Petviashvili type methods for traveling wave computations: I. Analysis of convergence

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Abstract

In this paper a family of fixed point algorithms for the numerical resolution of some systems of nonlinear equations is designed and analyzed. The family introduced here generalizes the Petviashvili method and can be applied to the numerical generation of traveling waves in some nonlinear dispersive systems. Conditions for the local convergence are derived and numerical comparisons between different elements of the family are carried out.

Key words: Petviashvili type methods, traveling wave generation, iterative methods for nonlinear systems, orbital convergence

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1 Introduction

Considered here is the construction and study of fixed point algorithms for the numerical resolution of nonlinear systems of the form

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Lu = N(u), \quad u \in \mathbb{R}^m, \quad m > 1, \quad (1)

where \( L \) is a nonsingular \( m \times m \) real matrix and \( N : \mathbb{R}^m \rightarrow \mathbb{R}^m \) is an homogeneous function of the components of \( u \) with degree \( p, \, |p| > 1 \). These systems are typical in many applications, including the approximation to equilibria in mechanical systems and the numerical generation of traveling waves and ground states in nonlinear dispersive systems for water waves and nonlinear optics. (In this last context, \( m \) would represent the number of discretization points.) More generally, (1) may appear when generating relative equilibria or coherent structures, \([11]\). We denote by \( u^* \) a solution of (1), that is

\[
Lu^* = N(u^*). \quad (2)
\]

The classical fixed point algorithm for (1) has the following formulation. If \( u_0 \neq 0 \), the approximation to \( u^* \) in (2) at the \( (n+1) \)-th iteration is given by the recurrence

\[
Lu_{n+1} = N(u_n), \quad n = 0, 1, \ldots \quad (3)
\]

The method (3) is not usually convergent for this kind of problems. Note that if

\[
S = L^{-1}N'(u^*), \quad (4)
\]

stands for the iteration matrix at \( u^* \) (and where \( N'(u) \) denotes the Jacobian of \( N \) at \( u \)), then the homogeneous character of \( N \) implies that \( N'(u^*)u^* = pN(u^*) \); therefore, using (2),

\[
S(u^*)u^* = L^{-1}N'(u^*)u^* = pL^{-1}N(u^*) = pu^*.
\]

Thus, \( u^* \) is an eigenvector of \( S \) associated to an eigenvalue \( \lambda = p \) with \( |p| > 1 \).

The methods presented here generalize the so-called Petviashvili method. From a starting iteration \( u_0 \neq 0 \), the Petviashvili method generates the recurrence

\[
m(u_n) = \frac{\langle Lu_n, u_n \rangle}{\langle N(u_n), u_n \rangle}, \quad (5)
\]

\[
Lu_{n+1} = m(u_n)\gamma N(u_n), \quad n = 0, 1, \ldots \quad (6)
\]

where here and in the rest of the paper \( \langle \cdot, \cdot \rangle \) stands for the Euclidean inner product and \( \gamma \) is a free real parameter. The term (5) is called stabilizing factor
and, in the case of convergence, must tend to one. The origin of the method is in [27], focused on the search for lump solitary waves of the Kadomtsev-Petviashvili I (KPI) equation

\[(u_t + 2uu_x + u_{xxx})_x = u_{yy}, \quad t > 0, x, y \in \mathbb{R} \tag{7}\]

of the form \(u(x, y, t) = c\varphi(X, Y) = c\varphi(\sqrt{c}(x - ct), cy), c > 0\). The profile \(\varphi\) must satisfy

\[\partial_{XX} (-\varphi + \partial_{XX}\varphi) - \partial_{YY}\varphi = -\partial_{XX}\varphi^2,\]

which, in terms of the 2-D Fourier Transform,

\[\hat{\varphi}(k_x, k_y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \varphi(x, y)e^{-ik_xx}e^{-ik_yy}dxdy,\]

is converted into an algebraic system

\[\hat{\varphi}(k_x, k_y) = G(k_x, k_y)A(k_x, k_y),\]
\[G(k_x, k_y) = \frac{k_x^2}{k_x^4 + k_x^2 + k_y^2}, \quad A(k_x, k_y) = \hat{\varphi}^2(k_x, k_y) \tag{8}\]

The divergence of the classical fixed point algorithm, applied to (8) forces to consider a new iteration system, of the form

\[\hat{\varphi}(k_x, k_y) = m(\varphi)\gamma G(k_x, k_y)A(k_x, k_y),\]

where the stabilizing factor \(m(\varphi)\) is defined as

\[m(\varphi) = \frac{s_1}{s_2}, \quad s_1 = \int \int |\hat{\varphi}|^2dk_xdk_y, \quad s_2 = \int \int \frac{k_x^2}{k_x^4 + k_x^2 + k_y^2} \hat{\varphi}^2dk_xdk_y,\]

(\(\hat{\varphi}\) denotes the complex conjugate of \(\varphi\)) where \(\gamma\) is a free real parameter. In the case of (7), \(\gamma\) is taken approximately 2, [27]. On the other hand, for the exact profile \(\varphi\), \(m(\varphi) = 1\).

The Petviashvili method has become popular as a technique to generate special solutions in partial differential equations of interest in water waves and nonlinear optics. It takes part of a large family of methods designed to this goal, which includes variants of the Newton’s method, [29], modified conjugate gradient methods applied to nonlinear problems, [20], squared operator
methods, \cite{32}, imaginary-time evolution methods, \cite{31} or different variational procedures, \cite{13,4,9}. Some literature about \cite{5,6}, from the original paper, \cite{27}, is now briefly reviewed. Pelinovsky and Stepanyants, \cite{26}, analyze the continuous version of the method to approximate solitary wave profiles of the nonlinear dispersive models

\[ u_t - \mathcal{L}u_x + pu^{p-1}u_x = 0, \quad p > 1, \quad t > 0, \quad x \in \mathbb{R}, \]

where \( \mathcal{L} \) is a pseudodifferential operator with positive Fourier symbol. On the other hand, Lakoba and Yang, \cite{21,22}, introduce a generalized version of the procedure, for more general systems of the form

\[ -Mu + F(x, u) = 0, \quad u \to 0, \quad |x| \to \infty \]

where \( M \) is positive definite, self-adjoint operator and \( F \) is nonlinear (see also \cite{30}). Finally, Ablowitz and Musslimani, \cite{1}, \( \text{see also } \cite{2} \) propose an alternative of the algorithm, the spectral renormalization method, with application to generate numerically ground state profiles for systems of NLS type

\[ iU_z + \Delta U - V(x)U + f(|U|^2)U = 0. \]

Some new results contained in this paper are described below.

- Based on the philosophy the Petviashvili method was devised with, new fixed point methods are derived. They can be considered as a Petviashvili type family of methods.
- From the view point of the classical algorithm, the corresponding iteration functions are designed to filter the harmful directions of the errors leading to divergence, in such a way that convergence results are obtained under the same hypotheses as those of the Petviashvili method. Here it is worth mentioning two types of convergence. The first one has the classical sense, with the requirement (among others) of isolated fixed points. However, in traveling wave generation, it is very typical that the system of equations admits a symmetry group (usually related to translational or rotational invariance of the system). In this case, fixed points cannot be isolated and the convergence must be understood in the orbital sense, that is, for the orbits of fixed points. Convergence results for both cases will be given. This study complements some previous results of convergence presented in the literature for the Petviashvili method, \cite{26,21,22}.

The structure of the paper is as follows: in Section 2 and starting from the Petviashvili method \cite{5,6}, the new family of fixed point algorithms are constructed and analyzed. A comparison of efficiency of some of them is also
carried out. Section 3 will treat the derivation of general conditions for the local convergence of the methods. The first part of the study assumes the existence of a neighborhood where the fixed point \( u^* \) is unique. The spectral analysis of the iteration matrix (4) of the classical fixed point algorithm (or, equivalently, the pencil \( A(\lambda) = \lambda L - N'(u^*) \)) is used. The local convergence of the methods can be achieved even when (4) admits eigenvalues with modulus greater than or equals one. The results are illustrated with several numerical examples, concerning the generation of localized ground state solutions of nonlinear Schrödinger type equations with potentials. On the other hand, some other applications of the methods suggest to analyze a case where the hypothesis of local uniqueness of the fixed point does not hold, in the sense that the system (1) admits a group of symmetries, generating orbits of solutions. From the point of view of the analysis, the existence of a symmetry group in (1) is associated to the formation of the eigenvalue one in the pencil, \([\lambda]\), and leads, in a natural way, to the concept of orbital convergence. Section 3 is finished off with the corresponding results of convergence for this case and they will be illustrated by the generation of soliton solutions of the nonlinear Schrödinger equation.

The present paper is a first part of a study of the methods carried out by the same authors. It will be followed by a second part, in which some particular, relevant cases of systems (1) are emphasized and where the effect of the introduction of acceleration techniques is studied.

2 Derivation and convergence analysis of the algorithms

2.1 Derivation

The following fixed point methods for the iterative resolution of (1) are introduced. If \( u_0 \neq 0 \), the iterations \( u_n, n = 1, 2, \ldots \) are generated by a formula of the form

\[
Lu_{n+1} = s(u_n)N(u_n), \quad n = 0, 1, \ldots
\]

(9)

where \( s : \mathbb{R}^m \to \mathbb{R} \) is a \( C^1 \) function satisfying the following properties:

(P1) A set of fixed points of the iteration operator

\[
F(u) = s(u)L^{-1}N(u),
\]

(10)

coincides with a set of fixed points of (1). This means that: (a) if \( u^* \) is a solution of (1) then \( s(u^*) = 1 \); (b) inversely, if the sequence \( \{u_n\}_{n=0}^\infty \),
generated by (9), converges to some \( y \), then \( s(y) = 1 \) (and, consequently, \( y \) is a solution of (1)).

(P2) \( s \) is homogeneous with degree \( q \) such that \( |p + q| < 1 \).

Note that, in particular, the choice

\[
s(u) = \left( \frac{\langle Lu, u \rangle}{\langle N(u), u \rangle} \right)^\gamma, \quad q = \gamma(1 - p),
\]

leads to the Petviashvili method (5), (6). Then, (9) can be considered as a generalization and justifies that \( s \) will be also called a stabilizing factor. Several examples are the following:

- The term (11) can be generalized by considering any \( C^1 \) homogeneous function \( f : \mathbb{R}^m \to \mathbb{R} \) with degree greater than or equals one and taking

\[
s_f(u) = \left( \frac{\langle Lu, f(u) \rangle}{\langle N(u), f(u) \rangle} \right)^\gamma, \quad q = \gamma(1 - p), \quad |p + q| < 1.
\]

- Another alternative is the use of norms, with

\[
s_r(u) = \left( \frac{||Lu||_r}{||N(u)||_r} \right)^\gamma, \quad q = \gamma(1 - p), \quad |p + q| < 1,
\]

where if \( u = (u_1, \ldots, u_m)^T \) then \( ||u||_r = (|u_1|^r + \ldots + |u_m|^r)^{1/r}, 1 \leq r \leq +\infty \), with \( r = +\infty \) standing for the usual maximum norm. The case \( r = 1 \) was considered in [2].

2.2 First numerical experiments

Displayed here are some numerical experiments concerning the performance of the methods, according to the choice of the stabilizing factor. As an example we consider the problem of generating lump solitary waves in the 2D Benjamin equation

\[
\left( \eta_t + \alpha(\eta^2)_x - \beta \mathcal{H}(\eta_{xx}) + \delta \eta_{xxx} \right)_x - \eta_{zz} = 0,
\]

where \( \alpha, \beta, \delta \geq 0 \) and \( \mathcal{H} \) stands for the Hilbert transform with respect to \( x \):

\[
\mathcal{H}f(x) = \frac{1}{\pi} P.V. \int_{-\infty}^{\infty} \frac{f(y)}{x - y} dy.
\]
Equation (14) is analyzed in [17,18,19]. It appears as an extension of the one-dimensional equation derived by Benjamin, [5,6,7], and modeling the propagation of waves at the interface of two ideal fluids, with a bounded upper layer and the heavier one with infinite depth, and under the presence of interfacial tension. The two-dimensional version incorporates weak transverse variations. The form (14) contains particular cases, such as the Kamdotsev-Petviashvili (KP-I) equation, [15,23] \((\beta = 0, \delta > 0)\) and the two-dimensional Benjamin-Davis-Ono (BDO) equation, corresponding to \(\delta = 0, \beta > 0\), [3]. A normalized form of (14)

\[
\left( \eta_t + (\eta^2)_x - 2\Gamma \mathcal{H}(\eta_{xx}) + \eta_{xxx} \right)_x - \eta_{zz} = 0,
\]

is derived in [19] and will be adopted here. The parameter \(\Gamma \geq 0\) is related to the interfacial tension and the densities of the fluids. Finally, for localized solutions, the constraint

\[
\int_{-\infty}^{\infty} \eta(x, z, t) dx = 0,
\]

(16) (zero total mass condition) is assumed, as in the KP and BDO equations [16].

The search for lump solitary wave solutions of (15)

\[
\eta(x, z, t) = \eta(X, Z), \quad X = x - c_s t, \quad Z = z,
\]
leads to the equation

\[( -c_s \eta + \eta^2 - 2\gamma \mathcal{H}(\eta x) + \eta xx )_{xx} - \eta zz = 0, \]  

(17)

for the profile \( \eta \). In [19] it is shown that (17) admits lumps of wavepacket type, as well as lumps of KP-I type (see Figures [1](d) and [1](a) respectively). The bifurcation point corresponds to \( \Gamma = 1 \). As an alternative to the numerical procedure performed in that paper, some lumps will be here generated numerically, by using numerical continuation in \( \Gamma \) from the known lump solitary wave solution of the KP-I equation (corresponding to \( \Gamma = 0 \)), [23]. Taking
two-dimensional Fourier transform in (17) we have

\[ \left( k_x^2 \left( c_s + 2 |k_x| + k_y^2 \right) + k_y^2 \right) \tilde{\eta}(k_x, k_y) = k_x^2 \left( \bar{n}^2 \right)(k_x, k_y). \]  

(18)

The continuation algorithm until the computation of the profile at certain value \( \Gamma^* \) consists of defining an homotopic path

\[ \Gamma_0 = 0 < \Gamma_1 < \cdots < \Gamma_M = \Gamma^* < 1, \]

and solving numerically (18) with the method (9) at each \( \Gamma_j \) and initial iterate given by the last computed iterate at the previous stage \( \Gamma_{j-1} \). The procedure starts with the exact KP-I lump at \( \Gamma = \Gamma_0 = 0 \). The numerical resolution of (18) with (9) is now described. Note that (18) for \( k_x = k_y = 0 \) leaves the \((0,0)\)-Fourier component free and the value \( \tilde{\eta}(0,0) = 0 \) is set by the zero total mass condition (16). System (18) is discretized by using a Fourier collocation scheme and, with the notation of (1), the corresponding discrete system leads to a singular matrix \( L \). In order to solve this, the \((0,0)\)-Fourier component of the approximation is set to zero, then the resulting system for the rest of the Fourier components is not singular and is therefore iteratively solved with (9), [26]. The numerical results are shown in Figure 1. (They correspond to \( c_s = 1 \).) On the left, different lump profiles, associated to several values of \( \Gamma \) are displayed. On the right, the corresponding \( X- \) and \( Z- \) cross sections are represented. The convergence of the procedure is illustrated by Figure 2.
For the case $\Gamma = 0.99$, it shows the limiting behaviour of the stabilizing factor (left) and the residual errors (right)

$$RE_n = \| Lx_n - N(x_n) \|, \quad (19)$$

(where here and in the rest of the paper $\| \cdot \|$ stands for the Euclidean norm) both as functions of the number of iterations as for several choices of the stabilizing factor, from the two families (12), (13). As a representative of (12), the original Petviashvili method ($f(x) = x$) has been compared with two methods with stabilizing factors of the form (13), corresponding to $r = 1, 2$. Figure 2(a) shows that the convergence of the stabilizing factor to one is more efficient with the Petviashvili method: it provides an error with less iterations and, for a fixed number of iterations, it gives a smaller discrepancy. This is also the conclusion when analyzing Figure 2(b), concerning the behaviour of the residual error with the number of iterations. However, this better performance of the Petviashvili method in this example is not big enough to be conclusive and to rule the rest of the methods out in a general situation. We have the impression that in terms of the computational effort, the methods are more or less equivalent, with a slight superiority of (5), (6). For that reason, this will be considered as a representative of (9) for the rest of the experiments in this paper (see Section 3).

Finally, although the main goal of the example is illustrating a comparison between some methods of the family (9), it is worth mentioning that (15) is translationally invariant. Thus, the convergence must be understood in the sense analyzed in Section 3.3 (orbital convergence).

### 3 Analysis of convergence

As mentioned in the Introduction, the convergence of the methods (9) can be divided in two cases, depending on the character of $u^*$ as fixed point of (1). In what follows, the Jacobian of the iteration operator (10) at a fixed point $u^*$ satisfying (2),

$$F'(u^*) = S + u^* \left( \nabla s(u^*) \right), \quad (20)$$

will be used. (In (20), the gradient $\nabla s(u^*)$ is taken as a row vector.)
Fig. 2. Convergence results of the Petviashvili type methods (9) for (17): (a) Discrepancy between the stabilizing factor vs number of iterations (semilog scale). (b) Logarithm of the residual errors vs number of iterations. Solid line: Petviashvili method (12) with $f(x) = x$; dashed line: (13) with $r = 2$; dashed-dotted line: (13) with $r = 1$. 

(b)
3.1 Convergence (classical sense)

We first define the pencil \( A(\lambda) = \lambda L - N'(u^*) \), where \( u^* \) satisfies (2). Note that, since \( L \) is nonsingular, the zeros of \( A(\lambda) \) coincide with the spectrum of the iteration matrix \([4, \text{ see } [12], \text{ Section 4.5 and } [14], \text{ Section 7.7}]. \) (In particular, \( \lambda = p \) is a zero of \( A(\lambda) \) with \( A(p)u^* = 0 \).) We also remind that an eigenvalue \( \lambda \) of a matrix is semisimple if the corresponding geometric and algebraic multiplicity are the same; that is, if the dimension of the associated eigenspace coincides with the order of \( \lambda \) as zero of the characteristic polynomial.

**Theorem 1** Assume that

*(H1)* There exists \( R > 0 \) such that \( u^* \) in (2) is the unique fixed point of (1) in \( B(u^*, R) = \{ u \in \mathbb{R}^m / ||u - u^*|| < R \} \).

Take \( u_0 \neq 0 \) and assume the following hypotheses on the zeros of \( A(\lambda) \):

(i) \( \lambda = p \) is simple.

(ii) The rest of \( \lambda \) satisfies \( |\lambda| \leq 1 \).

(iii) If \( |\lambda| = 1 \Rightarrow \{ \lambda \text{ is semisimple} \} \) does not have component in \( \text{Ker} A(\lambda) \).

Then the method (9), with \( s \) satisfying (P1) and (P2), is locally convergent, that is, there is a neighborhood \( W \) of \( u^* \) such that if \( u_0 \in W, u_0 \neq 0 \), the sequence \( \{u_n\}_{n=0}^{\infty} \) generated by (9), converges to \( u^* \). The optimal rate of convergence is obtained with \( q = -p \).

**Proof.** The errors \( e_n = u_n - u^*, n = 0, 1, \ldots \), satisfy

\[
e_{n+1} = F'(u^*)e_n + O(||e_n||^2), \quad n = 0, 1, \ldots, \tag{21}
\]

where \( F'(u^*) \) is given by (20). According to the hypotheses (i)-(iii), \( e_n \) can be decomposed

\[
e_n = \alpha_n u^* + z_n, \quad \alpha_n \in \mathbb{R}, \quad z_n \in V, \quad S(V) \subset V, \tag{22}
\]

where \( V \) is a \( S \) invariant supplementary subspace of \( \text{span}(u^*) \). (\( V \) is the sum of the \( S \)-invariant subspaces associated to the eigenvalues of \( S \) different from \( \lambda = p \).) Substituting (22) into (21) and neglecting second order terms the system

\[
\alpha_{n+1} = \alpha_n(p + (\nabla s(u^*))u^*) + (\nabla s(u^*))z_n = \alpha_n(p + q) + (\nabla s(u^*))z_n \tag{23}
\]

\[
z_{n+1} = Sz_n, \tag{24}
\]
is obtained. (Last equality in (23) comes from (P1) and (P2), which imply that \((\nabla s(u^*)) u^* = qs(u^*) = q\).) Due to hypotheses (ii) and (iii), the sequence \(\{z_n\}_{n=0}^{\infty}\) in (24) converges to zero. This and property (P2) imply then that \(\alpha_n \to 0\) in (23), leading to local convergence. Finally, the fastest rate of convergence occurs when the factor \(p + q\) in (23) is zero.

In summary, under the hypotheses of Theorem 1, the iteration map (10) is contractive in a neighborhood of the fixed point, with the fastest rate of convergence when \(q = -p\). Condition (iii) was already obtained in [26], for the equations treated there and the continuous version of the Petviashvili method. In this sense, Theorem 1 establishes the fact that (iii) is one of the sufficient conditions for the local convergence for more general methods and in more general systems.

Assumption (iii) also suggests a dependence of the convergence on the choice of the initial iterate, not only in the sense required by the local convergence, but also because \(u_0\) must contain the correct directions. The contribution to the iteration error of the components of \(u_0\) in these ‘harmful’ eigendirections that (iii) is concerned with, can be sketched as follows. Assume for simplicity that \(S\) contains one semisimple eigenvalue \(\lambda_0\) with \(|\lambda_0| = 1\) and the rest of the spectrum (except \(\lambda = p\)) is below one in modulus. In (22), we can decompose the term \(z_n\) in the form \(z_n = v_n + w_n\) with \(v_n \in \text{Ker}(\lambda_0 I - S), w_n \in V \setminus \text{Ker}(\lambda_0 I - S)\). (Thus, \(v_n\) can be written as a linear combination of a basis of \(\text{Ker}(\lambda_0 I - S)\), with the coordinates depending on \(n\).) Now, (23) and (24) can be written as

\[
\begin{align*}
\alpha_{n+1} &= \alpha_n (p + q) + (\nabla s(u^*)) v_n + (\nabla s(u^*)) w_n, \\
v_{n+1} &= S v_n = \lambda_0 v_n, \\
w_{n+1} &= S w_n.
\end{align*}
\]

Therefore, due to (27) and the previous assumptions on the spectrum of \(S\), \(w_n\) goes to zero, while (26) implies \(v_n = \lambda_0^n v_0\), \(n = 0, 1, \ldots\), being \(v_0\) the component of \(e_0\) in \(\text{Ker}(\lambda_0 I - S)\) (which is to say the component of \(u_0\) in \(\text{Ker}(\lambda_0 I - S)\)). Then (25) becomes

\[
\alpha_{n+1} = \alpha_n (p + q) + \lambda_0^n (\nabla s(u^*)) v_0 + (\nabla s(u^*)) w_n.
\]

Thus, in general, \(\alpha_n\) would be \(O(||v_0||)\) as \(n \to \infty\). As proved by Theorem 1 if \(v_0 = 0\) (condition (iii)) and using (P2), then \(\alpha_n\) tends to zero as \(n \to \infty\). The previous arguments also say that the errors would behave as the size of the component \(v_0\).

The comparison between the matrices \(S\) and \(F'(u^*)\) reveals that the stabilizing factor acts like a filter for the harmful direction of the error that leads to
the nonconvergence of the classical fixed-point algorithm in this case. The spectrum of $F'(x^\ast)$ differs from that of $S$ in the dominant eigenvalue $p$, which is transformed to some less than one (or, eventually, to zero eigenvalue if the optimal case is taken), leading to convergence if the rest of the spectrum of $S$, with probably the help of the initial iteration, behaves in the way described in Theorem 1 (see the numerical experiments in sections 3.2 and 3.4).

3.2 Some examples

As a first example, the application of the Petviashvili method to generate localized ground state solutions of the nonlinear Schrödinger (NLS) model

$$iu_t + \partial_{xx}u + V(x)u - |u|^2u = 0,$$  

(28)

with a potential $V(x)$ is considered. A ground state solution has the form $u(x, t) = e^{i\mu t}U(x)$, where $\mu \in \mathbb{R}$ and the profile $U(x)$ is assumed to be real and localized ($U \to 0$, $|x| \to \infty$) and then must satisfy

$$U''(x) + V(x)U(x) - \mu U(x) - U^3(x) = 0.$$  

(29)

The Petviashvili method (as a representative of the family \cite{9}, see Section 2.2) can be applied to a discretization of (29). One way to treat numerically the problem is approximating (29) on a sufficiently long interval $(-l, l)$ and then discretizing the corresponding system for the profile. As an illustration, the discretization based on a Fourier collocation method for the periodic problem is taken, in such a way that the corresponding discrete equations have the form (1) with

$$L = D^2 + \text{diag}(V) - \mu I, \quad N(U_h) = -U_h^3,$$

where $D$ is the pseudospectral differentiation matrix, (see \cite{8}, chapter 6 and \cite{10}, chapter 2), $\text{diag}(V)$ is the diagonal matrix with elements $V_j = V(x_j)$, $x_j = -l + jh, j = 0, \ldots, m - 1$, $I$ is the $m \times m$ identity matrix and the dot in the nonlinearity $N$ stands for the Hadamard product from the approximation $U_h \in \mathbb{R}^m$ to the exact values of the profile at the grid points $x_j$.

The ground state generation of (28) is illustrated with two potentials (see \cite{21,30} and references therein for applications). The first one is $V(x) = \text{sech}^2(x)$. For $\mu = 1.3$ and a Gaussian profile as initial iteration, the Petviashvili method has been run. Table 1 (first column) shows the six largest magnitude eigenvalues of the approximated iteration matrix at $u^* = U_f$, where $U_f$ is the last computed iterate (an analytical expression for the ground state profile is
The dominant eigenvalue $p = 3$ (corresponding to the degree of homogeneity for this case) is observed, with the rest below one. The effect of the method is observed in the second column of Table 1 that displays the dominant eigenvalues of the Jacobian (20). The magnitude of the eigenvalues is less than one, guaranteeing the convergence of the method, which is illustrated in Figure 3 (a). This shows the logarithm of the residual error (19) as function of the number of iterations. In approximately 25 iterations, a residual error of about $1.5 \times 10^{-12}$ is obtained. The ground state profile is shown in Figure 3 (b). The convergence of the stabilizing factor to one has also been checked, with a final discrepancy, in 25 iterations, of about $3 \times 10^{-14}$.

As a second example, we consider (28) with a double-well potential $V(x) = -6(\text{sech}^2(x - 1) + \text{sech}^2(x + 1))$. As indicated in [21], the Petviashvili method fails in the search for an anti-symmetric solution of (29) (see the profile in Figure 4, obtained for $\mu = 1.43$ with the AITEM method, [31]). This case of divergence can be justified using the previous results. For $\mu = 1.43$, Table 1 (third column) shows the six largest magnitude eigenvalues of the iteration matrix evaluated at the profile obtained with the AITEM method. Besides the eigenvalue $\lambda = 3$, associated to the degree of homogeneity of the nonlinear part, Table 1 reveals the existence of other eigenvalues with magnitude above one. This divergence is also confirmed by the eigenvalues of the Jacobian (20), shown in the fourth column of Table 1.

| $V(x) = \text{sech}^2(x)$ | $V(x) = -6(\text{sech}^2(x - 1) + \text{sech}^2(x + 1))$ |
|---------------------------|----------------------------------|
| $\mu = 1.3$               | $\mu = 1.43$                     |
| eigs $S$                  | eigs $(F'(u^*))$                  |
| 2.9999E+00                | 8.0032E+00                       |
| 7.0640E-01                | -5.6760E+00                      |
| 3.2731E-01                | 2.9999E+00                       |
| 1.9060E-01                | -1.5841E+00                      |
| 1.2518E-01                | 1.1350E+00                       |
| 8.8644E-02                | -9.7207E-01                      |
|                          |                                  |

Table 1
Ground state generation for (28) with $V(x) = \text{sech}^2(x), \mu = 1.3$ and $V(x) = -6(\text{sech}^2(x - 1) + \text{sech}^2(x + 1)), \mu = 1.43$. Six largest magnitude eigenvalues of the approximate iteration matrix (4) and of the Jacobian (20). Both are evaluated at the last computed iterate $U_f$ of the Petviashvili method for (29) and AITEM for (29), respectively.
3.3 Systems with symmetries. Orbital convergence

In many situations, the system (1) admits symmetries, \[25,24\]. This means that there is an \(\nu\)-parameter group of transformations \((\nu \geq 1)\)

\[G = \{G_\alpha : \mathbb{R}^m \to \mathbb{R}^m, \alpha = (\alpha_1, \ldots, \alpha_\nu) \in \mathbb{R}^\nu\},\]  
(30)

with the property of transforming solutions of (1) into other solutions:

\[Lu^* = N(u^*) \Rightarrow L(G_\alpha u^*) = N(G_\alpha u^*), \quad \alpha \in \mathbb{R}^\nu.\]  
(31)

For simplicity, we assume that the transformations \(G_\alpha\) in (30) are smooth and \(G\) is Abelian. (In traveling wave generation, typical examples are, as mentioned before, translations and phase rotations, see Section 3.4). The existence of a symmetry group for (1) has several consequences. We emphasize two of them:

- The group (30) defines orbits of solutions of (1):

\[\mathcal{G}(u^*) = \{G_\alpha u^* : \alpha \in \mathbb{R}^\nu\}.\]

The space of solutions of (1) is partitioned into these orbits, in such a way
that assumption (H1) in Theorem 1 does not hold in this case: a fixed point \( u^* \) cannot be isolated and the concept of convergence for the iterative methods must be redefined. Under these conditions, it is said that the iteration (9) is orbitally convergent to \( u^* \) if \( u_n \) converges to \( G_\alpha u^* \) for some \( \alpha \in \mathbb{R}^\nu \).

- The pencil \( A(\lambda) \) admits \( \lambda = 1 \) as eigenvalue, since differentiation with respect to \( \alpha \) in (31) implies

\[
(L - N'(u^*)) \frac{\partial}{\partial \alpha_j} |_{\alpha=0} G_\alpha(u^*) = 0, \quad j = 1, \ldots, \nu,
\]

and the infinitesimal generators of the group, 25

\[
u_j(u) = \frac{\partial}{\partial \alpha_j} |_{\alpha=0} G_\alpha(u), \quad j = 1, \ldots, \nu,
\]

(32)
evaluated at \( u = u^* \), are associated eigenvectors.
The convergence result in Theorem 1 can be adapted to this case as follows. First, hypothesis (H1) is substituted by

\[(H1)' \ G \text{ is a symmetry group of (1) with } \dim \ker A = \nu.\]

As far as the spectrum of \(A(\lambda)\) is concerned, we still assume (i) and (ii) of Theorem 1 while the third condition is now

(iii) If \(|\lambda| = 1 \Rightarrow \{ \lambda \text{ is semisimple} \} \lambda \neq 1 \Rightarrow u_0 \text{ does not have component in } \ker A(\lambda)\)

In this case the convergence is orbital, in the sense above defined. Note that now the errors \(e_n, n = 0, 1, \ldots\), can be decomposed in the form (cf. (22))

\[e_n = \alpha_n u^* + \sum_{k=1}^{\nu} \beta_{n,k} v_k(u^*) + z_n, \quad \alpha_n, \beta_{n,k} \in \mathbb{R}, k = 1, \ldots, \nu, \quad z_n \in V;\]

where \(\{v_k(u^*)\}_{k=1}^{\nu}\) is the basis (32) of \(\ker A(1)\) and now \(V\) is the (unique) supplementary \((m - \nu - 1)\) dimensional space of \(\text{span}(u^*) + \ker A(1)\) with \(S(V) \subset V\). Now, the sequences \(\alpha_n, \beta_{n,k}, \alpha_j \in \mathbb{R}, j = 1, \ldots, \nu\) and \(z_n\) satisfy

\[
\begin{align*}
\alpha_{n+1} &= \alpha_n (p + q) + \sum_{k=1}^{\nu} \beta_{n,k} (\nabla s(u^*)) v_k(u^*) + (\nabla s(u^*)) z_n, \\
z_{n+1} &= S z_n, \\
\beta_{n+1,k} &= \beta_{n,k}, \quad k = 1, \ldots, \nu.
\end{align*}
\]

(33) \hspace{1cm} (34) \hspace{1cm} (35)

Note, on the other hand, that (P1) and (31) imply

\[s(G_\alpha(u^*)) = 1, \quad \alpha = (\alpha_1, \ldots, \alpha_\nu) \in \mathbb{R}^\nu.\]  

(36)

Differentiating (36) with respect to each \(\alpha_j, \dot{j} = 1, \ldots, \nu\) and evaluating at \(\alpha = 0\) we have

\[\nabla s(u^*) v_j = 0, \quad j = 1, \ldots, \nu,\]

and (33)-(35) can be written as

\[
\begin{align*}
\alpha_{n+1} &= \alpha_n (p + q) + (\nabla s(u^*)) z_n, \\
z_{n+1} &= S z_n, \\
\beta_{n+1,k} &= \beta_{n,k}, \quad k = 1, \ldots, \nu \\
\Rightarrow \beta_{n,k} &= \beta_{0,k}, \quad k = 1, \ldots, \nu, \quad n \geq 0.
\end{align*}
\]

Consequently,
$$G_{(\beta_0, \ldots, \beta_0, \nu)}(u^*) + \alpha_n x^* + z_n$$

differs from

$$u_n = u^* + e_n = u^* + \sum_{k=1}^{\nu} \beta_{0,k} v_k(u^*) + z_n,$$

in $O(||e_n||^2)$ terms. Under the above mentioned hypotheses, the convergence is to the element $G_{(\beta_0, \ldots, \beta_0, \nu)}(u^*)$ of the orbit of $u^*$, determined by the component of the initial iteration in $\text{Ker}(I - S)$. As in Theorem 4, the fastest rate of convergence occurs when $q = -p$.

### 3.4 Some examples

This case is illustrated by the generation of solitary wave solutions of nonlinear Schrödinger equations of the form (see e. g. [28] and references therein)

$$iu_t + u_{xx} + |u|^{2\sigma} u = 0, \quad -\infty < x < \infty, \quad t > 0,$$

(37)

where $\sigma > 0$. The symmetry group for (37) consists of gauge transformations and translations

$$G_{\theta_0, x_0}(u(x)) = e^{i\theta_0} u(x + x_0), \quad \theta_0, x_0 \in \mathbb{R}.$$  

(38)

Solitary wave solutions of (37) can be obtained from profiles $U(x)$ satisfying

$$U'' + |U|^{2\sigma} u - \lambda_1 U - i\lambda_2 U' = 0,$$

(39)

for some real parameters $\lambda_1, \lambda_2$. This leads to the explicit formulas

$$U(x) = \rho(x)e^{i\theta(x)}$$

(40)

$$\rho(x) = (a(\sigma + 1))^{1/2\sigma} \left( \text{sech}(\sigma \sqrt{a}x) \right)^{1/\sigma}, \quad a = \lambda_1 - (\lambda_2^2)/4,$$

(41)

$$\theta(x) = \frac{\lambda_2}{2} x.$$  

(42)

Due to the symmetry group (38), the two-parameter orbit of the solution given by (40) is of the form

$$\mathcal{O}(\rho, \theta) = \{ \varphi = \rho(x - x_0)e^{i\theta(x-x_0)} : x_0, \theta_0 \in \mathbb{R} \}.$$  

(43)
| $\sigma = 1$ | $\sigma = 2$ |
|----------------|----------------|
| 2.9999E+00     | 4.9999E+00     |
| 9.9999E-01     | 9.9999E-01     |
| 9.9999E-01     | 9.9999E-01     |
| 4.9999E-01     | 4.2857E-01     |
| 3.3333E-01     | 2.3810E-01     |
| 2.9999E-01     | 1.9999E-01     |

Table 2
Solitary wave generation of (37). Six largest magnitude eigenvalues of the approximate iteration matrix (4) evaluated at the exact profile (40) with $\lambda_1 = \lambda_2 = 1, x_0 = \theta_0 = 0$ for $\sigma = 1$ (first column) and $\sigma = 2$ (second column).

The four-parameter family of solitary wave solutions of (37) is finally of the form

$$
\psi(x, t, a, c, x_0, \theta_0) = G(t \lambda_1, t \lambda_2) (\varphi) = \rho(x - ct x_0) e^{i\theta(x-ct-x_0)+i\theta_0+i(a+(c^2/4))t},
$$

(where $c = \lambda_1$). As far as the discretization is concerned, the corresponding Fourier collocation approximation of (39)

$$
D^2U_h + |(U_h)|^{2\sigma} U_h - \lambda_1 U_h - i\lambda_2 D U_h = 0,
$$

(the dot stands for the Hadamard product) inherits the symmetry group infinitesimally generated by (see (32))

$$
U_h \mapsto v_1(U_h) = iU_h, \quad U_h \mapsto v_2(U_h) = DU_h.
$$

They are associated, respectively, to phase rotations and spatial translations.

Local convergence of the Petviashvili method is first checked by Table 2. This shows, for $\sigma = 1, 2$, the first largest magnitude eigenvalues of the iteration matrix $S$ at the exact profile (40)-(42) with parameters $\lambda_1 = \lambda_2 = 1$, (where $x_0 = \theta_0 = 0$). The results guarantee the satisfaction of the conditions for local convergence. (Note that, in this case, since the symmetry group is two dimensional, the eigenvalue $\lambda = 1$ has geometric multiplicity equals two.)

The following results illustrate the orbital convergence. An exact profile of the form (40)-(42) with $\lambda_1 = \lambda_2 = 1, x_0 = \theta_0 = 0$, denoted by $U_{\text{exact}}$, is perturbed in the form

$$
U_0 = U_{\text{exact}} + \epsilon_1 iU_{\text{exact}} + \epsilon_2 D U_{\text{exact}}, \quad (44)
$$
(with small parameters $\epsilon_1, \epsilon_2$). Now the Petviashvili method is run with (44) as initial iteration. The results are illustrated by two experiments. Figure 5(a) (resp. Figure 5(b)) compares the real part (resp. the modulus) of the exact profile $U_{\text{exact}}$ with that of the last computed iterate, denoted by $U_f$ and obtained with a residual error below $10^{-13}$ and for $\epsilon_1 = 0.2, \epsilon_2 = 0$.

While moduli are practically indistinguishable, Figure 5(a) reveals a phase displacement of the computed profile with respect to the exact one. The phase of $U_f$ (computed as $\text{Im} \left( \log \left( U_f/|U_f| \right) \right)$, modulo $2\pi$) has been calculated. The resulting data are fitted to a line $y = mx + n$, see Figure 5(c). The computed slope is $m = 4.9934 \times 10^{-1}$ (approximating the corresponding value $\lambda_2/2$ of (40)-(42) for this case) while $n = 1.2764 \times 10^1$, which modulo $2\pi$ is $1.9751 \times 10^{-1}$, an approximation to the value of $\epsilon_1$. These results suggest that the computed profile is closer to the element of the orbit (43) of $U_{\text{exact}}$ with new phase $\theta_0 + \epsilon_1 = \epsilon_1$ and the same translational parameter $x_0 = 0$.

A second experiment is performed with the values $\epsilon_1 = 0.2, \epsilon_2 = 0.2$. Figure 6(a) (resp. Figure 6(b)) compares the real part (resp. the modulus) of the exact profile $U_{\text{exact}}$ with that of the last computed iterate $U_f$, after 35 iterations and with a residual error (19) below $10^{-11}$ (see Figure 6(c)). The error in the stabilizing factor is of the order of the machine precision (below $10^{-15}$). In this case, besides the phase shift, also the modulus is affected by a displacement (cf. Figure 5(b)). The corresponding fitting line to the phase data of the computed profile $U_f$, $y = mx + n$ has a slope $m = 4.9933 \times 10^{-1}$ while $n = 1.2852 \times 10^1$, which modulo $2\pi$ is approximately $2.8553 \times 10^{-1}$. This last value approximates $\epsilon_1 + (\lambda_2/2)\epsilon_2 = 0.3$, suggesting that the computed profile is close to the exact one of the form (40), (43) with group parameters $\theta_0 + \epsilon_1, x_0 + \epsilon_2$.

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Fig. 5. Solitary wave generation of (37). The parameters are $\lambda_1 = \lambda_2 = 1, x_0 = \theta_0 = 0, \epsilon_1 = 0.2, \epsilon_2 = 0$. (a) Real part of the last computed iterate $U_f$ obtained by the Petviashvili scheme (solid line) and of the exact profile $U_{\text{exact}}$ (dashed line). (b) Modulus of the last computed iterate $U_f$ obtained by the Petviashvili scheme (solid line) and of the exact profile $U_{\text{exact}}$ (dashed line). (c) Fitting line to the phase of the computed profile $U_f$. 

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Fig. 6. Solitary wave generation of (37). The parameters are $\lambda_1 = \lambda_2 = 1, x_0 = \theta_0 = 0, \epsilon_1 = 0.2, \epsilon_2 = 0.2$. (a) Real part of the last computed iterate $U_f$ obtained by the Petviashvili scheme (solid line) and of the exact profile $U_{\text{exact}}$ (dashed line). (b) Modulus of the last computed iterate $U_f$ obtained by the Petviashvili scheme (solid line) and of the exact profile $U_{\text{exact}}$ (dashed line). (c) Logarithm of the residual error against number of iterations.
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