.1), one can consider the abstract equation $U^\Delta(t)=AU(t)$, where U takes values in $\ell^\infty(\mathbb{Z})$, and $A:\ell^\infty(\mathbb{Z})\to\ell^\infty(\mathbb{Z})$ is a linear operator given by

$$A(\{u_n\}_{n\in\mathbb{Z}})=\{au_{n+1}+bu_n+cu_{n-1}\}_{n\in\mathbb{Z}}. \tag{1.2.2}$$

This operator is bounded and has norm $\|A\|=|a|+|b|+|c|$. In view of the graininess condition, $I+A\mu(t)$ is invertible for all $t\in[T_1,t_0)_{\mathbb{T}}$, which in turn implies the existence of a solution U. The proof of uniqueness is longer, but involves only elementary estimates.

The graininess condition $\mu(t)<\frac{1}{|a|+|b|+|c|}$ in Theorem 1.2.1 applies to backward solutions only, and cannot be omitted. For example, let $a=c=1$, $b=-2$, and consider the time scale $\mathbb{T}=\frac{1}{4}\mathbb{Z}=\{\frac{n}{4},\ n\in\mathbb{Z}\}$, which violates the graininess condition:

- For the zero initial condition at $t=0$, it is easy to check that $u(x,-1/4)=(-1)^x\alpha$, $x\in\mathbb{Z}$, satisfies Eq. (1.1.1) for every $\alpha\in\mathbb{R}$. Hence, in general, bounded backward solutions need not be unique.

- For the initial condition

  $$u(x,0)=\begin{cases}1 & \text{if } x=0,\\ 0 & \text{if } x\neq 0,\end{cases}$$

  one can show that it is impossible to find a bounded sequence $\{u(x,-1/4)\}_{x\in\mathbb{Z}}$ so that Eq. (1.1.1) is satisfied. Therefore, in general, bounded backward solutions need not exist once the graininess condition is violated.

Another basic result is the superposition principle. Eq. (1.1.1) is linear, and every finite linear combination of solutions is a solution again. The next theorem shows that under certain assumptions, it makes sense to consider infinite linear combinations as well.

Theorem 1.2.2. *Let $u_k : \mathbb{Z} \times [t_0, T]_{\mathbb{T}} \to \mathbb{R}$, $k \in \mathbb{N}$, be a sequence of bounded solutions of Eq.* (1.1.1). *Assume there exists a $\beta > 0$ such that $\sum_{k=1}^{\infty} |u_k(x, t_0)| \leq \beta$ for every $x \in \mathbb{Z}$. Then, for every bounded sequence $\{c_k\}_{k=1}^{\infty}$, the function $u(x,t) = \sum_{k=1}^{\infty} c_k u_k(x,t)$ is a solution of Eq.* (1.1.1) *on $\mathbb{Z} \times [t_0, T]_{\mathbb{T}}$.*

An important corollary is that for each arbitrary initial condition from $\ell^{\infty}(\mathbb{Z})$, we can express the corresponding unique bounded solution of (1.1.1) in terms of the so-called fundamental solution (the function u in the next statement).

Corollary 1.2.3. *Let $u : \mathbb{Z} \times [t_0, T]_{\mathbb{T}} \to \mathbb{R}$ be the unique bounded solution of Eq.* (1.1.1) *corresponding to the initial condition*

$$u(x, t_0) = \begin{cases} 1 & \text{if } x = 0, \\ 0 & \text{if } x \neq 0. \end{cases}$$

If $\{c_k\}_{k \in \mathbb{Z}}$ is an arbitrary bounded real sequence, then

$$v(x,t) = \sum_{k \in \mathbb{Z}} c_k u(x-k, t)$$

is the unique bounded solution of Eq. (1.1.1) *corresponding to the initial condition $v(x, t_0) = c_x$, $x \in \mathbb{Z}$.*

The next result shows that for equations with $a + b + c = 0$, the sum $\sum_{x \in \mathbb{Z}} u(x,t)$ is the same for all t.

Theorem 1.2.4. *Let $u : \mathbb{Z} \times [T_1, T_2]_{\mathbb{T}} \to \mathbb{R}$ be a bounded solution of Eq.* (1.1.1) *with $a + b + c = 0$. Assume that:*

- *For a certain $t_0 \in [T_1, T_2]_{\mathbb{T}}$, the sum $\sum_{x \in \mathbb{Z}} |u(x, t_0)|$ is finite.*
- *$\mu(t) < \frac{1}{|a|+|b|+|c|}$ for every $t \in [T_1, t_0)_{\mathbb{T}}$.*

Then $\sum_{x \in \mathbb{Z}} u(x,t) = \sum_{x \in \mathbb{Z}} u(x, t_0)$ for every $t \in [T_1, T_2]_{\mathbb{T}}$.

We conclude our survey of basic results with the minimum and maximum principles.

Theorem 1.2.5. *Let a, b, c be such that $a, c \geq 0$, $b \leq 0$. Consider a bounded solution $u : \mathbb{Z} \times [T_1, T_2]_{\mathbb{T}} \to \mathbb{R}$ of Eq.* (1.1.1). *Moreover, assume that $\mu(t) \leq -1/b$ for every $t \in [T_1, T_2)_{\mathbb{T}}$. Then the following statements are true for all $K \geq 0$:*

- *If $a+b+c \geq 0$ and $u(x,T_1) \geq K$ for every $x \in \mathbb{Z}$, then $u(x,t) \geq K$ for all $t \in [T_1,T_2]_{\mathbb{T}}$, $x \in \mathbb{Z}$.*
- *If $a+b+c \leq 0$ and $u(x,T_1) \leq K$ for every $x \in \mathbb{Z}$, then $u(x,t) \leq K$ for all $t \in [T_1,T_2]_{\mathbb{T}}$, $x \in \mathbb{Z}$.*

The proof is interesting because it utilizes some ideas from product integration theory. If $\mathbb{T}$ is purely discrete, one can obtain the values of the solution at any time t as a composition of monotone operators applied to the initial condition. For a general time scale, one passes to the limit and uses the fact that a limit of monotone operators is again monotone.

If $a+b+c=0$, both minimum and maximum principles hold, and we get two important consequences:

- *Stability of solutions.* If u,v is a pair of solutions of Eq. (1.1.1) such that $|u(x,T_1)-v(x,T_1)| \leq \varepsilon$ for every $x \in \mathbb{Z}$, we can apply Theorem 1.2.5 to the function $u-v$ and conclude that $|u(x,t)-v(x,t)| \leq \varepsilon$ for all $x \in \mathbb{Z}$, $t \geq T_1$.
- *Global boundedness.* We know from Theorem 1.2.1 that for every $t_1 \in [t_0,\infty)_{\mathbb{T}}$, Eq. (1.1.1) has a unique bounded solution on $\mathbb{Z} \times [t_0,t_1]_{\mathbb{T}}$. It follows from Theorem 1.2.5 that these solutions are always bounded by the same constant independent of t_1. Hence, Eq. (1.1.1) has a unique bounded solution on $\mathbb{Z} \times [t_0,\infty)_{\mathbb{T}}$. On the other hand, when $a+b+c \neq 0$, we still have a solution on $\mathbb{Z} \times [t_0,\infty)_{\mathbb{T}}$, but it need not be globally bounded (consider the case $a=c=0$, $b=1$).

1.3 More general problems

Most results of the previous section can be extended to more general equations having the form

$$u^{\Delta}(x,t) = \sum_{i=-m}^{m} a_i u(x+i,t), \quad x \in \mathbb{Z}, \quad t \in \mathbb{T},$$

where $m \in \mathbb{N}$, and $a_{-m},\dots,a_m \in \mathbb{R}$. We omit the details and refer the reader to the paper [AS3], which also discusses the relation between this type of equations and stochastic processes.

An even more general setting can be found in [AS4], which deals with multidimensional systems: Assume that $N \in \mathbb{N}$, $e_1,\dots,e_N$ is the canonical basis of $\mathbb{R}^N$, $n, r \in \mathbb{N}$, and $A^{(i_1,\ldots,i_N)} \in \mathbb{R}^{n\times n}$ for all $i_1, \ldots, i_N \in \{-r, \ldots, r\}$. One can consider systems of n first-order equations written in the vector form

$$u^{\Delta}(x,t) = \sum_{i_1,\ldots,i_N \in \{-r,\ldots,r\}} A^{(i_1,\ldots,i_N)} u\left(x + \textstyle\sum_{k=1}^N i_k e_k, t\right), \quad t \in \mathbb{T},\ x \in \mathbb{Z}^N, \tag{1.3.1}$$

with the unknown function $u : \mathbb{Z}^N \times \mathbb{T} \to \mathbb{R}^n$. Thus, each component of $u^{\Delta}(x,t)$ is a linear combination of the values of u lying in the N-dimensional hypercube centered at x and whose side has length $2r+1$. Special cases of this general problem include the N-dimensional discrete-space diffusion equation

$$u^{\Delta}(x,t) = a\left(\sum_{i=1}^N u(x+e_i,t) - 2Nu(x,t) + \sum_{i=1}^N u(x-e_i,t)\right),$$

as well as the N-dimensional discrete-space wave equation

$$u^{\Delta\Delta}(x,t) = c^2\left(\sum_{i=1}^N u(x+e_i,t) - 2Nu(x,t) + \sum_{i=1}^N u(x-e_i,t)\right),$$

which is equivalent to the first-order system

$$\begin{aligned} u^{\Delta}(x,t) &= v(x,t),\\ v^{\Delta}(x,t) &= \sum_{i=1}^N c^2 u(x+e_i,t) - 2Nc^2 u(x,t) + \sum_{i=1}^N c^2 u(x-e_i,t), \end{aligned}$$

i.e., it has the form (1.3.1) with $n = 2$, $r = 1$, $A^{(0,\ldots,0)} = \begin{pmatrix} 0 & 1 \\ -2Nc^2 & 0 \end{pmatrix}$, $A^{(i_1,\ldots,i_N)} = \begin{pmatrix} 0 & 0 \\ c^2 & 0 \end{pmatrix}$ if exactly one of the $i_1, \ldots, i_N$ is nonzero and equals ± 1, and $A^{(i_1,\ldots,i_N)} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ otherwise.

We refer the reader to [AS4] for more details.

1.4 Fundamental solutions

There are several methods for finding explicit formulas for fundamental solutions of linear discrete-space equations. Let us look for the unique bounded solution of the initial-value problem

$$\begin{aligned} u^{\Delta}(x,t) &= au(x+1,t)+bu(x,t)+cu(x-1,t), \\ u(x,t_0) &= \begin{cases} 1 & \text{if } x=0, \\ 0 & \text{if } x\neq 0, \end{cases} \end{aligned} \tag{1.4.1}$$

where a, b, c are arbitrary real numbers.

Perhaps the most powerful method is based on generating functions. Given a sequence $\{u_n\}_{n\in\mathbb{Z}}$, its generating function is the series $U(z) = \sum_{n=-\infty}^{\infty} u_n z^n$. Depending on the context, the series can be interpreted either as a classical Laurent series, or as a formal Laurent series.

Assume that u is the solution of the initial-value problem (1.4.1), and let $F(z,t) = \sum_{x=-\infty}^{\infty} u(x,t)z^x$; hence, for every fixed $t \in \mathbb{T}$, the function $z \mapsto F(z,t)$ is the generating function of $\{u(x,t)\}_{x\in\mathbb{Z}}$. Using (1.4.1) and some elementary manipulations, we obtain

$$F^{\Delta}(z,t) = (a/z+b+cz)F(z,t),$$

and $F(z,t_0) = \sum_{x=-\infty}^{\infty} u(x,t_0)z^x = 1$. Hence, we have a first-order linear dynamic equation for the function F. Its solution is given by the time scale exponential function $F(z,t) = e_{a/z+b+cz}(t,t_0)$.

Given a particular time scale $\mathbb{T}$, it is enough to calculate the value of $e_{a/z+b+cz}(t,t_0)$, find its Laurent series expansion with respect to z, and look at the coefficient of z^x to find an explicit formula for $u(x,t)$.

As an illustration, let $\mathbb{T} = \mathbb{R}$ and $t_0 = 0$. The time scale exponential function $e_{a/z+b+cz}(t,t_0)$ reduces to the classical exponential function $e^{(a/z+b+cz)t}$. Therefore, our generating function method gives

$$F(z,t) = e^{(a/z+b+cz)t} = e^{bt}e^{(a/z+cz)t}.$$

To obtain the series expansion of F, we need the identity

$$e^{w/2(z+1/z)} = \sum_{x=-\infty}^{\infty} I_x(w)z^x,$$

where $I_x(w) = \sum_{k=0}^{\infty} \frac{1}{\Gamma(k+x+1)k!}\left(\frac{w}{2}\right)^{2k+x}$ is the modified Bessel function of the first kind. Assuming that $a, c \neq 0$, we get

$$F(z,t) = e^{bt}e^{\sqrt{ac}\left(\frac{\sqrt{a}}{\sqrt{cz}}+\frac{\sqrt{cz}}{\sqrt{a}}\right)t} = e^{bt}\sum_{x=-\infty}^{\infty} I_x(2t\sqrt{ac})\left(\sqrt{\frac{c}{a}}\,z\right)^x,$$

which leads to the result

$$u(x,t) = e^{bt} I_x(2t\sqrt{ac}) \left(\sqrt{\frac{c}{a}}\right)^x, \quad x \in \mathbb{Z}, \quad t \in \mathbb{R}.$$

For symmetric right-hand sides with $a = c$, the solution simplifies to

$$u(x,t) = e^{bt} I_x(2at), \quad x \in \mathbb{Z}, \quad t \in \mathbb{R}. \tag{1.4.2}$$

Additional examples can be found in [AS2]. The same method also works for the discrete-space wave equation, see [AS4].

For $\mathbb{T} = \mathbb{Z}$, the fundamental solution of the purely discrete diffusion equation

$$u(x,t+1) - u(x,t) = d\big(u(x+1,t) - 2u(x,t) + u(x-1,t)\big) \tag{1.4.3}$$

obtained from the generating function method has the form

$$u(x,t) = \sum_{j=0}^{t} \binom{t}{j,\, t-2j-x,\, j+x} d^{2j+x} (1-2d)^{t-2j-x}.$$

Yet another approach was presented in [AS6]: Following the ideas of [3], one can introduce the modified discrete Bessel functions $\mathcal{I}_n^c$, which are defined on $\mathbb{N}_0$, and satisfy a certain difference equation similar to the modified Bessel differential equation. Consequently, it turns out that the fundamental solution of (1.4.3) can be expressed (for $d \neq 1/2$) as

$$u(x,t) = (1-2d)^t \mathcal{I}_{|x|}^{2d/(1-2d)}(t), \quad x \in \mathbb{Z}, \quad t \in \mathbb{N}_0,$$

which is formally similar to (1.4.2) (note that $(1-2d)^t$ is a discrete exponential function). An advantage of the latter formula is that we immediately see that for each $x \in \mathbb{Z}$, the function $t \mapsto u(x,t)$ is nonnegative if $d \in (0, 1/2)$, and oscillatory if $d > 1/2$.

In a similar way, one can express the fundamental solutions of the purely discrete wave equation in terms of the discrete Bessel functions $\mathcal{J}_n^c$, and study their oscillatory properties. For more details, see [AS6].

1.5 Unimodality

Recall that the fundamental solution of the semidiscrete equation

$$\frac{\partial u}{\partial t}(x,t) = au(x+1,t) + bu(x,t) + au(x-1,t), \quad x \in \mathbb{Z}, \quad t \geq 0,$$

is given by the formula $u(x,t) = e^{bt} I_x(2at)$, where I_x is the modified Bessel function of order x. For each fixed $t \geq 0$, the function $x \mapsto u(x,t)$ is increasing on the set of negative integers, attains its maximum at zero, and is decreasing on the set of positive integers. According to the following definition, the sequence $\{u(x,t)\}_{x\in\mathbb{Z}}$ is unimodal about zero.

Definition 1.5.1. A sequence $\{a_n\}_{n\in\mathbb{Z}}$ is unimodal about a mode $n_0 \in \mathbb{Z}$ if $a_n \geq a_{n-1}$ for all $n \leq n_0$, and $a_n \leq a_{n-1}$ for all $n \geq n_0 + 1$.

The situation is different when $\mathbb{T} = \mathbb{Z}$. For example, the fundamental solution of the discrete diffusion equation (1.4.3) with $d = 1/2$ is

$$u(x,t) = \begin{cases} \binom{t}{\frac{t+x}{2}} \frac{1}{2^t} & \text{if } t+x \text{ is even,} \\ 0 & \text{if } t+x \text{ is odd.} \end{cases}$$

Hence, $x \mapsto u(x,t)$ does not attain its maximum at $x = 0$ when t is odd, and it is unimodal only for $t = 0$.

We now provide necessary and sufficient conditions for unimodality of the fundamental solution for a wider class of discrete diffusion equations having the form

$$u(x,t+1) - u(x,t) = \sum_{i=-m}^{m} a_i u(x+i,t), \quad x \in \mathbb{Z}, \quad t \in \mathbb{N}_0, \quad (1.5.1)$$

where $m \in \mathbb{N}$. Consider the following conditions on $a_{-m}, \dots, a_m \in \mathbb{R}$:

(C1) $\sum_{i=-m}^{m} a_i = 0$.

(C2) $a_i = a_{-i}$ for each $i \in \{1, \dots, m\}$.

(C3) $-1 \leq a_0 \leq 0$, and $a_i \geq 0$ for all $i \in \{-m, \dots, m\} \setminus \{0\}$.

The proof of the following result uses the fact that the convolution of two symmetric discrete unimodal distributions is unimodal.

Theorem 1.5.2. *Suppose that (C1)–(C3) hold. Then the fundamental solution of* (1.5.1) *is unimodal for every $t \in \mathbb{N}_0$ if and only if*

$$1 + a_0 \geq a_1 \geq \dots \geq a_m. \quad (1.5.2)$$

In this case, the fundamental solution is unimodal about zero.

Even if the assumption (1.5.2) does not hold, weaker conditions suffice to ensure that the fundamental solution $\{u(x,t)\}_{x\in\mathbb{Z}}$ is unimodal for all sufficiently large $t \in \mathbb{N}_0$. The proof of the next theorem relies on a deep result on the unimodality of high convolutions proved in [26].

Theorem 1.5.3. *Suppose that conditions (C1)–(C3) hold, $a_m > 0$, and either $m > 1$ and $a_{m-1} > 0$, or $m = 1$ and $a_0 \in (-1, 0)$. Then there exists a $t_0 \in \mathbb{N}_0$ such that $\{u(x,t)\}_{x\in\mathbb{Z}}$ is unimodal about zero for every $t \geq t_0$.*

As an example, consider the discrete diffusion equation

$$u(x, t+1) - u(x,t) = a(u(x-1,t) - 2u(x,t) + u(x+1,t)).$$

In this case, the values of the fundamental solution for $t = 1$ are

$$(\ldots, 0, a, 1-2a, a, 0, \ldots).$$

Thus, $x \mapsto u(x, 1)$ has maximum at $x = 0$ if and only if $1 - 2a \geq a$, i.e., if $a \leq \frac{1}{3}$. In this case, condition (1.5.2) is satisfied, and Theorem 1.5.2 implies that for each $t \in \mathbb{N}_0$, $\{u(x,t)\}_{x\in\mathbb{Z}}$ is unimodal about zero and therefore has a global maximum at zero.

The assumptions of Theorem 1.5.3 require that $-2a \in (-1, 0)$. Thus, for $a \in (0, \frac{1}{2})$, Theorem 1.5.3 guarantees that $\{u(x,t)\}_{x\in\mathbb{Z}}$ is unimodal about zero for all sufficiently large t.

1.6 Asymptotic behavior of solutions

In this section, we investigate the asymptotic behavior of solutions to various types of linear diffusion equations on discrete domains.

The first result deals with the semidiscrete diffusion equation

$$\frac{\partial u}{\partial t}(x,t) = a(u(x+1,t) - 2u(x,t) + u(x-1,t)),\ x \in \mathbb{Z},\ t \geq 0, \quad (1.6.1)$$

$$u(x, 0) = c_x, \quad x \in \mathbb{Z}. \quad (1.6.2)$$

It says that if the average of the initial values $\lim_{k\to\infty} \frac{1}{2k+1} \sum_{l=-k}^{k} c_l$ exists and equals d, then $\lim_{t\to\infty} u(x,t) = d$ for each $x \in \mathbb{Z}$. Under additional assumptions, the limit is uniform with respect to x. In fact, the result is more general and provides information on the limit superior and limit inferior of $u(x,t)$ as $t \to \infty$ even in the case when the average of the initial values does not exist. The corresponding results for the classical one-dimensional diffusion equation $\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2}$ are well known; see e.g. [28, 31] and the references therein.

Theorem 1.6.1. *For each bounded real sequence $\{c_k\}_{k\in\mathbb{Z}}$, the unique bounded solution of* (1.6.1)–(1.6.2) *has the following properties:*

1. *For every $x \in \mathbb{Z}$,*

$$\liminf_{k\to\infty} \frac{\sum_{l=x-k}^{x+k} c_l}{2k+1} \le \liminf_{t\to\infty} u(x,t) \le \limsup_{t\to\infty} u(x,t) \le \limsup_{k\to\infty} \frac{\sum_{l=x-k}^{x+k} c_l}{2k+1}.$$

2. *If $x \in \mathbb{Z}$ and $\lim_{k\to\infty} \frac{1}{2k+1} \sum_{l=x-k}^{x+k} c_l = d$, then $\lim_{t\to\infty} u(x,t) = d$.*

3. *If $\lim_{k\to\infty} \frac{1}{2k+1} \sum_{l=x-k}^{x+k} c_l = d$ holds uniformly for all $x \in \mathbb{Z}$, then $\lim_{t\to\infty} u(x,t) = d$ uniformly with respect to $x \in \mathbb{Z}$.*

The proof is based on the explicit solution formula

$$u(x,t) = e^{-2at} \sum_{k\in\mathbb{Z}} c_k I_{x-k}(2at), \quad x \in \mathbb{Z}, \quad t \ge 0,$$

as well as summation by parts and certain properties of the modified Bessel functions. Here are two useful corollaries of Theorem 1.6.1.

Corollary 1.6.2. *If $\{c_k\}_{k\in\mathbb{Z}}$ is a bounded real sequence such that $\lim_{k\to\infty} \frac{1}{2k+1} \sum_{l=-k}^{k} c_l = d$, then the unique bounded solution of* (1.6.1)–(1.6.2) *satisfies $\lim_{t\to\infty} u(x,t) = d$ for each $x \in \mathbb{Z}$.*

Corollary 1.6.3. *If $\{c_k\}_{k\in\mathbb{Z}}$ is such that $\lim_{k\to\pm\infty} c_k = d$, then the unique bounded solution of* (1.6.1)–(1.6.2) *satisfies $\lim_{t\to\infty} u(x,t) = d$ uniformly with respect to x.*

In fact, it is not difficult to obtain a more general result: If $\{c_k\}_{k\in\mathbb{Z}}$ is almost convergent to d_1 for $k \to \infty$ and to d_2 for $k \to -\infty$, then the unique bounded solution to the initial-value problem (1.6.1)–(1.6.2) satisfies $\lim_{t\to\infty} u(x,t) = (d_1 + d_2)/2$ uniformly with respect to x.

Note that if $\{c_k\}_{k\in\mathbb{Z}} \in \ell^p(\mathbb{Z})$ for an arbitrary $p \in [1,\infty)$, then $\lim_{k\to\pm\infty} c_k = 0$, and Corollary 1.6.3 yields $\lim_{t\to\infty} u(x,t) = 0$ uniformly with respect to x. This generalizes a result from [13, Theorem 4] dealing with the case $p = 2$.

A result similar to Theorem 1.6.1 can be derived for the N-dimensional semidiscrete diffusion equation

$$\frac{\partial u}{\partial t}(x,t) = a\left(\sum_{i=1}^{N} u(x+e_i,t) - 2Nu(x,t) + \sum_{i=1}^{N} u(x-e_i,t)\right),$$

where $x \in \mathbb{Z}^N$, $t \ge 0$, and $e_1,\dots,e_N$ is the canonical basis of $\mathbb{R}^N$. We omit the details, and refer the reader to [AS12].

We conclude with the purely discrete case, where we are able to deal with a larger class of discrete-space equations having the form

$$u(x,t+1)-u(x,t)=\sum_{i=-m}^{m} a_i u(x+i,t), \quad x\in\mathbb{Z}, \quad t\in\mathbb{N}_0. \tag{1.6.3}$$

Theorem 1.6.4. *Suppose that $a_0>-1$, $a_1,\dots,a_m>0$, $a_i=a_{-i}$ for each $i\in\{1,\dots,m\}$, and $\sum_{i=-m}^{m} a_i=0$. Let $\{c_k\}_{k\in\mathbb{Z}}$ be a bounded real sequence, and denote $A_l(x)=\frac{1}{2l+1}\sum_{k=x-l}^{x+l} c_k$ for $l\in\mathbb{N}_0$, $x\in\mathbb{Z}$.*

Then the unique solution of (1.6.3) satisfying $u(x,0)=c_x$ for all $x\in\mathbb{Z}$ has the following properties:

1. *For every $x\in\mathbb{Z}$,*

$$\liminf_{l\to\infty} A_l(x)\le \liminf_{t\to\infty} u(x,t)\le \limsup_{t\to\infty} u(x,t)\le \limsup_{l\to\infty} A_l(x).$$

2. *If $x\in\mathbb{Z}$ and $\lim_{l\to\infty} A_l(x)=d$, then $\lim_{t\to\infty} u(x,t)=d$.*
3. *If $\lim_{l\to\infty} A_l(x)=d$ uniformly for all $x\in\mathbb{Z}$, then $\lim_{t\to\infty} u(x,t)=d$ uniformly for all $x\in\mathbb{Z}$.*

Interestingly, the proof is more complicated that in the semidiscrete case. The first step is to prove that for $t\to\infty$, the fundamental solution of (1.6.3) is uniformly convergent to zero. We do not have an explicit formula for this solution, but we have discovered two completely different proofs of this statement: The first one is based on the relation between diffusion-type equations and random walks. A random walk arises from the sum of independent and identically distributed random variables, and by the local limit theorem for random variables with lattice distribution, the distribution of these sums approaches a suitably scaled normal distribution. The second proof is based on the maximum principle; it is longer, but can be easily adapted to the multidimensional setting. The rest of the proof of Theorem 1.6.4 is similar to the semidiscrete case, and relies on the properties of the fundamental solution including the unimodality result from Theorem 1.5.3.

For the discrete diffusion equation

$$u(x,t+1)-u(x,t)=a(u(x-1,t)-2u(x,t)+u(x+1,t)),$$

the previous theorem guarantees that if $a\in(0,\frac{1}{2})$, then $\lim_{t\to\infty} u(x,t)=\lim_{l\to\infty} A_l(x)$ whenever the latter limit exists. One can show that the same conclusion no longer holds for $a\ge\frac{1}{2}$ (see [AS11]).

Chapter 2

Reaction-diffusion equations on $\mathbb{Z}$

The present chapter is based on the papers [AS5], [AS7].

2.1 Well-posedness and maximum principles for scalar equations

The classical reaction-diffusion equation $\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + f(u)$ is frequently used to describe the evolution of chemical concentrations, temperatures, populations, etc., in phenomena that combine a local dynamics (via the reaction function f) and a spatial dynamics (via the diffusion).

Various authors have also considered the semidiscrete lattice reaction-diffusion equation [7, 8, 37, 38]

$$\frac{\partial u}{\partial t}(x,t) = k(u(x+1,t) - 2u(x,t) + u(x-1,t)) + f(u(x,t))$$

with $x \in \mathbb{Z}$, $t \in [0,\infty)$, as well as the purely discrete reaction-diffusion equation [9, 8, 16]

$$u(x,t+1) - u(x,t) = k(u(x+1,t) - 2u(x,t) + u(x-1,t)) + f(u(x,t))$$

with $x \in \mathbb{Z}$, $t \in \mathbb{N}_0$. Both equations are interesting from the viewpoint of numerical mathematics (since they correspond to semi- or full discretization of the original reaction-diffusion equation [16]) as well as potential applications (e.g., in population dynamics).

As before, in order to consider both cases at once, we use the language of the time scale calculus. We do not restrict ourselves to symmetric diffusion and consider the nonautonomous reaction-diffusion equation

$$u^{\Delta}(x,t) = au(x+1,t)+bu(x,t)+cu(x-1,t)+f(u(x,t),x,t), \qquad (2.1.1)$$

where $x \in \mathbb{Z}$, $t \in \mathbb{T}$, $a,b,c \in \mathbb{R}$, $\mathbb{T} \subseteq \mathbb{R}$ is a time scale, and the symbol u^{Δ} denotes the delta derivative with respect to time. Our results are new even in the special cases $\mathbb{T} = \mathbb{R}$ (when u^{Δ} becomes the partial derivative $\frac{\partial u}{\partial t}$) and $\mathbb{T} = \mathbb{Z}$ (when u^{Δ} is the partial difference $u(x,t+1) - u(x,t)$).

If $a = c$ and $b = -2a$, then (2.1.1) becomes the symmetric lattice reaction-diffusion equation. The asymmetric case $a \neq c$, $b = -(a+c)$ corresponds to the lattice reaction-advection-diffusion equation. Next, if $c = 0$ and $b = -a$, or if $a = 0$ and $b = -c$, then (2.1.1) reduces to the lattice reaction-transport equation.

We focus on well-posedness results as well as maximum principles for the equation (2.1.1). We begin with the local existence and global uniqueness of solutions to the initial-value problem

$$\begin{aligned} u^{\Delta}(x,t) &= au(x+1,t) + bu(x,t) + cu(x-1,t) + f(u(x,t),x,t), \\ u(x,t_0) &= u_x^0, \end{aligned} \qquad (2.1.2)$$

where $\{u_x^0\}_{x\in\mathbb{Z}}$ is a bounded real sequence and t_0, $T \in \mathbb{T}$.

We impose the following conditions on $f : \mathbb{R} \times \mathbb{Z} \times [t_0,T]_{\mathbb{T}} \to \mathbb{R}$:

(H_1) f is bounded on each set $B \times \mathbb{Z} \times [t_0,T]_{\mathbb{T}}$, where $B \subset \mathbb{R}$ is bounded.

(H_2) f is Lipschitz-continuous in the first variable on each set $B \times \mathbb{Z} \times [t_0,T]_{\mathbb{T}}$, where $B \subset \mathbb{R}$ is bounded.

(H_3) For each bounded set $B \subset \mathbb{R}$ and each choice of $\varepsilon > 0$ and $t \in [t_0,T]_{\mathbb{T}}$, there exists a $\delta > 0$ such that if $s \in (t-\delta, t+\delta) \cap [t_0,T]_{\mathbb{T}}$, then $|f(u,x,t) - f(u,x,s)| < \varepsilon$ for all $u \in B$, $x \in \mathbb{Z}$.

Theorem 2.1.1. *Assume that $f : \mathbb{R} \times \mathbb{Z} \times [t_0,T]_{\mathbb{T}} \to \mathbb{R}$ satisfies (H_1)–(H_3). Then for each $u^0 \in \ell^{\infty}(\mathbb{Z})$, the initial-value problem* (2.1.2) *has a bounded local solution on $\mathbb{Z} \times [t_0, t_0+\delta]_{\mathbb{T}}$, where $\delta > 0$ and $\delta \geq \mu(t_0)$.*

Recall that even in the linear case $f \equiv 0$, the solutions of (2.1.2) are not unique in general, and uniqueness can be expected only in the class of bounded solutions.

Theorem 2.1.2. *Assume that $f : \mathbb{R} \times \mathbb{Z} \times [t_0, T]_\mathbb{T} \to \mathbb{R}$ satisfies (H_1) and (H_2). Then for each $u^0 \in \ell^\infty(\mathbb{Z})$, the initial-value problem* (2.1.2) *has at most one bounded solution $u : \mathbb{Z} \times [t_0, T]_\mathbb{T} \to \mathbb{R}$.*

Our next task is to investigate the maximum principles. For an initial condition $u^0 \in \ell^\infty(\mathbb{Z})$, let

$$m = \inf_{x \in \mathbb{Z}} u_x^0, \quad M = \sup_{x \in \mathbb{Z}} u_x^0.$$

We introduce the notation

$$\overline{\mu}_\mathbb{T} = \max_{t \in [t_0, T)_\mathbb{T}} \mu(t)$$

as well as the following conditions.

(H_4) a, b, $c \in \mathbb{R}$ are such that $a, c \geq 0$ and $a + b + c = 0$.

(H_5) $b < 0$ and $\overline{\mu}_\mathbb{T} \leq -1/b$.

(H_6) There exist $r, R \in \mathbb{R}$ such that $r \leq m \leq M \leq R$, and one of the following statements holds:

- $\overline{\mu}_\mathbb{T} = 0$ and $f(R, x, t) \leq 0 \leq f(r, x, t)$ for all $x \in \mathbb{Z}$, $t \in [t_0, T]_\mathbb{T}$.
- $\overline{\mu}_\mathbb{T} > 0$ and $\dfrac{1 + \overline{\mu}_\mathbb{T} b}{\overline{\mu}_\mathbb{T}}(r - u) \leq f(u, x, t) \leq \dfrac{1 + \overline{\mu}_\mathbb{T} b}{\overline{\mu}_\mathbb{T}}(R - u)$ for all $u \in [r, R]$, $x \in \mathbb{Z}$, $t \in [t_0, T]_\mathbb{T}$.

Condition (H_6) defines forbidden areas that the function $f(\cdot, x, t)$ cannot intersect for any x and t, similarly to [30] (see Figure 2.1).

We are now able to state the weak maximum principle for (2.1.2).

Theorem 2.1.3. *Assume that (H_1)–(H_6) hold. If $u : \mathbb{Z} \times [t_0, T]_\mathbb{T} \to \mathbb{R}$ is a bounded solution of* (2.1.2)*, then*

$$r \leq u(x, t) \leq R \quad \text{for all} \quad x \in \mathbb{Z}, \quad t \in [t_0, T]_\mathbb{T}. \tag{2.1.3}$$

The proof consists of two parts: First, one proves the result for time scales having only isolated points. Second, one uses continuous dependence of solutions on $\mathbb{T}$ to approximate the solution of (2.1.2) on any time scale by solutions of (2.1.2) defined on isolated time scales.

The classical maximum principle guarantees that $m \leq u(x, t) \leq M$, i.e., it corresponds to the case when $r = m$ and $R = M$. However, for this choice of r and R, (H_6) need not be satisfied. Choosing $r < m$

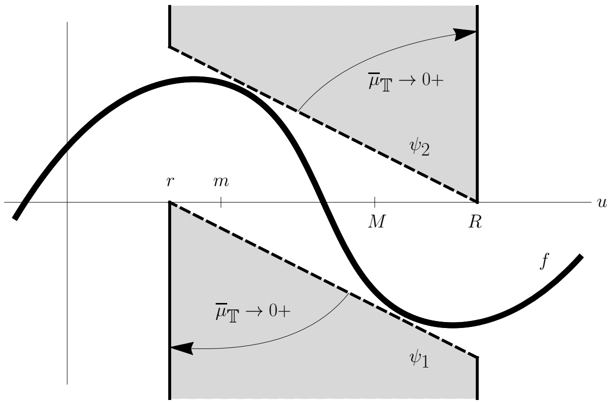

Figure 2.1: Illustration of (H_6). The values r, R are chosen so that the function $f(\cdot, x, t)$ does not intersect the gray forbidden areas. The slope of the boundary dashed lines is determined by the values of $\overline{\mu}_{\mathbb{T}}$.

and $R > M$, we can soften (H_6), and obtain the weaker estimate $r \le u(x,t) \le R$.

As an application of the weak maximum principle, we obtain the following global existence theorem.

Theorem 2.1.4. *If $u^0 \in \ell^\infty(\mathbb{Z})$ and (H_1)–(H_6) hold, then* (2.1.2) *has a unique bounded solution $u : \mathbb{Z} \times [t_0, T]_{\mathbb{T}} \to \mathbb{R}$.*

Moreover, the solution depends continuously on u^0 in the following sense: For every $\varepsilon > 0$, there exists a $\delta > 0$ such that if $v^0 \in \ell^\infty(\mathbb{Z})$, $r \le v^0_x \le R$ for all $x \in \mathbb{Z}$, and $\|u^0 - v^0\|_\infty < \delta$, then the unique bounded solution $v : \mathbb{Z} \times [t_0, T]_{\mathbb{T}} \to \mathbb{R}$ of (2.1.2) *corresponding to the initial condition v^0 satisfies $|u(x,t) - v(x,t)| < \varepsilon$ for all $x \in \mathbb{Z}$, $t \in [t_0, T]_{\mathbb{T}}$.*

To be able to state the strong maximum principle, we need the following stronger versions of (H_4)–(H_6):

$(\overline{H_4})$ a, b, $c \in \mathbb{R}$ are such that $a, c > 0$ and $a + b + c = 0$.

$(\overline{H_5})$ $b < 0$ and $\overline{\mu}_{\mathbb{T}} < -1/b$.

$(\overline{H_6})$ There exist $r, R \in \mathbb{R}$ such that $r \le m \le M \le R$, and the following statements hold for all $x \in \mathbb{Z}$ and $t \in [t_0, T]_{\mathbb{T}}$:

- $f(R, x, t) \le 0 \le f(r, x, t)$.

- If $\overline{\mu}_{\mathbb{T}} > 0$, then $f(u,x,t) > \dfrac{1+\overline{\mu}_{\mathbb{T}} b}{\overline{\mu}_{\mathbb{T}}}(r-u)$ for all $u \in (r,R]$.
- If $\overline{\mu}_{\mathbb{T}} > 0$, then $f(u,x,t) < \dfrac{1+\overline{\mu}_{\mathbb{T}} b}{\overline{\mu}_{\mathbb{T}}}(R-u)$ for all $u \in [r,R)$.

The strong maximum principle now reads as follows. Its statement involves the backward jump operator ρ defined by

$$\rho(t) = \sup\{s \in \mathbb{T} : s < t\}, \quad t \in \mathbb{T}.$$

Theorem 2.1.5. *Assume that (H_1), (H_2), (H_3), $(\overline{H_4})$, $(\overline{H_5})$, $(\overline{H_6})$ hold with $r = m \le M = R$ and $u : \mathbb{Z} \times [t_0,T]_{\mathbb{T}} \to \mathbb{R}$ is a bounded solution of (2.1.2). If $u(\bar{x},\bar{t}) \in \{r,R\}$ for some $\bar{x} \in \mathbb{Z}$ and $\bar{t} \in (t_0,T]_{\mathbb{T}}$, then the following statements hold:*

(a) *If $[t_0,\bar{t}]_{\mathbb{T}}$ contains only isolated points, i.e., $t_0 = \rho^k(\bar{t})$ for some $k \in \mathbb{N}$, then $u(x,t) = u(\bar{x},\bar{t})$ for all (x,t) with $t = \rho^j(\bar{t})$ for a certain $j \in \{0,\dots,k\}$, and $x = \bar{x} \pm i$ for a certain $i \in \{0,\dots,j\}$.*

(b) *Otherwise, if $[t_0,\bar{t}]_{\mathbb{T}}$ contains a point which is not isolated, then u is constant on $\mathbb{Z} \times [t_0,T]_{\mathbb{T}}$.*

Corollary 2.1.6. *Assume that (H_1), (H_2), (H_3), $(\overline{H_4})$, $(\overline{H_5})$, $(\overline{H_6})$ hold with $r = m \le M = R$ and $u : \mathbb{Z} \times [t_0,T]_{\mathbb{T}} \to \mathbb{R}$ is a bounded solution of (2.1.2). If there is a point $t_d \in [t_0,T)_{\mathbb{T}}$ that is not isolated and if the initial condition u^0 is not constant, then*

$$r < u(x,t) < R \quad \text{for all} \quad x \in \mathbb{Z}, \quad t \in (t_d,T]_{\mathbb{T}}.$$

Examples illustrating the weak and strong maximum principles are available in [AS7].

2.2 Invariant regions for systems of equations

Some results of the previous section can be extended to systems of the form

$$\frac{\partial u}{\partial t}(x,t) = A(x,t)u(x+1,t) + B(x,t)u(x,t) + C(x,t)u(x-1,t) + f(u(x,t),t), \tag{2.2.1}$$

where $x \in \mathbb{Z}$, $t \ge 0$, u takes values in $\mathbb{R}^m$ and A, B, C are matrix-valued functions.

The basic well-posedness results can be obtained similarly as in the scalar case, and we do not discuss them here. Instead, we focus on an invariance result, which can be interpreted as a generalization of the weak maximum principle: In the scalar case, the weak maximum principle says that under suitable assumptions on the reaction function f, the values of the solution always remain in the interval determined by the infimum and supremum of the initial values. Thus, the interval is an invariant region for the given equation. In the higher-dimensional setting, the interval is replaced by a closed convex set $S \subset \mathbb{R}^m$, and the problem is to find sufficient conditions guaranteeing that S is an invariant region, i.e., that solutions with initial values in S never leave this set.

We will consider compact convex sets S described as intersections of sublevel sets of certain functions $G_1, \dots, G_k$. More precisely, we introduce the following condition:

(S) Assume that $k \in \mathbb{N}$, $U_1, \dots, U_k \subseteq \mathbb{R}^m$ are open sets, and for each $i \in \{1, \dots, k\}$, $G_i : U_i \to \mathbb{R}$ is a $\mathcal{C}^1$ function. Suppose also that the closed sets $S_i = \{u \in U_i;\ G_i(u) \leq 0\}, \quad i \in \{1, \dots, k\}$, are convex, their intersection

$$S = S_1 \cap \cdots \cap S_k = \{u \in U_1 \cap \cdots \cap U_k;\ G_1(u) \leq 0, \dots, G_k(u) \leq 0\}$$

is bounded and has nonempty interior, and that $\nabla G_i(u) \neq 0$ for each $i \in \{1, \dots, k\}$, $u \in \partial S_i$.

To avoid technical difficulties, we consider only the case when f does not explicitly depend on x, and impose the following conditions:

(D_1) f is Lipschitz-continuous in the first variable on each set $B \times [0, T]$, where $B \subset \mathbb{R}^m$ is bounded.

(D_2) f is continuous in the second variable.

Our goal is to obtain sufficient conditions for S to be an invariant region for bounded solutions of Eq. (2.2.1), ensuring that each bounded solution of Eq. (2.2.1) with $u(x, 0) \in S$, $x \in \mathbb{Z}$, satisfies $u(x, t) \in S$ for each $t \in [0, T]$, $x \in \mathbb{Z}$. We need the following conditions:

(A_1) A, B, $C : \mathbb{Z} \times [0, T] \to \mathbb{R}^{m \times m}$ are bounded.

(A_2) For each $j \in \{-k, \dots, k\}$, $\varepsilon > 0$ and $t \in [0, T]$, there exists a $\delta > 0$ such that if $s \in (t - \delta, t + \delta) \cap [0, T]$, then $\|A(x, t) - A(x, s)\| < \varepsilon$ for all $x \in \mathbb{Z}$. The same condition holds for B and C.

(C_1) For all $i \in \{1, \dots, k\}$ and $u \in \partial S_i \cap S$, we have $\nabla G_i(u) \cdot f(u,t) \le 0$ for all $t \in [0,T]$.

(C_2) For all $i \in \{1, \dots, k\}$, $u \in \partial S_i \cap S$, $x \in \mathbb{Z}$ and $t \in [0,T]$, there exist numbers $a \ge 0$, $b \le 0$, $c \ge 0$ such that

$$\nabla G_i(u)^\top A(x,t) = a \nabla G_i(u)^\top, \quad \nabla G_i(u)^\top B(x,t) = b \nabla G_i(u)^\top,$$
$$\nabla G_i(u)^\top C(x,t) = c \nabla G_i(u)^\top.$$

(C_3) $A(x,t) + B(x,t) + C(x,t) = 0$ for each $x \in \mathbb{Z}$ and $t \in [0,T]$.

The assumption (C_1) says that the vector field f points inside S or is tangent to the boundary at all boundary points of S. This condition is well known from the invariance results for classical parabolic equations; see [2, 10, 27, 34, 36]. The fact that the condition (C_3) is necessary for the validity of the weak maximum principle in the scalar case was already noticed in the previous section. Condition (C_2) says that $\nabla G_i(u)$ is a left eigenvector of the matrices $A(x,t)$, $B(x,t)$, $C(x,t)$ for each $x \in \mathbb{Z}$ and $t \in [0,T]$. Moreover, it is required that the corresponding eigenvalues a, c are nonnegative, while b is nonpositive (note that the eigenvalues might depend on x and t). A condition of a similar type can be found in [10, 11, 12, 35], and it is also implicitly present in [34]. If A, B, C are not scalar multiples of the identity matrix, then condition (C_2) imposes a serious restriction on the shape of S – it says that the boundary of S has to be such that the normal vectors ∇G_i are left eigenvectors of A, B, C. In general, a condition of this type cannot be avoided. The necessity of an analogous condition for systems of parabolic differential equations was proved in [10, Theorem 4.2]. For example, if we have a decoupled system of two linear diffusion equations with different diffusion coefficients, it can easily happen that a solution leaves a compact convex set that has a non-rectangular shape; a convincing pictorial argument can be found in [11, Section 3.4].

The main result of this section is as follows.

Theorem 2.2.1. *Assume that conditions* (S), (D_1), (D_2), (A_1), (A_2), (C_1)–(C_3) *are satisfied. If* $u : \mathbb{Z} \times [0,T] \to \mathbb{R}^m$ *is a bounded solution of Eq.* (2.2.1) *with* $u(\cdot, 0) \in \ell^\infty(\mathbb{Z})^m$ *and* $u(x,0) \in S$ *for each* $x \in \mathbb{Z}$, *then* $u(x,t) \in S$ *for all* $t \in [0,T]$, $x \in \mathbb{Z}$.

The proof is technical and different from existing proofs for parabolic PDEs. The main idea is to derive an invariance result for the Euler approximations to Eq. (2.2.1), and then pass to the continuous-time limit.

Chapter 3

Reaction-diffusion equations on graphs

The present chapter is based on the papers [AS8], [AS10].

3.1 Lotka-Volterra model on graphs

In population dynamics, there exist three basic types of models describing the interaction between two species: predator-prey models, competition models, and mutualism/symbiosis models [25, Chapter 3]. We focus on a model of the second type, where two species compete against each other for the same resources. The basic competition model describing this situation is the classical Lotka-Volterra model, which can be written in the form

$$\begin{aligned} u'(t) &= \rho_1 u(t)(1 - u(t) - \alpha v(t)), \\ v'(t) &= \rho_2 v(t)(1 - \beta u(t) - v(t)), \end{aligned} \tag{3.1.1}$$

The quantities $u(t)$, $v(t)$ correspond to the number of individuals at time t, the parameters ρ_1, $\rho_2 > 0$ are the intrinsic growth rates, and α, $\beta > 0$ correspond to the strength of the competition. A detailed analysis of this model can be found in a large number of sources devoted to differential equations or mathematical biology, e.g. [25, Section 3.5].

One drawback of the above-mentioned model is that it does not take into account the spatial distribution of both species. For this reason, various authors have considered the so-called diffusive Lotka-Volterra model, which describes not only the competition between the two species, but also the migration of individuals within each population. The model is expressed as a system of two reaction-diffusion partial differential equations, and was studied in a large number of papers; see e.g. [6] and the references cited therein.

On the other hand, mathematical biology often deals with models where the spatial domain consists of discrete patches, corresponding to fragmented habitats (such as islands, ponds, etc.). Such models might be more realistic from the biological viewpoint, and their solutions often display behavior different from that of the continuous-space models. For example, the discrete-space Lotka-Volterra competition model that we consider here is known to have stable spatially heterogeneous stationary states [20], and this fact is in stark contrast to the continuous-space model, which has no stable nonconstant stationary states [19].

Suppose we have a finite number of discrete patches, each being inhabited by both species. Such a domain can be described by a finite graph $G = (V, E)$, where $V = \{1, \dots, n\}$ is the set of patches, and an edge $\{i, j\} \in E$ means that the species can move between patches i and j. Our model corresponds to the system of differential equations

$$\begin{aligned} u_i'(t) &= d_1 \sum_{j \in N(i)} (u_j(t) - u_i(t)) + \rho_1 u_i(t)(1 - u_i(t) - \alpha v_i(t)), \qquad i \in V, \\ v_i'(t) &= d_2 \sum_{j \in N(i)} (v_j(t) - v_i(t)) + \rho_2 v_i(t)(1 - v_i(t) - \beta u_i(t)), \qquad i \in V, \end{aligned} \tag{3.1.2}$$

where $d_1, d_2 \geq 0$ are diffusion constants (or migration rates), and $N(i) = \{j \in V; \{i, j\} \in E\}$ denotes the set of all neighbors of a vertex $i \in V$.

Let us begin by recalling some basic facts about the classical Lotka-Volterra competition model (3.1.1). To avoid technical difficulties, we restrict ourselves to the case when $\alpha \neq 1$ and $\beta \neq 1$. Also, due to the biological interpretation, we are interested only in nonnegative solutions of (3.1.1). The system (3.1.1) always has at least three equilibria:

$$E_0 = (0, 0), \quad E_1 = (1, 0), \quad E_2 = (0, 1). \tag{3.1.3}$$

Moreover, if $\alpha\beta \neq 1$, there is a fourth equilibrium

$$E_3 = \left(\frac{1 - \alpha}{1 - \alpha\beta}, \frac{1 - \beta}{1 - \alpha\beta} \right). \tag{3.1.4}$$

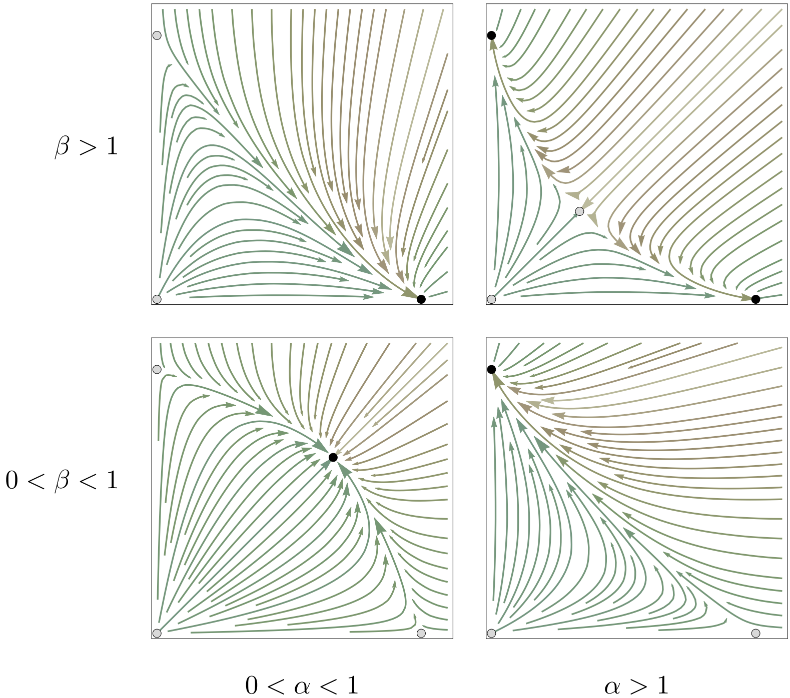

Figure 3.1: Phase portraits of the classical Lotka-Volterra competition system, depending on the values of α and β. The black/gray points correspond to stable/unstable equilibria.

Taking into account our restriction to $\alpha, \beta \neq 1$, we see that E_3 lies in the 1st quadrant if and only if $\alpha > 1$ and $\beta > 1$, or $\alpha < 1$ and $\beta < 1$. In both cases, E_3 is contained in the open square $(0, 1) \times (0, 1)$.

The equilibrium E_0 is always unstable. The equilibrium E_1 is unstable for $\beta < 1$, and asymptotically stable for $\beta > 1$. Similarly, E_2 is unstable for $\alpha < 1$, and asymptotically stable for $\alpha > 1$. Finally, if $\alpha > 1$ and $\beta > 1$, then E_3 is unstable (a saddle point), while if $\alpha < 1$ and $\beta < 1$, then E_3 is asymptotically stable.

Except the case $\alpha, \beta > 1$, exactly one of the three equilibrium points E_1, E_2, E_3 is stable. Moreover, it attracts all solutions with positive initial values (see Figure 3.1).

We now turn our attention to the spatial competition model (3.1.2).

From now on, we always assume that G is a connected graph (otherwise, it is possible to treat each component separately). Using Bony's theorem on positively invariant regions, it is not too difficult to prove that for nonnegative initial conditions, the system (3.1.2) has a unique solution defined on $[0, \infty)$, which remains nonnegative for all time.

To be able to investigate the qualitative behavior of solutions, the first task is to look for stationary states of the system (3.1.2). We begin with equilibria having the form $u_i(t) = u^* \geq 0$ and $v_i(t) = v^* \geq 0$ for all $i \in V$, $t \geq 0$, which are called spatially *homogeneous* (as opposed to spatially *heterogeneous* equilibria, where the components of u or v need not coincide). Substituting into (3.1.2), we get

$$\begin{aligned} 0 &= \rho_1 u^*(1 - u^* - \alpha v^*), \\ 0 &= \rho_2 v^*(1 - v^* - \beta u^*). \end{aligned} \tag{3.1.5}$$

Hence, a pair $E = (u^*, v^*)$ determines a homogeneous stationary state of the system (3.1.2) if and only if E is a stationary state of the classical Lotka-Volterra system (3.1.1), i.e., if E coincides with one of the four equilibrium points E_0, E_1, E_2, E_3.

We will use the symbol $\boldsymbol{E}_i$ to denote the homogeneous stationary state of the system (3.1.2) satisfying $(u_i(t), v_i(t)) = E_i$ for all $i \in V$, $t \geq 0$. Note that we use boldface to distinguish homogeneous stationary states of (3.1.2) from stationary states of (3.1.1). Thus, $\boldsymbol{E}_i \in \mathbb{R}^{2n}$, while $E_i \in \mathbb{R}^2$.

The local stability of the homogeneous stationary states can be determined from the Jacobian matrix using some properties of the Kronecker product of matrices.

Theorem 3.1.1. *If $\alpha, \beta > 0$ and $\alpha, \beta \neq 1$, then:*

- $\boldsymbol{E}_0$ *is always unstable.*
- $\boldsymbol{E}_1$ *is unstable if $\beta < 1$, and asymptotically stable if $\beta > 1$.*
- $\boldsymbol{E}_2$ *is unstable if $\alpha < 1$, and asymptotically stable if $\alpha > 1$.*
- $\boldsymbol{E}_3$ *is unstable if $\alpha > 1$ and $\beta > 1$, and asymptotically stable if $\alpha < 1$ and $\beta < 1$.*

The next result describes the asymptotic behavior of solutions to the system (3.1.2) in all cases when at least one of α, β is less than 1. The proof is based on the construction of appropriate Lyapunov functions and application of LaSalle's invariance principle.

Theorem 3.1.2. *Suppose that $d_1, d_2, \rho_1, \rho_2 > 0$.*

- *If $0 < \alpha < 1$ and $\beta > 1$, then each solution $u, v : [0, \infty) \to \mathbb{R}^n$ of* (3.1.2) *with $u(0) > 0$ and $v(0) \geq 0$ approaches $\boldsymbol{E}_1$ as $t \to \infty$.*
- *If $\alpha > 1$ and $0 < \beta < 1$, then each solution $u, v : [0, \infty) \to \mathbb{R}^n$ of* (3.1.2) *with $u(0) \geq 0$ and $v(0) > 0$ approaches $\boldsymbol{E}_2$ as $t \to \infty$.*
- *If $0 < \alpha < 1$ and $0 < \beta < 1$, then each solution $u, v : [0, \infty) \to \mathbb{R}^n$ of* (3.1.2) *with $u(0) > 0$ and $v(0) > 0$ approaches $\boldsymbol{E}_3$ as $t \to \infty$.*

In all cases except $\alpha, \beta > 1$, Theorem 3.1.2 implies that all solutions with positive initial values are attracted to one of the homogeneous stationary states $\boldsymbol{E_1}$, $\boldsymbol{E_2}$, $\boldsymbol{E_3}$. In particular, there are no heterogeneous stationary states in the positive orthant. It remains to settle the case $\alpha, \beta > 1$, which leads to a much more interesting dynamics. We will see that the system (3.1.2) might possess a large number of heterogeneous stationary states, some of which are asymptotically stable.

We will assume that ρ_1, ρ_2, α, β and G are fixed, and we study the effect of diffusion on the existence of heterogeneous stationary states. The next result shows that if the diffusion is sufficiently large, there are no heterogeneous stationary states, and all solutions with nonnegative initial conditions tend to a homogeneous stationary state. The proof is somewhat lengthy, and has two parts: First, some calculations involving the Laplacian matrix of G and its eigenvectors show that each solution tends to a spatially homogeneous function. In the second part, one verifies that the spatially homogenous function tends to a homogeneous stationary state; this part involves a comparison with a solution of the classical Lotka-Volterra system.

Theorem 3.1.3. *For each $\rho_1, \rho_2 > 0$, $\alpha, \beta > 0$, and graph G, there exists a $D \geq 0$ such that if $\min(d_1, d_2) > D$, then all solutions of* (3.1.2) *with nonnegative initial conditions tend to a homogeneous stationary state. In particular,* (3.1.2) *has no heterogeneous stationary state with nonnegative components.*

We now proceed to the opposite case when the diffusion is small. If $d_1 = d_2 = 0$ and $\rho_1, \rho_2 > 0$, the situation is simple: All stationary points of the system (3.1.2) have the form

$$\boldsymbol{E}_\sigma = (E_{\sigma(1)}, \ldots, E_{\sigma(n)}), \tag{3.1.6}$$

where $\sigma = (\sigma(1), \ldots, \sigma(n)) \in \{0, 1, 2, 3\}^n$. If $\alpha > 1$ and $\beta > 1$, then all four points E_0, E_1, E_2, E_3 have nonnegative components, and hence the system (3.1.2) has 4^n nonnegative stationary states; four of them are homogeneous (namely $\boldsymbol{E}_0$, $\boldsymbol{E}_1$, $\boldsymbol{E}_2$, $\boldsymbol{E}_3$), and the remaining $4^n - 4$ are heterogeneous.

However, we are primarily interested in what happens if $d_1, d_2 > 0$. It is reasonable to expect that if d_1, d_2 are small, the system (3.1.2) will possess 4^n stationary solutions close to $\boldsymbol{E}_\sigma$, $\sigma \in \{0, 1, 2, 3\}^n$; this is the content of the next lemma, whose proof is based on the implicit function theorem.

Lemma 3.1.4. *For each $\rho_1, \rho_2 > 0$, $\alpha, \beta > 1$ and graph G, there exist disjoint sets $U(\boldsymbol{E}_\sigma) \subset \mathbb{R}^{2n}$, $\sigma \in \{0, 1, 2, 3\}^n$, an $\varepsilon > 0$, and smooth functions $F_\sigma : [0, \varepsilon] \times [0, \varepsilon] \to U(\boldsymbol{E}_\sigma)$, $\sigma \in \{0, 1, 2, 3\}^n$, with the following properties:*

- *$F_\sigma(0, 0) = \boldsymbol{E}_\sigma$ for each $\sigma \in \{0, 1, 2, 3\}^n$.*
- *If $\sigma \in \{0, 1, 2, 3\}^n$ and $d_1, d_2 \in [0, \varepsilon]$, then $F_\sigma(d_1, d_2)$ is a stationary state of the system* (3.1.2)*. This state is asymptotically stable if and only if $\sigma \in \{1, 2\}^n$, and unstable otherwise.*

The lemma says that if $d_1, d_2 \geq 0$ are sufficiently small, then (3.1.2) has 4^n stationary solutions of the form

$$F_\sigma(d_1, d_2) = (u_1(d_1, d_2), \ldots, u_n(d_1, d_2), v_1(d_1, d_2), \ldots, v_n(d_1, d_2)),$$

where $\sigma \in \{0, 1, 2, 3\}^n$; four of them corresponding to $\sigma = (i, \ldots, i)$ with $i \in \{0, 1, 2, 3\}$ are homogeneous, while the remaining $4^n - 4$ are heterogeneous (this follows from the fact that the neighborhoods $U(\boldsymbol{E}_\sigma)$ are disjoint) and $2^n - 2$ of them are asymptotically stable.

The idea of using the implicit function theorem to study stationary states of networks consisting of weakly coupled bistable units can be found e.g. in [23]. However, in the present problem, we have to be careful, since the heterogeneous equilibria need not be nonnegative. If $\sigma(i) = 3$, then $(u_i(d_1, d_2), v_i(d_1, d_2))$ is close to E_3, and therefore nonnegative. On the other hand, if $\sigma(i) \in \{0, 1, 2\}$, we do not a priori know whether $u_i(d_1, d_2)$ and $v_i(d_1, d_2)$ are nonnegative.

To settle this question, we will assume that $d_1 = d\delta_1$ and $d_2 = d\delta_2$, where $\delta_1, \delta_2 > 0$ are fixed, and d is a variable. In other words, the ratio of diffusion coefficients is fixed to be δ_1/δ_2, but their magnitudes are allowed to vary. Then we determine which of the stationary states $F_\sigma(d\delta_1, d\delta_2)$ have nonnegative components for sufficiently small $d > 0$. If $\sigma = (i, \ldots, i)$ for some $i \in \{0, 1, 2, 3\}$, then $F_\sigma(d\delta_1, d\delta_2) = \boldsymbol{E}_i$. Thus, it suffices to consider only n-tuples $\sigma \in \{0, 1, 2, 3\}^n$ whose components do not all coincide.

Theorem 3.1.5. *Consider a graph G and assume that $\alpha, \beta > 1$, $\delta_1, \delta_2 > 0$, and $F_\sigma : [0, \varepsilon] \times [0, \varepsilon] \to U(\boldsymbol{E}_\sigma)$, $\sigma \in \{0, 1, 2, 3\}^n$, are as in Lemma 3.1.4. There exists a $\Delta > 0$ with the following properties:*

- *Suppose that $\sigma \in \{0, 1, 2, 3\}^n$, $\sigma \neq (0, \dots, 0)$, and there exists an $i \in V$ with $\sigma(i) = 0$. Then at least one component of $F_\sigma(d\delta_1, d\delta_2)$ is negative for all $d \in (0, \Delta]$.*

- *Suppose that $\sigma \in \{1, 2, 3\}^n$ and not all components of σ coincide. Then for each $d \in (0, \Delta]$, $F_\sigma(d\delta_1, d\delta_2)$ is a heterogeneous stationary state of* (3.1.2)*, where $d_1 = d\delta_1$ and $d_2 = d\delta_2$, with positive components.*

We see that if $\alpha, \beta > 1$, $d_1 = d\delta_1$, $d_2 = d\delta_2$, and $d \geq 0$ is sufficiently small, then (3.1.2) has $3^n - 3$ heterogeneous stationary states with nonnegative components. Moreover, Lemma 3.1.4 implies that $2^n - 2$ of them are asymptotically stable. The biological interpretation is as follows: For each of the n patches, we can choose among the following three possible scenarios:

1. The patch will be dominated by species 1; species 2 will survive, but its population will be negligible.

2. The patch will be dominated by species 2; species 1 will survive, but its population will be negligible.

3. Both species will coexist in the given patch.

For each of the 3^n choices, it is possible to find a corresponding stationary state of (3.1.2), provided that d_1 and d_2 are sufficiently small. Moreover, this state will be stable if and only if we restrict our choices to the first two possibilities.

As a simple illustration, we consider a graph with two vertices connected by an edge. We take $\rho_1 = \rho_2 = 1$, $\alpha = \beta = 2$, and $\delta_1 = \delta_2 = 1$, i.e., $d_1 = d_2 = d$.

If $d = 0$, there are two stable heterogeneous equilibria $(E_1, E_2) = (1, 0, 0, 1)$ and $(E_2, E_1) = (0, 1, 1, 0)$. Figure 3.2 shows a numerically calculated solution of (3.1.2) approaching the latter stationary state. The initial conditions are $u_1(0) = 0.1$, $v_1(0) = 0.7$, $u_2(0) = 0.9$, $v_2(0) = 0.3$. We see that species 1 becomes extinct at vertex 1, and species 2 becomes extinct at vertex 2.

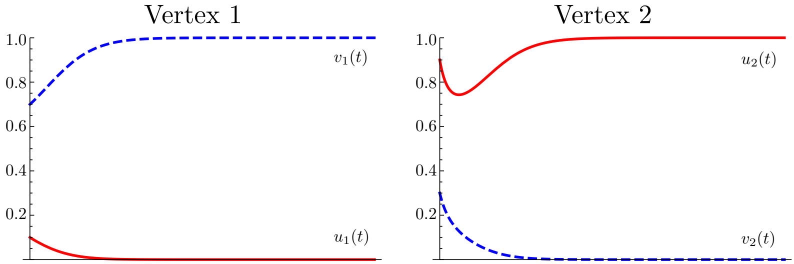

Figure 3.2: Numerical solution of the Lotka-Volterra model (3.1.2) on a graph with 2 vertices and 1 edge. Diffusion coefficients are $d_1 = d_2 = 0$.

If d is small and positive, Theorem 3.1.5 predicts the existence of stable heterogeneous stationary states with positive components close to $(E_1, E_2) = (1, 0, 0, 1)$ and $(E_2, E_1) = (0, 1, 1, 0)$. For example, if $d = 0.05$, a numerical calculation finds stable equilibrium points approximately at $(u_1, v_1, u_2, v_2) = (0.85, 0.05, 0.05, 0.85)$ and $(u_1, v_1, u_2, v_2) = (0.05, 0.85, 0.85, 0.05)$. Figure 3.3 shows a numerically calculated solution of (3.1.2) approaching the latter stationary state. We see that species 2 dominates at vertex 1, while species 1 dominates at vertex 2. However, no species becomes extinct: In each vertex, the tendency of the weaker population to extinction is compensated by diffusion from the other vertex.

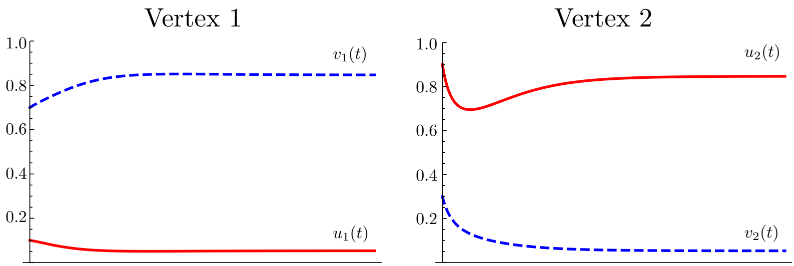

Figure 3.3: Numerical solution of the same Lotka-Volterra model as in Figure 3.2, but with diffusion coefficients increased to $d_1 = d_2 = 0.05$.

If we increase the diffusion to $d = 0.2$, numerical calculation finds no heterogeneous stationary states with nonnegative components. Fig-

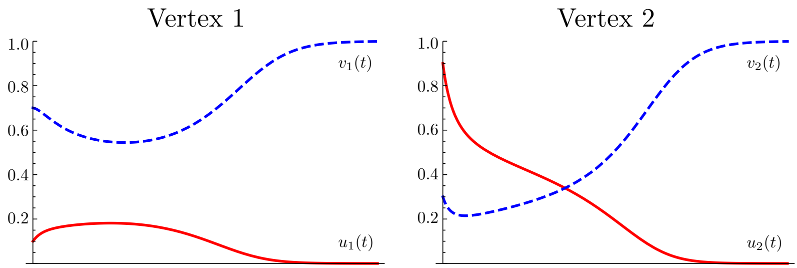

Figure 3.4: Numerical solution of the same Lotka-Volterra model as in Figure 3.3, but with diffusion coefficients increased to $d_1 = d_2 = 0.2$.

ure 3.4 shows the solution with the same initial conditions as before. The solution now approaches the homogeneous stationary state $\boldsymbol{E}_2 = (0, 1, 0, 1)$, in which species 2 wins the competition at both vertices, and species 1 is driven to extinction.

3.2 Nonnegative heterogeneous equilibria of reaction-diffusion systems on graphs

In the present section, we provide a closer look on the existence of nonnegative heterogeneous stationary states. We do not restrict ourselves to specific reaction functions, but consider a general class of reaction-diffusion systems, which are obtained as follows. First, consider a dynamical system governed by the system of differential equations

$$(x_k)'(t) = h_k(x_1(t), \dots, x_N(t)), \quad k \in \{1, \dots, N\}. \tag{3.2.1}$$

Suppose that $\Sigma = \{S_1, \dots, S_s\} \subset \mathbb{R}^N$ is a finite set of stationary states of this system. Next, we take an arbitrary undirected graph G with vertex set $V(G) = \{1, \dots, n\}$ and edge set $E(G)$ (consisting of unordered pairs of vertices). The local dynamics inside each vertex will be driven by the above-mentioned N-dimensional dynamical system. Moreover, we suppose that these n systems are coupled via diffusion along the edges of G. If $\{i, j\} \in E(G)$, let $d_k^{ij} = d_k^{ji} \geq 0$ be the intensity of diffusion for the k-th component of x between vertices i and j. In this way, we obtain the system of $n \cdot N$ reaction-diffusion equations

$$(x_k^i)'(t) = \sum_{j \in \mathcal{N}(i)} d_k^{ij}(x_k^j(t) - x_k^i(t)) + h_k(x_1^i(t), \dots, x_N^i(t)), \qquad (3.2.2)$$

where $i \in V(G)$, $k \in \{1, \dots, N\}$, and $\mathcal{N}(i) = \{j \in V(G); \{i,j\} \in E(G)\}$ denotes the set of all neighbors of a vertex $i \in V(G)$.

The system (3.2.2) has s stationary states in which no diffusion takes place, and $(x_1^i(t), \dots, x_N^i(t)) = S$ for a certain $S \in \Sigma$ and all $i \in V(G)$, $t \geq 0$; such stationary states are called spatially homogeneous. The system might also possess other stationary states, which are called spatially heterogeneous. To see this, we follow the idea from the previous section: First, if $d_k^{ij} = 0$ for all i, j, k, we have n decoupled systems. For each $i \in V(G)$, we might choose an arbitrary $\sigma(i) \in \{1, \dots, s\}$, and let $(x_1^i(t), \dots, x_N^i(t)) = S_{\sigma(i)}$ for all $t \geq 0$. If $\sigma(1), \dots, \sigma(n)$ do not all coincide, we obtain a heterogeneous stationary state $S_\sigma = (S_{\sigma(1)}, \dots, S_{\sigma(n)})$ of (3.2.2). Now, if $h_1, \dots, h_N$ are smooth, and the Jacobian matrix J_h of $h = (h_1, \dots, h_N)$ is invertible at each of the points $S_{\sigma(1)}, \dots, S_{\sigma(n)}$, then the implicit function theorem guarantees that if d_k^{ij} are small, then (3.2.2) still possesses a heterogeneous stationary state close to S_σ.

In some applications, for example in population dynamics, the only meaningful stationary states of (3.2.2) are those with nonnegative components. Note that the stationary states obtained using the implicit function theorem by continuation from S_σ depend continuously on the diffusion coefficients. Hence, if S_σ has strictly positive components, then the stationary state obtained by continuation from S_σ will be also positive, at least for sufficiently small d_k^{ij}. On the other hand, if at least one component of S_σ is strictly negative, it will remain negative for small d_k^{ij}. Hence, the only nontrivial case occurs if all components of S_σ are nonnegative, and at least one of them is zero. In such case, further analysis is needed to find out whether the corresponding stationary states obtained by continuation from S_σ have nonnegative components.

Our goal is to provide a criterion for checking whether the heterogeneous stationary states obtained by continuation from S_σ with at least one zero component remain nonnegative if the diffusion coefficients are small. To simplify the calculation, we will assume that the diffusion coefficients in (3.2.2) have the form $d_k^{ij} = d\delta_k^{ij}$ for all i, j, k, where $\delta_k^{ij} > 0$ are fixed, and $d \geq 0$ is a variable. This means that the ratio of the diffusion coefficients is fixed, but their magnitudes are allowed to vary. Although this assumption might seem too restrictive, the setting suffices for determining the existence/nonexistence of heterogeneous stationary states with nonnegative components.

Recall that $\Sigma = \{S_1, \ldots, S_s\} \subset \mathbb{R}^N$ is a finite set of (not necessarily all) equilibrium points of the system (3.2.1) such that the Jacobian matrix J_h of $h = (h_1, \ldots, h_N)$ is invertible at each $S \in \Sigma$. For each choice $S_\sigma = (S_{\sigma(1)}, \ldots, S_{\sigma(n)}) \in \Sigma^n$, the implicit function theorem yields the existence of an $\varepsilon > 0$ and continuously differentiable functions $u_k^i : [0, \varepsilon] \to \mathbb{R}$, $i \in V(G)$, $k \in \{1, \ldots, N\}$, such that

$$\sum_{j \in \mathcal{N}(i)} d\delta_k^{ij}(u_k^i(d) - u_k^j(d)) = h_k(u_1^i(d), \ldots, u_N^i(d)), \quad d \in [0, \varepsilon], \quad (3.2.3)$$

where $(u_1^i(0), \ldots, u_N^i(0)) = S_{\sigma(i)}$ for all $i \in V(G)$. Hence, the values $u_k^i(d)$ determine an equilibrium state of (3.2.2) with $d_k^{ij} = d\delta_k^{ij}$ obtained by continuation from S_σ. We keep in mind that the functions u_k^i depend on the choice of S_σ, although we do not write this dependence explicitly.

In the following main result, we assume that G is a connected undirected graph; otherwise, one can examine each connected component separately. The symbol $\operatorname{diam} G$ denotes the diameter of a graph G, i.e., the maximum distance between two vertices in G.

Theorem 3.2.1. *Suppose that $S_\sigma \in \Sigma^n$ has nonnegative components, each of $h_1, \ldots, h_N$ is real analytic at the points $S_{\sigma(1)}, \ldots, S_{\sigma(n)}$, and if $k \in \{1, \ldots, N\}$ and $i \in V(G)$ are such that $u_k^i(0) = 0$, then*

$$\frac{\partial^q h_k}{\partial x_{m_1} \cdots \partial x_{m_q}}(u_1^i(0), \ldots, u_N^i(0)) = 0$$

for all $q \in \{1, \ldots, \operatorname{diam} G\}$ and $m_1, \ldots, m_q \in \{1, \ldots, N\} \setminus \{k\}$. Then the continuation of S_σ is nonnegative for all sufficiently small $d > 0$ if and only if for each $k \in \{1, \ldots, N\}$ and $i \in V(G)$ for which $u_k^i(0) = 0$, either $u_k^j(0) = 0$ for all $j \in V(G)$, or $\frac{\partial h_k}{\partial x_k}(u_1^i(0), \ldots, u_N^i(0)) < 0$.

The idea of the proof is as follows: To decide whether the continuation of S_σ has nonnegative components, we examine all vertices $i \in V(G)$. For each zero component of $S_{\sigma(i)}$, we determine the sign of the first nonvanishing derivative (with respect to the strength of the diffusion). The assumptions on the right-hand sides $h_1, \ldots, h_N$ make this possible without having to calculate the inverse Jacobian matrix.

Under the assumptions of Theorem 3.2.1, we see that the fact whether the continuation of S_σ is nonnegative depends only on the set $\{\sigma(i) : i \in V(G)\}$, and not on the distribution of the values $\sigma(1), \ldots, \sigma(n)$ among the vertices. This leads us to the following concept of an admissible set – a set of equilibria of (3.2.1) that can be combined together in an arbitrary way in order to get a nonnegative stationary state of the spatial system (3.2.2) for small $d \geq 0$.

Definition 3.2.2. If $\Sigma = \{S_1, \ldots, S_s\} \subset \mathbb{R}^N$ is a finite set of stationary states of the system (3.2.1), we say that $\mathcal{A} \subset \Sigma$ is an *admissible set* for (3.2.2) if it has the following property: If $S_{\sigma(1)}, \ldots, S_{\sigma(n)} \in \mathcal{A}$, then the continuation of $S_\sigma = (S_{\sigma(1)}, \ldots, S_{\sigma(n)})$ is nonnegative for small $d \geq 0$.

We say that an admissible set $\mathcal{A}$ is *maximal* if it is not contained in any larger admissible set.

Note that each admissible set contains only nonnegative states S_i, and each nonnegative state S_i gives rise to the singleton admissible set $\mathcal{A} = \{S_i\}$, but it need not be maximal.

It follows from Theorem 3.2.1 that the problem of determining all choices $\sigma(1), \ldots, \sigma(n) \in \{1, \ldots, s\}$ such that the continuation of $S_\sigma = (S_{\sigma(1)}, \ldots, S_{\sigma(n)})$ is nonnegative can be solved by finding all maximal admissible sets for (3.2.2). In particular, all $S_{\sigma(1)}, \ldots, S_{\sigma(n)}$ have to be elements of a certain maximal admissible set.

The next result provides a formula for the number of nonnegative heterogeneous stationary states; the symbol $|X|$ stands for the number of elements of a set X.

Theorem 3.2.3. *Suppose that $\mathcal{A}_1, \ldots, \mathcal{A}_r$ is the collection of all distinct maximal admissible sets for the system* (3.2.2). *Assume that $|\mathcal{A}_i \cap \mathcal{A}_j| \leq 1$ whenever $i \neq j$. Then, if $d_k^{ij} = d\delta_k^{ij}$ for all i, j, k, the system* (3.2.2) *has at least $\sum_{i=1}^r (|\mathcal{A}_i|^n - |\mathcal{A}_i|)$ nonnegative heterogeneous stationary states for all sufficiently small $d \geq 0$.*

We illustrate our results on the simplest possible example: When $N = 1$, the system (3.2.1) reduces to the single equation $x'(t) = h(x(t))$, and (3.2.2) becomes

$$(x^i)'(t) = \sum_{j \in \mathcal{N}(i)} d^{ij}(x^j(t) - x^i(t)) + h(x^i(t)), \quad i \in V(G). \qquad (3.2.4)$$

Suppose that $h : \mathbb{R} \to \mathbb{R}$ has the zero equilibrium and several positive equilibria, i.e., $\Sigma = \{S_1, S_2, \ldots, S_s\}$ with $0 = S_1 < S_2 < \cdots < S_s$. To be able to apply Theorem 3.2.1, we assume that $d^{ij} = d\delta^{ij}$ and that for each $x \in \Sigma$, h is real analytic at x and $h'(x) \neq 0$.

An arbitrary $S_\sigma = (S_{\sigma(1)}, \dots, S_{\sigma(n)}) \in \Sigma^n$ is a stationary state for (3.2.4) with $d^{ij} = 0$. Clearly, if $S_{\sigma(i)} \neq 0$ for all $i \in V(G)$, then the continuation of S_σ is nonnegative for small $d > 0$. If $S_{\sigma(i)} = 0$ for some $i \in V(G)$, Theorem 3.2.1 implies that the continuation of S_σ is nonnegative for small $d > 0$ if and only if either $S_{\sigma(j)} = 0$ for all $j \in V(G)$, or $h'(0) < 0$. In other words, if $h'(0) < 0$, then the unique maximal admissible set for (3.2.4) is Σ and we get $s^n - s$ nonnegative heterogeneous stationary states, while if $h'(0) > 0$, then the maximal admissible sets are $\mathcal{A}_1 = \{0\}$ and $\mathcal{A}_2 = \{S_2, \dots, S_s\}$, and we get $(s-1)^n - (s-1)$ nonnegative heterogeneous stationary states.

For example, if $h(x) = \rho x(x-a)(b-x)$, where $0 < a < b$, then (3.2.4) is the Nagumo equation considered in [29]. We have $\Sigma = \{0, a, b\}$, $h'(a) = \rho a(b-a) \neq 0$, $h'(b) = \rho b(a-b) \neq 0$ and $h'(0) = -\rho ab < 0$. Hence, the unique maximal admissible set is Σ, and we get $3^n - 3$ nonnegative heterogenenous stationary states for $d^{ij} = d\delta^{ij}$ and small $d > 0$, as proved in [29].

Another possible choice is the logistic nonlinearity $h(x) = \rho x(a-x)$, where $a > 0$. Then $\Sigma = \{0, a\}$, $h'(a) = -\rho a \neq 0$, and $h'(0) = \rho a > 0$. Hence, the maximal admissible sets are $\mathcal{A}_1 = \{0\}$, $\mathcal{A}_2 = \{a\}$, which lead only to homogeneous stationary states.

More complicated examples (Lotka-Volterra models with two or three species, a competition model for two species with an Allee effect, and the Gause predator-prey model) can be found in [AS10].

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