Various types of solutions of graph and lattice reaction diffusion equations

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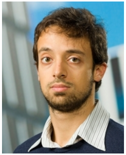

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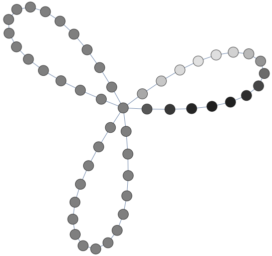

Interesting encounter of analysis, numerics, linear algebra, graph theory and applied mathematics

Reaction diffusion equation

$$u_t = du_{xx} + \lambda f(u), \quad x \in \mathbb{R}, t > 0.$$

- spatial dynamics - diffusion (d - diffusion parameter)
- local dynamics - reaction function (λ - reaction parameter)
- rich behaviour, several phenomena (biological, physical, chemical...)

Prototypical example for

- pattern formation,
- travelling wave solutions.

Why lattices and graphs?

Discrete-space domains:
Lattices - $\mathbb{Z}$, $\mathbb{Z}^d$, $d \in \mathbb{N}$
Graph - $G = (V, E)$ (in this talk undirected graph, no loops, no multiple edges...)

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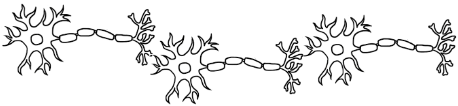
numerics - finite differences, method of lines - don't carry coal to Newcastle...

analysis - richer behaviour earlier (both patterns and travelling waves)



Neurology -

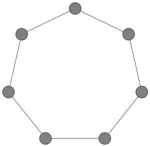
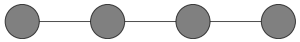
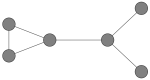
- cortical travelling waves, EEG, Berger (1929),
- travelling waves and propagation failure

Ecology - Real world populations:

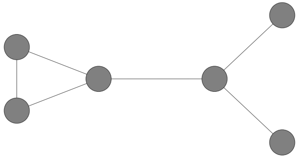
- spatial configurations are not always homogeneous (obstacles, coasts),
- diffusion may differ (slopes, ...)
- habitats form a connected undirected and finite graph $G = (V, E)$.

(source: imageshack)

Motivation - RDE on discrete structures

 (cycles)	Turing(1952)	cells	morphogenesis
 (1D lattices)	Bell(1984) Allen(1987)	neurons islands	persistence persistence
nD lattices	Keener(1997)	neurons	patterns and waves
	???		

(only in continuous time)



Reaction-diffusion equations on graphs with constant diffusion

$$u_i'(t) = d \sum_{j \in N(i)} (u_j(t) - u_i(t)) + \lambda f(u_i(t)), \quad i \in V, \quad t \in [0, \infty),$$

or alternatively with non-constant diffusion

$$u_i'(t) = \sum_{j \in N(i)} d_{ij}(u_j(t) - u_i(t)) + \lambda f(u_i(t)), \quad i \in V, \quad t \in [0, \infty).$$

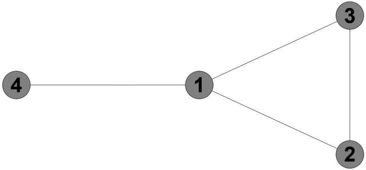
PDE $\rightarrow$ (in)finite systems of ODEs

$$u'(t) = \mathcal{L}u(t) + \lambda F(u(t)).$$

see, e.g., Bapat et al. (2001), de Abreu(2007), Fiedler(1973), Merris(1994), Mohar(1992)

Laplacian matrix of a graph $\mathcal{L} = D - A(G)$

- D is the diagonal matrix of vertex degrees,
- $A(G)$ is the adjacency matrix,



$$\mathcal{L} = \begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

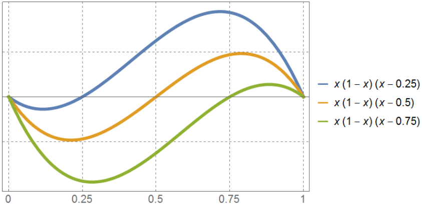
since

$$D = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad A(G) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Reaction functions

We consider the bistable (strong Allee) nonlinearity ($\lambda > 0$ and $0 < a < 1$)

$$f(u) = g(u; a) = \lambda u(u - a)(1 - u),$$



We use the nonlinear operator $\mathbb{R}^{|V|} \to \mathbb{R}^{|V|}$ defined by

$$F(v) := \begin{bmatrix} f(v_1) \\ f(v_2) \\ \vdots \\ f(v_3) \end{bmatrix}.$$

The reaction-diffusion equation on graphs (Nagumo equation on graphs) can then be written as a vector (or abstract) ODE

$$u'(t) = \mathcal{L}u(t) + \lambda F(u(t)), \quad u(t) \in \mathbb{R}^{|V|} \text{ (or a sequence space)}, t > 0.$$

We discuss the dependence of various properties of stationary solutions on the

- diffusion parameters d_{ij}
- reaction function parameters λ, a,
- graph parameters (number of vertices, connectedness, graph diameter ...)

Finite differences of a Neumann problem

$$\begin{cases} -x''(t) = \lambda f(t, x(t)), \quad t \in (0, 1, \\ x'(0) = x'(1) = 0. \end{cases}$$

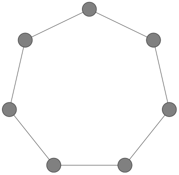
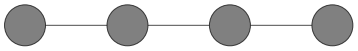
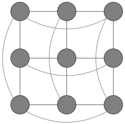
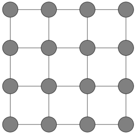
or directly a discrete problem

$$\begin{cases} -\Delta^2 x(k-1) = \lambda f(k, x(k)), \quad k = 1, 2..., n, \\ \Delta x(0) = \Delta x(n) = 0. \end{cases}$$

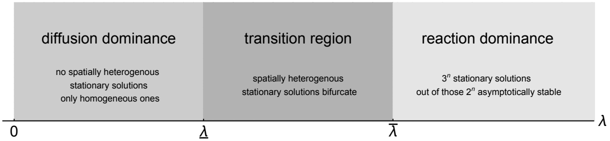
leads to $L_N \mathbf{x} = F(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^n$ with

$$L_N = \begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix},$$

Graph Laplacians and finite differences II.

boundary conditions	graph G	illustration
1D periodic	cycle C_n	
1D Neumann	path P_n	
2D periodic	cyclic grid $CG_{m,n}$	
2D Neumann	grid $G_{m,n}$	

Emergence of spatially heterogeneous stationary solutions

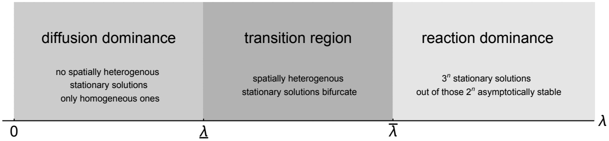


Stationary solutions satisfy the nonlinear matrix equation (an abstract difference equation) in $\mathbb{R}^{|V|}$

$$o = \mathcal{L}v + F(v)$$

- trivial stationary solutions - zeroes of $g(u; a)$
  - $u_1(t) \equiv 1$,
  - $u_2(t) \equiv a$,
  - $u_3(t) \equiv 0$,
- nontrivial stationary solutions - spatially heterogeneous
- implicit function theorem works perfectly if we are not interested in bounds

Emergence of spatially heterogeneous solutions



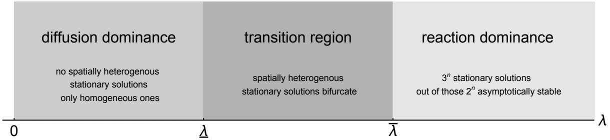
Theorem

For a given graph there exists $\underline{\lambda}$ such that for all $\lambda < \underline{\lambda}$ there are only trivial (spatially homogeneous) solutions. Moreover,

$$\frac{d_{\max}(\Delta(G)-1)}{a(1-a)\left(\left(\frac{d_{\max}}{d_{\min}}(\Delta(G)-1)+1\right)^{diam(G)-1}-1\right)} < \underline{\lambda} < \frac{\rho(A)}{a(1-a)}.$$

Conjecture: $\underline{\lambda} = \frac{\lambda_2}{a(1-a)}$

Exponential number of solutions



Theorem

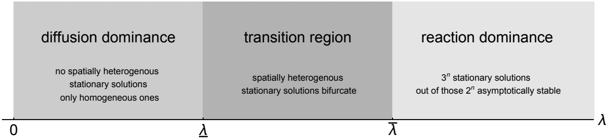
For a given graph there exists $\overline{\lambda}$ such that for all $\lambda > \overline{\lambda}$ there exist at least 3^n stationary solutions out of which 2^n are asymptotically stable. Moreover,

$$\overline{\lambda} < \frac{4 \cdot d_{max} \cdot \Delta(G)}{\min\{a^2, (1-a)^2\}}.$$

Simple example

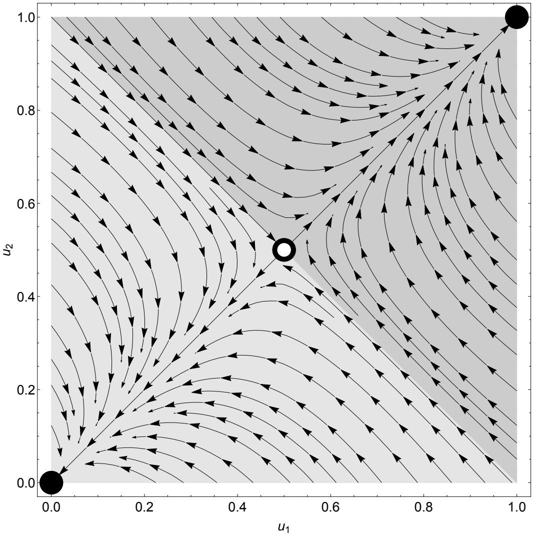
- two vertices (patches) - the simplest nontrivial graph K_2,

- $d = 1$,
- $a = .5$,
- what happens if we change λ?

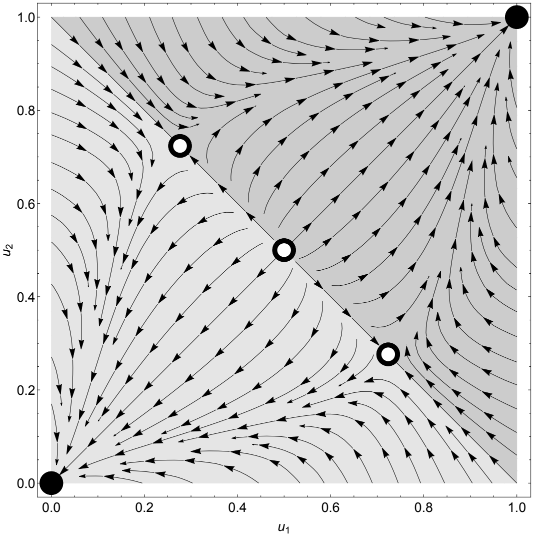


- In this case, everything can be computed analytically.
- Moreover, we will use it later...

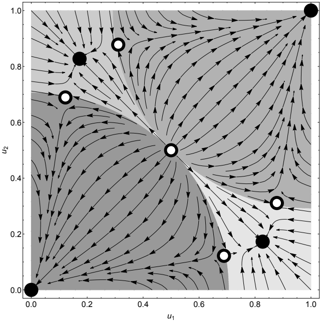
$d = 1$, $a = .5$, K_2, $0 < \lambda < 8$



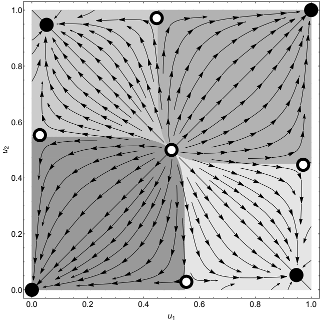
$d = 1$, $a = .5$, K_2, $8 < \lambda < 12$



$d = 1$, $a = .5$, K_2, $\lambda > 12$

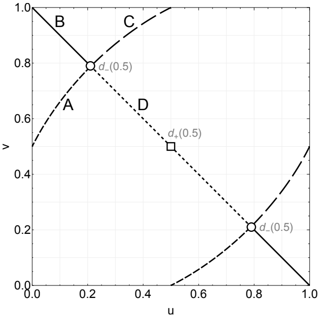


$\lambda = 15$



$\lambda = 40$

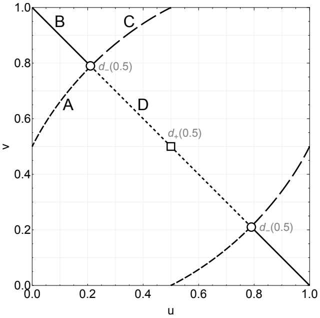
Spatially heterogeneous solutions only



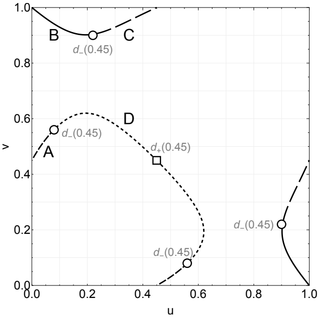
$a = .5$

Aggregate bifurcation diagrams

Spatially heterogeneous solutions only



$a = .5$



$a = .45$

Bichromatic and multichromatic waves - background

(a) (Monochromatic) travelling waves for continuous reaction-diffusion equation
(b) (Monochromatic) travelling waves for lattice reaction-diffusion equation
(c) Bichromatic and multichromatic travelling waves for lattice reaction-diffusion equation.
(d) Connection to graph reaction-diffusion equation

Fife, McLeod (1977) studied

$$u_t = du_{xx} + \lambda g(u; a), \quad x \in \mathbb{R}^N, t > 0, x \in \mathbb{R},$$

where $g(u; a) = u(1-u)(u-a)$.

They used phase-plane analysis to show the existence of a travelling wave solution

$$u(x,t) = \Phi(x - ct), \qquad \Phi(-\infty) = 0, \qquad \Phi(+\infty) = 1$$

for some smooth waveprofile Φ and wavespeed c with

$$\mathrm{sign}(c) = \mathrm{sign}\left(a - \frac{1}{2}\right).$$

- large basin of attraction. Any solution with an initial condition $u(x,0) = u_0(x)$ that has $u_0(x) \approx 0$ for $x \ll -1$ and $u_0(x) \approx 1$ for $x \gg +1$ will converge to a shifted version of the travelling wave.
- building blocks for more complex waves $(\alpha_1 \geq \alpha_0)$

$$u(x,t) = \Phi(x - ct + \alpha_0) + \Phi(-x - ct + \alpha_1) - 1$$

The situation with the LDE

$$u_j'(t) = d\big[u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\big] + g\big(u_j(t); a\big), \quad j \in \mathbb{Z}, t > 0,$$

becomes more complicated. The wave profile $\Phi(x - ct)$ satisfies

$$-c\Phi'(\xi) = d\big[\Phi(\xi - 1) - 2\Phi(\xi) + \Phi(\xi + 1)\big] + g\big(\Phi(\xi); a\big).$$

For a fixed $a \in (0, 1) \setminus \{\frac{1}{2}\}$:

- Keener (1987) - $c_{\mathrm{mc}}(a, d) = 0$ for $0 < d \ll 1$
- Zinner (1992) established that $c_{\mathrm{mc}}(a, d) \neq 0$ for $d \gg 1$
- Mallet-Paret (1996) - showed that for each d there exists $\delta > 0$ so that $c_{\mathrm{mc}}(a, d) = 0$ whenever $|a - \frac{1}{2}| \leq \delta$.

Thus, travelling waves don't exist for small values of d, this phenomenon is called **pinning**.

Pinning

- Keener (1987) - $c_{\mathrm{mc}}(a, d) = 0$ for $0 < d \ll 1$
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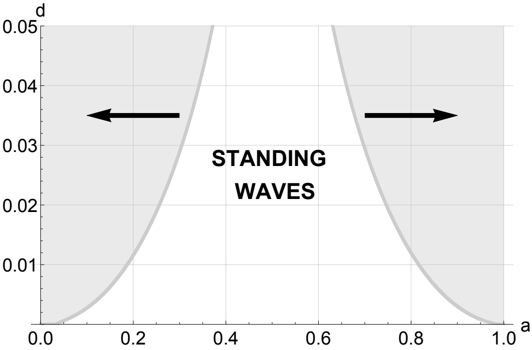
- Mallet-Paret (1996) - showed that there exists $\delta > 0$ so that $c_{\mathrm{mc}}(a, d) = 0$ whenever $|a - \frac{1}{2}| \leq \delta$.



Nagumo graph differential equation (GDE), $j \in V$, $t > 0$

$$u_i'(t) = d \sum_{j \in N(i)} (u_j(t) - u_i(t)) + g\big(u_i(t); a\big),$$

Nagumo lattice differential equation (LDE), $j \in \mathbb{Z}$, $t > 0$

$$\dot{u}_j(t) = d\big[u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\big] + g\big(u_j(t); a\big),$$

Nagumo lattice difference equation (LΔE), $j \in \mathbb{Z}$, $t \in \mathbb{N}_0$

$$\frac{u_j(t+h) - u_j(t)}{h} = d\big[u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\big] + g\big(u_j(t); a\big),$$

Theorem

If $(x_1, \ldots, x_n)$ is (one of 3^n) stationary solution of Nagumo equation on a cyclic graph C_n then its periodic extension is an n-periodic stationary solution of LDE and LΔE. Moreover, the asymptotic stability of corresponding stationary solutions of GDE and LDE coincides.

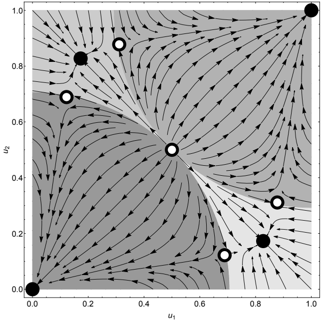
2-periodic stationary solutions of the lattice reaction-diffusion equation

$$u_j'(t) = d\big[u_{j-1}(t) - 2u_j(t) + u_{j+1}(t)\big] + g\big(u_j(t); a\big), \quad j \in \mathbb{Z}, t > 0,$$

satisfy

$$\begin{pmatrix} 2d(v-u) + g(u;a) \\ 2d(u-v) + g(v;a) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} =$$

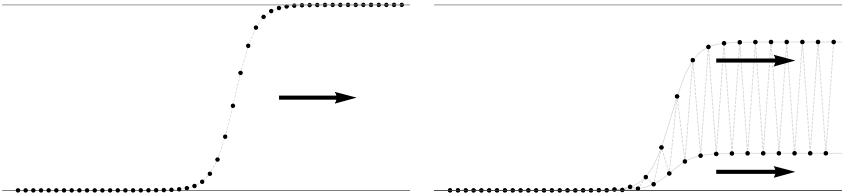
i.e., they are stationary solution of the graph reaction-diffusion equation with $\tilde{d} = 2d$!



We construct a new type of travelling wave solutions that connect homogeneous stationary solutions with 2-periodic stationary solutions.

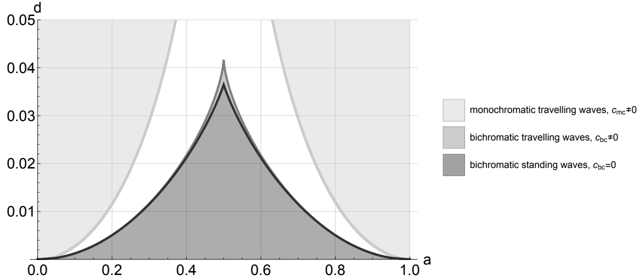
We consider bichromatic travelling wave solutions

$$x_j(t) = \begin{cases} \Phi_u(j - ct) & \text{if } j \text{ is even,} \\ \Phi_v(j - ct) & \text{if } j \text{ is odd.} \end{cases}$$



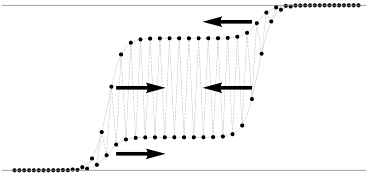
Bichromatic waves - results summary

Regions for the existence of bichromatic travelling waves:



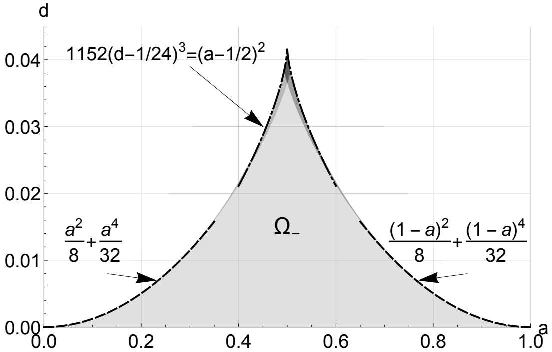
Most importantly,

- In contrast to monochromatic waves, the bichromatic waves exist and move for $a = \frac{1}{2}$.
- In contrast to monochromatic waves, both 0 and 1 can spread.

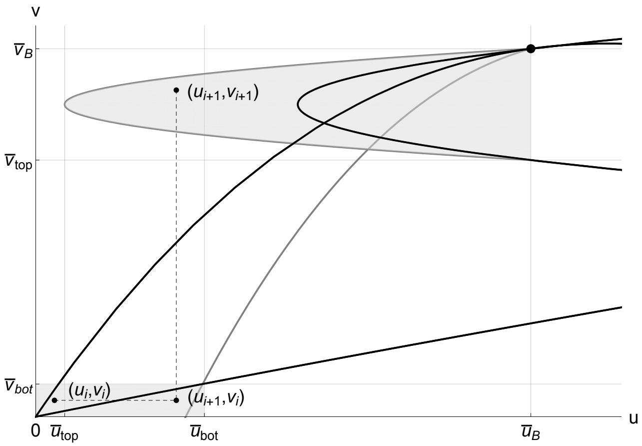


Bifuraction curves (rise of stable 2-periodic solutions) cannot be described analytically (bifurcation of 9th order polynomial, but

- we describe a cusp bifurcation around $(a, d) = (1/2, 1/24)$, and
- provide estimates near $a = 1$ and $a = 0$.



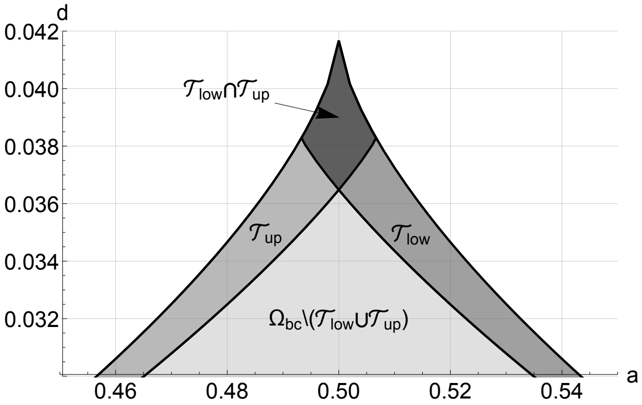
Standing wave must be a solution of an infinite system of difference equations. Using the so-called reflection principle we show that there is no solution near the bifurcation points.



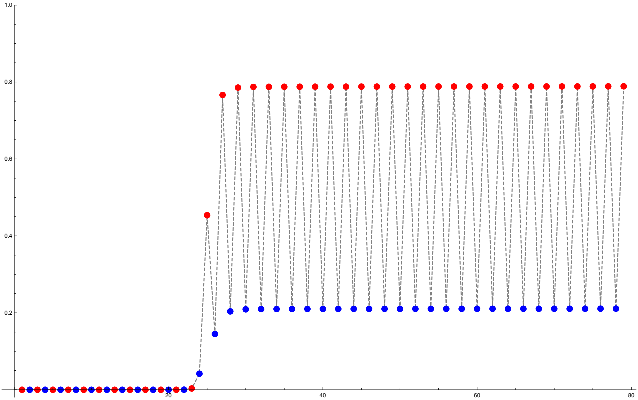
We introduce sets

$$\mathcal{T}_{\mathrm{low}} = \{(a, d) \in \Omega_{\mathrm{bc}} : c_{\mathrm{low}} > 0\},$$
$$\mathcal{T}_{\mathrm{up}} = \{(a, d) \in \Omega_{\mathrm{bc}} : c_{\mathrm{up}} < 0\},$$

and get the following situation near $a = \frac{1}{2}$.



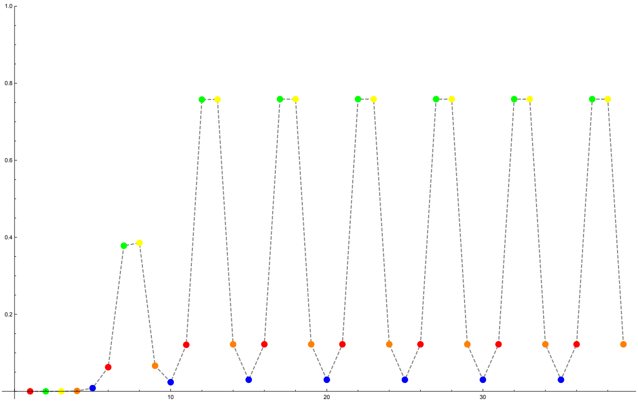
Bichromatic waves - numerical simulation



Multichromatic waves

Similar ideas can be used to get travelling waves with more colours

- trichromatic waves - three colours, connect stationary 3-periodic solutions which can be derived from stationary solutions of the graph reaction-diffusion on $G = C_3$,
- n-chromatic waves - n colours, connect stationary n-periodic solutions which can be derived from stationary solutions of the graph reaction-diffusion on $G = C_n$
- Only numerical results - bifurcation analysis of polynomials of order 3^n.



Motivated by the question of stability of 2^n solutions of graph Nagumo equation we pose the following question.

- L is a weighted graph Laplacian,
- $D = P - N$ is a diagonal matrix, where $P = (p_{ij})$ and $N = (n_{ij})$ are positive semidefinite diagonal matrices

Under which conditions is the matrix $L + D = L + P - N$ positive (semi)definite?

Example, let $\alpha, \beta, \gamma > 0$

$$\begin{pmatrix} 2+\alpha & -1 & -1 \\ -1 & 2+\beta & -1 \\ -1 & -1 & 2-\gamma \end{pmatrix}$$

$$L = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad N = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \gamma \end{pmatrix}$$

Notation

We use the following notation

- the set of positive entries of a diagonal matrix D,

$$\mathcal{I}^+(D) = \{i \in \mathcal{V} : d_{ii} > 0\}$$

- the number of positive entries of a diagonal matrix D,

$$\mathrm{nonz}(D) = |\mathcal{I}^+(D)|$$

Example

$$P = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{I}^+(P) = \{1, 2\}, \mathrm{nonz}(P) = 2.$$

Main result

Let L be a weighted Laplacian matrix, $\lambda_2 > 0$ its second eigenvalue, $P = (p_{ij})$ and $N = (n_{ij})$ positive semidefinite diagonal matrices. Assume that

(i) [magnitude assumption] there exists a constant d satisfying

$$0 \leq d \leq \frac{\lambda_2}{3},$$

such that $0 \leq n_{ii} \leq d$ for all $i \in \mathcal{V}$ and $p_{jj} \geq d$ for all $j \in \mathcal{I}^+(P)$,

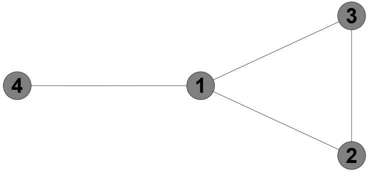
(ii) $p_{ii} n_{ii} = 0$ for all $i \in \mathcal{V}$,

(iii) [sum assumption]

$$\sum_i n_{ii} \leq \frac{d \cdot \mathrm{nonz}(P)}{3}.$$

Then the matrix $L' = L + P - N$ is positive semidefinite.

Example



$$L = \begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

Perturbing matrix

$$\begin{pmatrix} 3+\alpha & -1 & -1 & -1 \\ -1 & 2-\beta & -1 & 0 \\ -1 & -1 & 2-\gamma & 0 \\ -1 & 0 & 0 & 1-\delta \end{pmatrix}$$

is positive semidefinite for all $\alpha \geq \frac{1}{3}$ and $\beta, \gamma, \delta \geq 0$ satisfying $\beta + \gamma + \delta \leq \frac{1}{9}$ (note that $\mathrm{nonz}(P) = 1$).

Generalization - arbitrary PSD matrix

Let A be a positive semidefinite matrix, such that $\lambda_1 = 0$ is a simple eigenvalue of A with a corresponding eigenvector $\mathbf{x}_1 = (\xi_1, \xi_2, \ldots, \xi_n)^\top$. Let $\lambda_2 > 0$ be the second eigenvalue of A and let $P = (p_{ij})$ and $N = (n_{ij})$ be positive semidefinite diagonal matrices. Assume that

(i) there exists a constant d satisfying

$$0 \leq d \leq \frac{\lambda_2}{3},$$

such that $0 \leq n_{ii} \leq d$ for all $i \in \mathcal{V}$ and $p_{jj} \geq d$ for all $j \in \mathcal{I}^+(P)$,

(ii) $p_{ii} n_{ii} = 0$ for all $i \in \mathcal{V}$,

(iii)

$$\sum_i \xi_i^2 n_{ii} \leq \frac{\sum_i d \cdot \xi_i^2 \cdot \mathrm{sign}(p_{ii})}{3}.$$

Then the matrix $A' = A + P - N$ is positive semidefinite.

Example

$$A = \begin{pmatrix} 16 & 1 & -22 \\ 1 & 61 & 23 \\ -22 & 23 & 40 \end{pmatrix}$$

- eigenvalues - $0, 39, 78$,
- the first eigenvector is $\mathbf{x}_1 = (7, -2, 5)^\top$
- The sum assumption then implies

$$d = \frac{\lambda_2}{3} = 13, \quad p_{ii} \geq 13, n_{ii} \leq 13.$$

Consequently, our result implies that the perturbed matrix,

$$\begin{pmatrix} 16 + \alpha & 1 & -22 \\ 1 & 61 + \beta & 23 \\ -22 & 23 & 40 - \gamma \end{pmatrix}$$

is positive semidefinite for all $\alpha, \beta \geq 13$ and $\gamma \leq \frac{689}{75} \approx 9.19$.

Thank you for your attention