Lattices, Travelling Waves, and Differential Equations with Retarded and Advanced Arguments

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Many lattice differential equations appear to admit standing or travelling wave solutions. In applications (e.g., crystal growth, nerve conduction) it is important to know which occurs. However, this is a difficult question to answer, because travelling waves on lattices are defined by Advanced-Retarded Functional Differential Equations with the propagation failure limit as the wave speed vanishes being singular, whereas standing waves are defined by difference equations.
A typical LDE has the form

\[ \dot{u}_i = g_i(\{u_j\}_{j \in \Lambda}), \quad i \in \Lambda. \]

\( \Lambda \subset \mathbb{R}^n \) is a lattice; a discrete subset of \( \mathbb{R}^n \), finite or infinite number of points, regular spatial structure (e.g. \( \mathbb{Z}^n \))

- \( u_i(t) \) for each \( i \in \Lambda \) may be scalar or vector
- Continuous in time, discrete in space
- Today will restrict attention to 1D lattices for simplicity
Travelling Pulse Model

Discrete Fitzhugh-Nagumo Equation

\[ \dot{u}_i = (u_{i+1} - 2u_i + u_{i-1}) - f(u_i) - v_i \]
\[ \dot{v}_i = b(u_i - rv_i) \]

Models a Myelinated Nerve fibre

- Lattice points \( i \) represent nodes of Ranvier; gaps in myelin sheath where nerve may be excited
- \( u_i \) represents transmembrane potential at node \( i \)
- \( v_i \) is a recovery variable (potassium current)

Normal myelinated Fibre [Experiment] [Hugh Bostock, University of London].
\begin{equation*}
\dot{u}_i = (u_{i+1} - 2u_i + u_{i-1}) - \beta f(u_i) \quad \beta > 0,
\end{equation*}

Models leading edge behaviour of pulse. Two examples:
Leading Edge Model
Discrete Nagumo Equation

\[ \dot{u}_i = (u_{i+1} - 2u_i + u_{i-1}) - \beta f(u_i) \quad \beta > 0, \]

Models leading edge behaviour of pulse. Two examples:

1. Cubic nonlinearity

\[ f(u) = u(u - a)(u - 1) \]

2. McKean’s caricature of cubic

\[ f(u) = \begin{cases} 
    u - 1, & u > a, \\
    [u - 1, u], & u = a, \\
    u, & u < a.
\end{cases} \]
Consider the PDE
\[ u_t = u_{xx} - f(u), \quad x \in \mathbb{R}, \]
with cubic nonlinearity \( f(u) = u(u - a)(u - 1) \) models leading edge behaviour of pulse in the squid giant axon.

Homogeneous steady states satisfy \( f(u) = 0 \) implies \( u = 0, u = a \) or \( u = 1 \). Natural to look for solutions
\[ \lim_{x \to -\infty} u(x, t) = 0, \lim_{x \to +\infty} u(x, t) = 1. \]
Travelling Wave ansatz:

- Let $u(x, t) = \varphi(x - ct) = \varphi(\xi)$, where $c$ is unknown wave speed

$u_t = u_{xx} - f(u)$
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• Let $u(x,t) = \varphi(x - ct) = \varphi(\xi)$, where $c$ is unknown wave speed

\[ u_t = u_{xx} - f(u) \Rightarrow -c\varphi'(\xi) = \varphi''(\xi) - f(\varphi(\xi)), \]
Travelling Wave Ansatz: 

- Let \( u(x, t) = \varphi(x - ct) = \varphi(\xi) \), where \( c \) is unknown wave speed

\[
 u_t = u_{xx} - f(u) \Rightarrow -c\varphi'(\xi) = \varphi''(\xi) - f(\varphi(\xi)),
\]

- TW ansatz reduces PDE to ODE
- \( \xi \) is time-like variable
- Boundary conditions
  \( \varphi(-\infty) = 0, \varphi(\infty) = 1 \).
- Solutions not unique (translational invariance)
Functional Differential Equation Reduction
Travelling Waves for Discrete Nagumo Equation

\[ \dot{u}_i = (u_{i+1} - 2u_i + u_{i-1}) - \beta f(u_i) \]

- Travelling Wave ansatz \( u_i(t) = \varphi(i - ct) = \varphi(\xi) \) gives

\[ -c \varphi'(\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta f(\varphi(\xi)) \]
Functional Differential Equation Reduction

Travelling Waves for Discrete Nagumo Equation

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- \( i \in \mathbb{Z} \) but \( \xi = i - ct \in \mathbb{R} \) is time-like and \( \varphi : \mathbb{R} \to \mathbb{R} \).
- \( \varphi(\xi - 1) = \text{delay}, \varphi(\xi + 1) = \text{advance} \).
- Both nonlinearities have three constant solutions \( \varphi \equiv 0, a \) and \( 1 \). Seek solutions with \( \varphi(-\infty) = 0, \varphi(\infty) = 1 \).
- Propagation Failure \( c \to 0 \) is singular limit
- TW ansatz “reduces” LDE to a mixed-type FDE !!
Another Example Of Mixed Type Functional Differential Equations

\[ m_e \ddot{e} = F_{ep} = \frac{1}{2} (F_{ep}^+ + F_{ep}^-) \]
\[ m_p \ddot{p} = F_{pe} = \frac{1}{2} (F_{pe}^+ + F_{pe}^-) \]
\[ F_{ep}^\pm (t) = -K \frac{p(t \pm \tau) - e(t)}{|p(t \pm \tau) - e(t)|^3} \]
\[ F_{pe}^\pm (t) = -K \frac{e(t \pm \tau) - p(t)}{|e(t \pm \tau) - p(t)|^3} \]
\[ |p(t \pm \tau) - e(t)| = c\tau \]
\[ |e(t \pm \tau) - p(t)| = c\tau \]

- [Wheeler Feynman 1945&1949], [Schild 1963], [Many Others...]
Nonlinear FDE BVP
Existence and Uniqueness

\[-c\varphi'(\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta \varphi(\xi)(\varphi(\xi) - a)(\varphi(\xi) - 1)\]

\[\varphi(-\infty) = 0, \quad \varphi(\infty) = 1.\]

- [ZINNER 1991]: Uniqueness and Stability of Monotonic TWs
- [ZINNER 1992]: Existence of Monotonic TWs for \(\beta\) suff small.
- Zinner’s theory covers larger class of \(f\). More recent extensions include, in particular [MALLET-PARET 1999A],[MALLET-PARET 1999B].
- When is wave travelling or standing?
- Question has practical relevance to problem of waveblock in for example MS where signals fail to propagate along a demyelinated nerve.
- Solve TW equations numerically using a mixed-type DDE collocation code written for the purpose [ABELL ET AL 2005], (built on colmod [CASH ET AL 1995]).
Nonlinear Nagumo Equation

\[ \dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta u_i (u_i - a) (u_i - 1), \quad \beta > 0 \]

\[ -c \varphi'(\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta \varphi(\xi) (\varphi(\xi) - a) (\varphi(\xi) - 1), \]

\[ \beta \text{ small} \implies c = 0 \iff a = 1/2 \]

\[ \beta \text{ large} \implies c = 0 \text{ for growing range of } a: \]

= Propagation Failure
Nonlinear Nagumo Equation

Evolution of Wave Profile for $\beta = 1$ and $\beta = 8$.

\[-c\phi'(\xi) = \phi(\xi + 1) - 2\phi(\xi) + \phi(\xi - 1) - \beta \phi(\xi)(\phi(\xi) - a)(\phi(\xi) - 1)\]

- Consider evolution of wave profile as $c \to 0$
Nonlinear Nagumo Equation

Evolution of Wave Profile for $\beta = 1$ and $\beta = 8$.

\[-c\varphi'(\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta\varphi(\xi)(\varphi(\xi) - a)(\varphi(\xi) - 1)\]

- Consider evolution of wave profile as $c \to 0$
- Step profile explains this
- TW equation becomes a difference equation
Propagation Failure & Standing Waves

$c = 0$: A difference Equation

\[ 0 = -c \varphi'(\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta f(\varphi(\xi)) \]

\[ 0 = \dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta f(u_i) \]

McKean’s caricature of cubic

\[ f(\varphi) = \begin{cases} 
\beta(\varphi - 1), & \varphi > a, \\
\beta[\varphi - 1, \varphi], & \varphi = a, \\
\beta \varphi, & \varphi < a. 
\end{cases} \]

where $H$ is heaviside function.
Propagation Failure & Standing Waves

\( c = 0: \) A difference Equation

\[
0 = u_{i+1} - 2u_i + u_{i-1} - \begin{cases} 
\beta(u_i - 1), & u_i > a, \\
\beta u_i, & u_i < a.
\end{cases}
\]

Consider monotonic solution s.t.

\[
\begin{cases}
    u_i < a, & i < 0, \\
    u_i > a, & i \geq 0.
\end{cases}
\]

\[
x^2 - (2 + \beta)x + 1 = 0 \implies x = 1 + \frac{\beta}{2} + \frac{1}{2} \sqrt{4\beta + \beta^2}
\]

Solution:

\[
u_i = \frac{x^{i+1}}{x + 1}, \quad i \leq 0, \quad u_i = 1 - \frac{1}{x^i(x + 1)}, \quad i \geq -1
\]

valid for

\[
u_{-1} = \frac{1}{1 + x} < a < 1 - \frac{1}{1 + x} = u_0
\]
Propagation Failure & Standing Waves

$c = 0$: A difference Equation

$$0 = -c \varphi' (\xi) = \varphi(\xi + 1) - 2\varphi(\xi) + \varphi(\xi - 1) - \beta f(\varphi(\xi))$$

$$0 = \dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta f(u_i)$$
Propagation Failure

McKean and Cubic Nonlinearities

- McKean: \( \forall \beta > 0 \ \exists \epsilon > 0 : c = 0 \) for \( a \in [1/2 - \epsilon, 1/2 + \epsilon] \)
- Cubic: \( \beta \gg 0 \) = ditto
- Cubic: \( \beta \approx 0 \): \( \epsilon = 0 \) or \( O(e^{-1/\beta}) \) ???
- Why not always steps in wave profile as \( c \to 0 \) ???
Discrete Nagumo Standing Waves
As Hamiltonian Discretizations

\[
0 = \dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta f(u_i)
\]

Let \( h = \sqrt{\beta} \) and \( v_{j+1} = (u_{j+1} - u_j)/h \). Then

\[
\begin{align*}
  u_{j+1} &= u_j + hv_{j+1}, \\
  v_{j+1} &= v_j + hf(u_j)
\end{align*}
\]

Standing wave of LDE is a heteroclinic connection of this mapping between
\((0, 0)\) and \((1, 0)\) in \((u, v)\)-plane.
Discrete Nagumo Standing Waves 
As Hamiltonian Discretizations

\[ 0 = \dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta f(u_i) \]

Let \( h = \sqrt{\beta} \) and \( v_{j+1} = (u_{j+1} - u_j)/h \). Then

\[ u_{j+1} = u_j + hv_{j+1}, \quad v_{j+1} = v_j + hf(u_j) \]

Which is **symplectic Euler** applied to the Hamiltonian system

\[ \dot{v} = -H_u(u, v), \quad \dot{u} = v = H_v(u, v) \]

where

\[ H(u, v) = \frac{v^2}{2} - W(u), \quad W'(u) = f(u) \]

For cubic \( f \), \( W \) is a quartic double-well potential
The standing wave is a heteroclinic connection between \((u, v) = (0, 0)\) and \((1, 0)\). But we can do better...
Discrete Nagumo Standing Waves
Stormer-Verlet Discretization

\[ u_{i+1} - 2u_i + u_{i-1} = h^2 f(u_i) \]

Let \( v_j = \frac{1}{2h}(u_{j+1} - u_{j-1}) \) then

\[ u_{j+1} = u_j + hv_j + \frac{1}{2}h^2 f(u_j), \quad v_{j+1} = v_j + \frac{h}{2} f(u_j) + \frac{h}{2} f(u_{j+1}), \]

or

\[ v_{j+\frac{1}{2}} = v_j + \frac{h}{2} f(u_j), \]
\[ u_{j+1} = u_j + hv_{j+\frac{1}{2}}, \]
\[ v_{j+1} = v_{j+\frac{1}{2}} + \frac{h}{2} f(u_{j+1}). \]

Which is Stormer-Verlet method for \( \dot{u} = v, \dot{v} = f(u) \).
Discrete Nagumo Standing Waves
Stormer-Verlet Discretization

Standing wave of LDE is a heteroclinic connection of Stormer-Verlet method

\[ u_{j+1} = u_j + hv_j + \frac{1}{2} h^2 f(u_j), \quad v_{j+1} = v_j + \frac{h}{2} f(u_j) + \frac{h}{2} f(u_{j+1}), \]

between \((0, 0)\) and \((1, 0)\) in \((u, v)\)-plane, again applied to the Hamiltonian system

\[
\dot{v} = -H_u(u, v), \quad \dot{u} = v = H_v(u, v)
\]

where

\[ H(u, v) = \frac{v^2}{2} - W(u), \quad W'(u) = f(u) \]

Stormer-Verlet as well as being symplectic and explicit is also second order and symmetric.
Recall TW for \( u_t = u_{xx} - f(u) \) given by \( u(x, t) = \varphi(x - ct) = \varphi(\xi) \) satisfying ODE
\[
-c\varphi'(\xi) = \varphi''(\xi) - f(\varphi(\xi)).
\]
Note standing wave \( c = 0 \) is not a singular limit.

Nagumo PDE
Standing Wave
\[ \varphi''(\xi) = f(\varphi(\xi)), \]

or

\[ \varphi'(\xi) = \psi(\xi), \quad \psi'(\xi) = f(\varphi(\xi)), \]

which is Hamiltonian System

\[ \psi' = -H_{\varphi}(\varphi, \psi), \quad \varphi' = \psi = H_{\psi}(\varphi, \psi) \]

where

\[ H(\varphi, \psi) = \frac{\psi^2}{2} - W(\varphi), \quad W_{\varphi}(\varphi) = f(\varphi) \]

• Thus for all \( \beta > 0 \) discrete Nagumo Standing Wave problem corresponds to a Stormer-Verlet discretization with \( h = \sqrt{\beta} \) of continuous Nagumo Standing Wave Problem
Nagumo PDE
Standing Wave

\[ \psi' = -H_\varphi(\varphi, \psi, a), \quad \varphi' = H_\psi(\varphi, \psi, a) \]

\[ H(\varphi, \psi, a) = \frac{\psi^2}{2} - W(\varphi, a), \quad W_\varphi(\varphi, a) = f(\varphi, a) \]
Nagumo PDE
Standing Wave

\[ \psi' = -H_\varphi(\varphi, \psi, a), \quad \varphi' = H_\psi(\varphi, \psi, a) \]

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\[ \psi' = -H_\varphi(\varphi, \psi, a), \quad \varphi' = H_\psi(\varphi, \psi, a) \]

\[ H(\varphi, \psi, a) = \frac{\psi^2}{2} - W(\varphi, a), \quad W_\varphi(\varphi, a) = f(\varphi, a) \]

- For Nagumo PDE \( c = 0 \) iff \( a = 1/2 \)
- Then unstable manifold of \( (0, 0) \) and stable manifold of \( (1, 0) \) intersect tangentially
\[ u_{j+1} = u_j + h v_j + \frac{1}{2} h^2 f(u_j), \quad v_{j+1} = v_j + \frac{h}{2} f(u_j) + \frac{h}{2} f(u_{j+1}) , \]

\[ \beta = 8 \]
\[ h = \sqrt{\beta} \]
\[ a = 0.5 \]

Manifolds intersect transversally
Discrete Nagumo
Standing Wave

\[ u_{j+1} = u_j + hv_j + \frac{1}{2} h^2 f(u_j), \quad v_{j+1} = v_j + \frac{h}{2} f(u_j) + \frac{h}{2} f(u_{j+1}), \]

\[ \beta = 8 \]
\[ h = \sqrt{\beta} \]
\[ a = 0.5265 \]

Connections persist for \( a \neq 1/2 \)
Discrete Nagumo Standing Wave

\[ u_{j+1} = u_j + hv_j + \frac{1}{2} h^2 f(u_j), \quad v_{j+1} = v_j + \frac{h}{2} f(u_j) + \frac{h}{2} f(u_{j+1}), \]

\[ h^2 = \beta = 8 \]
\[ h = \sqrt{\beta} \]
\[ a = 0.55 \]
Discrete Nagumo
Standing/Travelling Wave Boundary
Discrete Nagumo
Standing/Travelling Wave Boundary

\[ h^2 = \beta = 8 \quad a = 0.5265 \]
• Expect heteroclinic connection for discretization for nearby parameter value [BEYN, 1990], [DOEDEL & FRIEDMAN, 1990]

• In general stable-unstable manifold intersection for discrete map generally transversal; so heteroclinic orbit will persist over (exponentially) small parameter range [FIEDLER & SCHEURLE, 1996]

• Manifolds 'touch' at boundary of interval of propagation failure

• Generically should expect propagation failure for cubic for $\beta$ small

• Missing steps as $c \rightarrow 0$ in numerical computations for $\beta \approx 0$, are result of modified equations argument. Computed wave form is spurious, but is "exact" solution for perturbed continuous problem, and has exponentially small residual for stated problem
Conclusions

- Advanced-Retarded FDE theory is incomplete
- Good numerics are needed to inform analysis
- Analysis is needed to inform numerics
- Can exploit discrete dynamical systems & symplectic method theory
- And difference equations are just numerical methods in disguise!