Theory and Numerics of Solitary Waves

- Numerical iterative methods for computing solitary waves -

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Problem Setup

Consider

$$y_t + \mathcal{N}(y) = 0 \text{ on } \Omega \subset \mathbb{R}^d \qquad \text{plus BC on} \quad \partial\Omega$$

$\mathcal{N} \dots$ nonlinear differential (in space) operator, $y \in \mathbb{C}^n, t \geq 0$.

Examples:

$$y_t + yy_x + y_{xxx} = 0, \quad |y| \to 0 \text{ as } |x| \to \infty \qquad (KdV) \tag{1}$$

$$iy_t + \triangle y + |y|^{p-1}y = 0, \quad |y| \to 0 \text{ as } |x| \to \infty \qquad (NLS) \tag{2}$$

(I) Assume **stationary (or travelling wave) ansatz**

(a) $y(x,t) = u(x - vt; v) = u(\zeta; v), \qquad \zeta := x - vt, v \in \mathbb{R}^d$ e.g. for (1)

(b) $y(x,t) = e^{-i\omega t}u(x;\omega),\ \omega \in \mathbb{R}$ (or $y = e^{-i\omega(v)t}u(\zeta;\omega,v)$) e.g. for (2)

(c) ...

so that the problem for u becomes $t-$independent. For $d = 1$ the $u-$equation can be sometimes integrated exactly or shooting methods can be applicable.

Problem Setup

To avoid writing gradients and dot products let's restrict to $d = 1$, i.e. $x \in \mathbb{R}$

$$y_t + \mathcal{N}(y) = 0 \text{ on } \Omega \subset \mathbb{R} \qquad \text{plus BC on} \quad \partial\Omega$$

(a) gives

$$-vu_\zeta + \mathcal{N}(u) = 0 \quad \text{plus BC.}$$

If $\mathcal{N}(y) = \tilde{\mathcal{N}}(|y|)y$, then (b) gives

$$-i\omega u + \tilde{\mathcal{N}}(|u|)u = 0 \quad \text{plus BC.}$$

(II) spatial discretization: m spatial grid points. Discretization of u denoted as $\vec{u}$

$$v\vec{u}_\zeta + N(\vec{u}) = 0 \text{ for (a)} \quad N \text{ discretization of } -\mathcal{N} \text{ (plus BC)} \quad (3)$$

$$\omega\vec{u} + \tilde{N}((|u_1|, \dots |u_m|)^T)\vec{u} = 0 \text{ for (b)} \quad \tilde{N} \text{ discretization of } i\tilde{\mathcal{N}} \text{ (plus BC)} \quad (4)$$

(3), (4) are $\begin{cases} \text{systems of nonlin. algebraic equations} & \text{if } \omega \text{ or } v \text{ fixed} \\ \text{nonlin. eigenvalue problems} & \text{if } \omega \text{ or } v \text{ not known} \end{cases}$

Problem Setup

Note: Solitary waves with exponentially decaying tails must have ω outside the continuous spectrum of the linear differential operator, i.e.

$$\omega \in \mathbb{R} \setminus \sigma_c(i\mathcal{L}), \qquad \mathcal{L} \ldots \text{linearization of } \mathcal{N} \text{ about } u = 0$$

This is because if $\omega \in \sigma_c(i\mathcal{L})$, then $\omega y + i\mathcal{L}y = 0$ has nondecaying solutions y. These linear solutions would be excited in the tails of the assumed solitary wave where it is small and behaves linearly. Thus the exponential decay is contradicted.

Example: stationary solitary waves to the 1−D NLS

$$iy_t + y_{xx} + |y|^2 y = 0, \quad |y| \to 0 \text{ as } |x| \to \infty$$

Ansatz: $y = e^{-i\omega t} u(x;\omega)$

$$\omega u + u_{xx} + |u|^2 u = 0$$

After discretization on a sufficiently large interval impose zero Dirichlet BC's (other BC's possible)

$$(\omega I + D)\vec{u} + \text{diag}\left((|u_1|^2, |u_2|^2, \ldots, |u_m|^2)^T\right)\vec{u} = 0$$

For a second order finite difference discretization $D = \frac{1}{dx^2}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}$

Newton's iteration

Assume ω or v fixed. Let $\vec{F}(\vec{u}) := v\vec{u} + N(\vec{u})$ for (a)
and $\vec{F}(\vec{u}) := \omega\vec{u} + \tilde{N}((|u_1|, \ldots |u_m|)^T)\vec{u}$ for (b).

Need to solve $\boxed{\vec{F}(\vec{u}) = 0}$.

Newton's iteration

$$\begin{aligned}
&\vec{u}^{(0)} \text{ given}, \; n = 0\\
&\text{while } \|\vec{r}\| > \text{ tol.}\\
&\quad \vec{u}^{(n+1)} = \vec{u}^{(n)} - {J^{(n)}}^{-1}\vec{F}(\vec{u}^{(n)}), \quad J^{(n)} = \vec{F}'(\vec{u}^{(n)})\\
&\quad \vec{r} = \vec{F}(\vec{u}^{(n+1)}), \; n = n+1\\
&\text{end}
\end{aligned}$$

Theorem (see C.T. Kelly, Iterative Methods for Lin. and Nonlin. Eqs., 1995)

$$\|\vec{u}^{(n+1)} - \vec{u}\| \le c\|\vec{u}^{(n)} - \vec{u}\|^2, c = c(\vec{u}; \vec{F})$$

if $\vec{F}$ is Lipschitz, $\vec{F}'(\vec{u})$ nonsingular and $\vec{u}^{(0)}$ sufficiently close to $\vec{u}$.

Newton's iteration

- fast (quadratic) convergence but only locally $\Rightarrow$ need for a good initial guess $\vec{u}^{(0)}$
- if $J^{(n)}$ is sparse, use a sparse solver for ${J^{(n)}}^{-1}\vec{F}(\vec{u}^{(n)})$
- instead of testing $\|\vec{r}\|$ we can test $\|s\|, s := \vec{u}^{(n+1)} - \vec{u^{(n)}} = -{J^{(n)}}^{-1}\vec{F}(\vec{u}^{(n)})$ because

$$\|\vec{u}^{(n)} - \vec{u}\| = \|s\| + \mathcal{O}(\|\vec{u}^{(n)} - \vec{u}\|^2)$$

This is proved as follows

$$c\|\vec{u}^{(n)} - \vec{u}\|^2 \geq \|\vec{u}^{(n+1)} - \vec{u}\| = \|\vec{u}^{(n)} - \vec{u} - {J^{(n)}}^{-1}\vec{F}(\vec{u}^{(n)})\| \geq \|\vec{u}^{(n)} - \vec{u}\| - \|s\|$$

$$\|\vec{u}^{(n)} - \vec{u}\| \leq \|s\| + c\|\vec{u}^{(n)} - \vec{u}\|^2$$

And also

$$\|\vec{u}^{(n)} - \vec{u}\| = \|\vec{u}^{(n)} - \vec{u}^{(n+1)} + \vec{u}^{(n+1)} - \vec{u}\| \geq \|s\| - \|\vec{u}^{(n+1)} - \vec{u}\| \geq \|s\| - c\|\vec{u}^{(n)} - \vec{u}\|^2$$

Hence

$$\|s\| - c\|\vec{u}^{(n)} - \vec{u}\|^2 \leq \|\vec{u}^{(n)} - \vec{u}\| \leq \|s\| + c\|\vec{u}^{(n)} - \vec{u}\|^2.$$

Self consistency iteration

Let's restrict to $iy_t + \mathcal{L}y + \tilde{\mathcal{N}}(|y|)y = 0, \mathcal{L}$ self adjoint and $\tilde{\mathcal{N}}$ a function with solutions $y = e^{-i\omega t}u(x)$ (e.g. cubic NLS $\mathcal{L} = \triangle,\ \tilde{\mathcal{N}}(|y|) = |y|^2$)
Self consistency iteration tries to find both ω and u.

Remark: (ω, u) is an eigenpair of the **linear** eigenvalue problem

$$\lambda\phi + (\mathcal{L} + \tilde{\mathcal{N}}(|u|))\phi = 0.$$

Denote: $L, \tilde{N}$ discretizations of $\mathcal{L}, \tilde{\mathcal{N}}$ (with the BC)

self consistency iteration

choose: $\vec{u}^{(0)}$, L^2 norm ρ (or maximum amplitude) for u
while $\|\vec{r}\| >$ tol.

$\lambda\phi + (L + \tilde{N}^{(n)})\phi = 0$ (get m eigenpairs (λ_j, ϕ_j))

$(\omega^{(n+1)}, \vec{u}^{(n+1)}) := (\lambda_i, \phi_i)$ for a chosen $i \in \{1, \dots, m\}$

$$\vec{u}^{(n+1)} = \frac{\vec{u}^{(n+1)}}{\|\vec{u}^{(n+1)}\|}\rho \qquad \text{(scale the eigenvector)}$$

$\vec{r} = (\omega + L + \tilde{N}^{(n+1)})\vec{u}^{(n+1)},\ n = n + 1$

end

Self consistency iteration

Problem: choice of i
Which linear eigenpair do we choose as the update?

Easy case:

when $\lambda\phi + (L + \tilde{N}^{(n)})\phi = 0$ is a Sturm- Liouville problem and we are looking for u with no zeros.

$\Rightarrow$ choose i corresponding to the smallest eigenvalue

General case:

- choose i s.t. $\|\frac{\phi_i}{\|\phi_i\|}\rho - \vec{u}^{(n)}\| = \min_{i\in\{1,\ldots,m\}}$
- may break down in case of multiple eigenvalues (proper BC often avoid it)
- useful information: range of ω for solitary wave existence

Analogy: travelling waves $y = u(x - vt; v) =: u(\zeta; v)$ for KdV satisfy

$$-vu_\zeta + uu_\zeta + u_{\zeta\zeta\zeta} = 0, u, u_\zeta \to 0 \text{ as } |x| \to 0$$

After one integration $\int_{-\infty}^{x}$ obtain an eigenvalue problem

$$-vu + \frac{1}{2}u^2 + u_{\zeta\zeta} = 0, u \to 0 \text{ as } |x| \to 0$$

Apply self consistency iteration to (v, u).

Petviashvili iteration (spectral renormalization method)

Let's restrict to $iy_t + \mathcal{L}y + |y|^{p-1}y = 0,\ p > 1, y \in \mathbb{C}, \mathcal{L}$ linear, with solutions $y = e^{-i\omega t}u(x), \omega \in \mathbb{R}$.
u satisfies

$$\omega u + \mathcal{L}u + |u|^{p-1}u = 0$$

After Fourier transform $\mathcal{F}(u)(k) = \hat{u}(k) = \int_{\mathbb{R}} u(x)e^{-ikx}dx$ (for const. coeff. $\mathcal{L}$)

$$\omega\hat{u} + \hat{\mathcal{L}}\hat{u} + \mathcal{F}(|u|^{p-1}u) = 0$$

Iteration scheme idea

$$\hat{u}^{(n+1)}(k) = \frac{-\mathcal{F}(|u^{(n)}|^{p-1}u^{(n)})(k)}{\omega + \hat{\mathcal{L}}(k)} \tag{5}$$

(5) usually diverges!
Explanation: if at some n we have $u^{(n)} = Cu, C \in \mathbb{C}$, then

$$\hat{u}^{(n+1)}(k) = |C|^{p-1}C\frac{-\mathcal{F}(|u|^{p-1}u)(k)}{\omega + \hat{\mathcal{L}}(k)} = |C|^{p-1}C\hat{u}(k)$$

$|C| > 1 \Rightarrow\ \|u^{(n)}\|_{L^2} \to \infty$ as $n \to \infty$
$|C| < 1 \Rightarrow\ \|u^{(n)}\|_{L^2} \to 0$ as $n \to \infty$

Petviashvili iteration

We need to prevent $\|\hat{u}^{(n)}\|_{L^2}$ from going to 0 or ∞!

Note that u satisfies $$\|\hat{u}\|_2^2 = \int_{\mathbb{R}} \frac{-\mathcal{F}(|u|^{p-1}u)(k)\hat{u}^*(k)}{\omega + \hat{\mathcal{L}}(k)} dk \qquad (6)$$

but $u^{(n)}$ does not.
Define $u^{(n+1/2)} := C_n u^{(n)}$ s.t. $u^{(n+1/2)}$ satisfies (6).

$$|C_n|^2 \underbrace{\|\hat{u}^{(n)}\|_2^2}_{=:\,\alpha_n} = \int \frac{\mathcal{F}(|C_n u^{(n)}|^{p-1} C_n u^{(n)}) C_n^* \widehat{u^{(n)}}^*}{-(\omega + \hat{\mathcal{L}})} = |C_n|^{p+1} \underbrace{\int \frac{\mathcal{F}(|u^{(n)}|^{p-1} u^{(n)}) \widehat{u^{(n)}}^*}{-(\omega + \hat{\mathcal{L}})}}_{=:\,\beta_n}$$

$$C_n = (\alpha_n/\beta_n)^{1/(p-1)}$$

Now apply the iteration step (5) to $u^{(n+1/2)}$

$$\hat{u}^{(n+1)}(k) = \frac{-\mathcal{F}(|u^{(n+1/2)}|^{p-1} u^{(n+1/2)})(k)}{\omega + \hat{\mathcal{L}}(k)} = -\left(\frac{\alpha_n}{\beta_n}\right)^{\frac{p}{p-1}} \frac{\mathcal{F}(|u^{(n)}|^{p-1} u^{(n)})(k)}{\omega + \hat{\mathcal{L}}(k)}$$

Petviashvili iteration

Generalization: $iy_t + \mathcal{L}y + \tilde{\mathcal{N}}(|y|)y = 0$
Now C_n satisfies

$$|C_n|^2 \int_{\mathbb{R}} |\hat{u}^{(n)}|^2 dk = \int_{\mathbb{R}} \frac{-\mathcal{F}(\tilde{\mathcal{N}}(|C_n u^{(n)}|)C_n u^{(n)})C_n^* \widehat{u^{(n)}}^*}{\omega + \hat{\mathcal{L}}(k)} dk$$

$$\int_{\mathbb{R}} |\hat{u}^{(n)}|^2 dk = \int_{\mathbb{R}} \frac{-\mathcal{F}(\tilde{\mathcal{N}}(|C_n u^{(n)}|)u^{(n)})\widehat{u^{(n)}}^*}{\omega + \hat{\mathcal{L}}(k)} dk$$

which may have to be solved numerically (e.g. Newton) for C_n.

Analogy: KdV $y_t + yy_x + y_{xxx} = 0, y = u(x - vt; v) =: u(\zeta; v)$ with zero asymptotic BC at $\pm\infty$

$$-vu_\zeta + uu_\zeta + u_{\zeta\zeta\zeta} = 0$$

After one integration

$$-vu + u_{\zeta\zeta} + u^2 = 0$$

Apply Petviashvili iteration replacing

$$\omega \rightsquigarrow -v, \ \tilde{\mathcal{N}}(|u|)u \rightsquigarrow u^2, \ L = \partial_\zeta^2$$