Travelling Waves for Fully Discretized Bistable Reaction-Diffusion Problems

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Reaction-Diffusion System

\[ \partial_t u = \Delta u - G'(u) \]

- Continuous spatial variable: \( x \in \mathbb{R} \).
- Continuous temporal variable: \( t \in \mathbb{R} \).
- \( 0 \leq u(x, t) \leq 1 \)
- Prototype for Pattern formation.
Think of $G(u)$ as a potential.

Ignoring spatial variations, $u$ moves through potential landscape.

Two competing rest states $u = 0$ and $u = 1$.
### Diffusion Term

\[
\partial_t u = \Delta u - G'(u)
\]

- **Rate of change**
- **Diffusion**
  - Mixes points
- **Reaction**
  - Single point

- Diffusion: flattens wrinkles.
Travelling Waves

Basic pattern: travelling waves connecting $u = 0$ to $u = 1$.

- Building blocks for more complex patterns.
Nonlinearity

For concreteness, will use quartic potential; i.e.

\[-G''(u) = -G''(u; a) = g_{\text{cub}}(u; a) = u(1 - u)(u - a)\]
Travelling wave: PDE

Nagumo PDE with $g_{\text{cub}}(\cdot; a)$:

$$\partial_t u = \partial_{xx} u + u(1 - u)(u - a).$$

Starting step [Fife, McLeod]: travelling waves.

Travelling wave $u(x, t) = \Phi(x + ct)$ satisfies:

$$c\Phi'(\xi) = \Phi''(\xi) + \Phi(\xi) (1 - \Phi(\xi)) (\Phi(\xi) - a).$$

Interested in pulse solutions connecting 0 to 1, i.e.

$$\lim_{\xi \to -\infty} \Phi(\xi) = 0, \quad \lim_{\xi \to +\infty} \Phi(\xi) = 1.$$
Recall travelling wave ODE

\[ c\Phi'(\xi) = \Phi''(\xi) + \Phi(\xi)(a - \Phi(\xi)) (\Phi(\xi) - 1). \]

\[ \lim_{\xi \to -\infty} \phi(\xi) = 0, \]
\[ \lim_{\xi \to +\infty} \phi(\xi) = 1. \]

Explicit solutions available:

\[ \Phi(\xi) = \frac{1}{2} + \frac{1}{2} \tanh\left(\frac{1}{4} \sqrt{2} \xi\right), \]
\[ c(a) = \frac{1}{\sqrt{2}}(1 - 2a). \]
Continuous space

Speed

one wins!

zero wins!

\( G(u) \)

\( u = 0 \)

\( u = 1 \)

balance

standoff!
Step 1 - Spatial Discretization

- Translational symmetry broken

- Gaps in discrete space: barriers

- Fundamental difference between Moving Waves and Standing Waves
**Reaction-Diffusion System**

\[ \dot{u}_j(t) = [\Delta_\mathbb{Z} u(t)]_j - G'(u_j(t)). \]

- **Discrete** spatial variable: \( j \in \mathbb{Z} \).
- **Continuous** temporal variable: \( t \in \mathbb{R} \).
- \( 0 \leq u_j(t) \leq 1 \)
Diffusion Term

\[ \dot{u}_j(t) = \left[ \Delta_Z u(t) \right]_j - G'(u_j(t)). \]

- Diffusion: flattens variations between neighbours.

\[ \left[ \Delta_Z u(t) \right]_j = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) \]
Travelling Waves

Again: Basic pattern: travelling waves connecting $u = 0$ to $u = 1$.

Different times see different discrete samples of smooth underlying profile.
Consider the Nagumo LDE

\[
\frac{d}{dt} u_j(t) = [u_{j+1}(t) + u_{j-1}(t) - 2u_j(t)] + g_{\text{cub}}(u_j(t); a), \quad j \in \mathbb{Z}.
\]

Travelling wave profile \( u_j(t) = \Phi(j + ct) \) must satisfy:

\[
c\Phi'() = \Phi(\xi + 1) + \Phi(\xi - 1) - 2\Phi(\xi) + g_{\text{cub}}(\Phi(\xi); a)
\]

\[
\lim_{\xi \to -\infty} \Phi(\xi) = 0,
\]

\[
\lim_{\xi \to +\infty} \Phi(\xi) = 1.
\]

• Notice that wave speed \( c \) enters in singular fashion.

• When \( c \neq 0 \), this is a functional differential equation of mixed type (MFDE).

• When \( c = 0 \), this is a difference equation.
Recall travelling wave MFDE:

\[ c\Phi'(\xi) = [\Phi(\xi + 1) + \Phi(\xi - 1) - 2\Phi(\xi)] + g_{\text{cub}}(\Phi(\xi); a) \]

\[ \lim_{\xi \to -\infty} \phi(\xi) = 0, \]
\[ \lim_{\xi \to +\infty} \phi(\xi) = 1. \]

When \( c = 0 \), can restrict to \( \xi \in \mathbb{Z} \): recurrence relation!

With \( p_j = \Phi(j) \) and \( r_j = \Phi(j + 1) \), we find

\[ p_{j+1} = r_j \]
\[ r_{j+1} = -p_j + 2r_j - r_j(r_j - a)(1 - r_j). \]

Saddles \((0, 0)\) and \((1, 1)\).
Propagation Failure

\[ p_{j+1} = r_j \]
\[ r_{j+1} = -p_j + 2r_j - r_j(r_j - a)(1 - r_j). \]

For \( a = \frac{1}{2} \), site-centered (orange) and bond-centered (black) solutions. Generically:

\[ \mathcal{W}^u(0,0)^{(1,1)} \]
Propagation Failure

\[ p_{j+1} = r_j \]
\[ r_{j+1} = -p_j + 2r_j - r_j(r_j - a)(1 - r_j). \]

Two branches coincide and annihilate at \( a = a_* \).
Propagation

Typical wave speed $c$ versus $a$ plot for discrete reaction-diffusion systems:

Wave speed $c$ depends uniquely on $a$.

In case $a_* < \frac{1}{2}$, then we say that LDE suffers from propagation failure.

Propagation failure common for LDEs [Keener, Mallet-Paret, Hoffman, ...].
Discrete space

Speed

$G(u_j)$

$u_j = 0$

$u_j = 1$

one wins!

standoff!

$(\ln)$balance

zero wins!
Discrete Nagumo LDE - Propagation failure

Travelling waves for the discrete Nagumo LDE connecting $0 \rightarrow 1$. 

![Graph showing travelling waves for the discrete Nagumo LDE connecting $0 \rightarrow 1$.]
Step Two - Temporal Discretization

Apply Backward-Euler time discretization with time-step $\Delta t$:

$$\frac{1}{\Delta t} [u_j(t) - u_j(t - \Delta t)] = [\Delta_Z u(t)]_j - G'(u_j(t)).$$

- Temporal variable $t$ now in $(\Delta t)\mathbb{Z}$ (discrete).
- Spatial variable $j \in \mathbb{Z}$ still discrete.

Travelling wave Ansatz $u_j(t) = \Phi(j + ct)$ now yields

$$c[D_{1,M}\Phi](\zeta) = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) - G'(\Phi(\zeta))$$

in which $M = (c\Delta t)^{-1}$ and

$$[D_{1,M}\Phi](\zeta) = M[\Phi(\zeta) - \Phi(\zeta - M^{-1})]$$

Domain of $\zeta$ depends on $M$. Dense in $\mathbb{R}$ if $M$ irrational; otherwise periodic.
BDF Methods

- Backward-Euler discretization is the order $k = 1$ BDF (Backward Differentiation Formula) method.
- These methods are L-stable (slightly worse than A-stable); much better than forward Euler.
- Methods available up to order $k = 6$.

With BDF order $k$ discretization, wave must solve:

$$c[D_{k,M} \Phi](\zeta) = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) - G'(\Phi(\zeta)).$$

Example for $k = 2$:

$$[D_{2,M} \Phi](\zeta) = \frac{3}{2} M \left[ \Phi(\zeta) - \frac{4}{3} \Phi(\zeta - M^{-1}) + \frac{1}{3} \Phi(\zeta - 2M^{-1}) \right].$$

For smooth functions $\phi$:

$$[D_{k,M} \phi - \phi'](\zeta) = O(M^{-k} \| \phi^{(k+1)} \|_\infty).$$
**Backward-Euler: restatement**

For backward-Euler one can look for solutions to

\[
\tilde{c}\Phi'(\xi) = \frac{1}{\Delta t}[\Phi(\xi - c\Delta t) - \Phi(\xi)] + \Phi(\xi + 1) + \Phi(\xi - 1) - 2\Phi(\xi) - G'(\Phi(\xi); a)
\]

with \(\tilde{c} = 0\).

All shifted terms have **positive** coefficients. Allows framework of Mallet-Paret for **spatial discretization** to be applied for fixed \(c\) and \(\Delta t\).

This gives unique \(\tilde{c} = \tilde{c}(c, a)\).

**Thm.** [H., Van Vleck based on Mallet-Paret] Fix \(\Delta t\). For all \(c\) sufficiently small, there is at least one \(a\) for which \(\tilde{c}(c, a) = 0\).

**Numerical insights** Generically, \(\tilde{c}(c, a) = 0\) for range of \(a\) [propagation failure]. Wave speed \(c\) is no longer a unique function of \(a\). [Critical intervals \([a_-(c), a_+(c)]\) overlap for different values of \(c\)]
Backward-Euler: non-uniqueness of wave speed

Regions in \((c, a)\) space where solutions exist.
Singular perturbation

For orders 2, 3, ... 6, this monotonic structure is not available.

Goal here is to fix \( a \) and look at \( cT \to 0 \), writing

\[
\Phi(\zeta) = \Phi_*(\zeta) + v(\zeta), \quad c = c_* + c'
\]

where \((c_*, \Phi_*)\) is the wave for the **spatially discrete** problem.

However the bifurcation is **singular**, in the sense that one must solve

\[
\mathcal{L}_{k,M}v = O(v^2 + M^{-1} + c'),
\]

with

\[
[\mathcal{L}_{k,M}v](\zeta) = -c_* D_{k,M}v + v(\zeta + 1) + v(\zeta - 1) - 2v(\zeta) + g'(\Phi_*(\zeta))v(\zeta).
\]

We only know that

\[
[\mathcal{L}_*v](\xi) = -c_* v'(\xi) + v(\xi + 1) + v(\xi - 1) - 2v(\xi) + g'(\Phi_*(\xi))v(\xi).
\]

is Fredholm with index zero as \( H^1 \to L^2 \) map, with \( \text{Ker} \mathcal{L}_* = \{ \Phi_* \} \). Can we lift?
Spectral convergence

• Comparison between $\mathcal{L}_{k,M}$ and $\mathcal{L}_*$ can be studied based by adapting 'spectral convergence' technique [Bates, Chen, Chmaj].

• Compares resolvents of linear operators $\mathcal{A}$ and $\mathcal{A}_M$ assuming that $\sigma(\mathcal{A}_M) \to \sigma(\mathcal{A})$ as $M \to \infty$ on compact subsets of $\mathbb{C}$.

• Step A: use weak convergence to pass to a weak limit.

• Step B: recover 'missing' information by exploiting equation.
Step A: Weak Convergence

Need to build an $H^1$-function from sequence

Here $M = \frac{3}{2}$ so $\zeta \in \frac{1}{3}\mathbb{Z}$.

Cannot directly do interpolation in a controlled fashion.
Step A: Weak Convergence

After splitting; can interpolate. Size of derivative controlled by $D_{k,M}v$. 

$v_1(\zeta)$

$v_2(\zeta)$
Step B: Missing information

- Bounded sequence of $H^1$ functions converge (after subsequence) weakly in $H^1$ and **strongly** on $L^2([a,b])$.

- Weak limit $V$ satisfies limiting problem $\mathcal{L}_* V = 0$.

- Task: rule out $V = 0$.

- Here exploit **bistable** nature of equation plus monotonic structure of discrete Laplacian

- Can show that $\mathcal{D}_{k,M} v$ can not get too big as $M \to \infty$

- This gives lower bound on $L^2([a,b])$ norm of limit $V$. 
The result

Looking for travelling wave \((c, v)\) of form

\[ \Phi(\zeta) = \Phi_*(\vartheta + \zeta) + v(\zeta) \]

to system

\[ cD_{k,M} \Phi = \Phi(\zeta + 1) + \Phi(\zeta - 1) - 2\Phi(\zeta) + g_{\text{cub}}(\Phi(\zeta); a) \]

Thm. [H., Van Vleck] Fix integer \(q_* > 1\). There exists \(M_* \gg 1\) so that for all \(M \geq M_*\) and \(M = \frac{p}{q}\) with \(q \leq q_*\) there are unique solutions \(c_M(a, \vartheta)\) and \(v_M(a, \vartheta)\).

- \(\Delta t\) can be recovered via \(M^{-1} = c\Delta t\)
- Speed \(c_M(a, \vartheta) = c_* + O(M^{-1})\)
- Periodicity \(c_M(a, \vartheta + M^{-1}) = c_M(a, \vartheta)\).
- Monotonicity \(\partial_\vartheta c_M(a, \vartheta) < 0\).

We have non-uniqueness of wave speed \(c\) as a function of \(a\) and \(a\) as a function of \(c\) provided we can show that \(\partial_\vartheta c_M(a, \vartheta) \neq 0\). But this is \(O(e^{M^{-1}})\).