Rotational Quotient Procedure: a Tracking Control Continuation Method for PDEs on Radially Symmetric Domains

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Abstract

Continuation methods are capable of finding multiform solutions by tracking solution curves. However, these methods may fail to track some desired solution curves due to the interference of the rotational equivalent solutions on a radially symmetric domain. We propose a rotational quotient procedure that applies extra constraints to standard continuation which overcomes this difficulty. We solve a time-independent nonlinear Schrödinger equation on a disk domain to demonstrate the functionality of the proposed method.

Key words: Continuation methods, radially symmetric domain, rotation invariant solutions.

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1 Introduction

Mathematical models based on partial differential equations (PDEs) play an important role in scientific discovery. Among existing numerical schemes, continuation methods have been used to solve PDEs in various settings [1–3]. One advantage of continuation methods is their capability to find various types of solutions. Starting from an initial solution, continuation methods track a solution curve to other different solutions. The methods can also track multiple solution curves bifurcated at the singular points and produce informative bifurcation diagrams.

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While continuation methods have been used to solve many PDEs successfully, limitations exist in some circumstances. As a result, the methods may proceed along the solution curves inefficiently or even fail to track the next solution [3]. One of such obstacles occurs in PDEs defined on radially symmetric domains such as two dimensional disks or three dimensional balls. Taking a disk domain as an example, Figure 1 illustrates such numerical issues conceptually. Suppose there is a non-radially symmetric solution (represented by the green dot in Figure 1(a)). It is clear that arbitrary many equivalent solutions can be generated by rotating this particular solution through different angles. Four of such equivalent solutions are shown in Figure 1(b). These equivalent solutions thus form a solution curve (represented by the blue-dashed circles in Figure 1(a) and 1(b).) Such equivalent solution curves can be generated from any non-radially symmetric solutions and all of these equivalent solution curves actually form a two-dimensional manifold. As a standard continuation method may fail to proceed on this manifold, it is our goal to design a numerical scheme to extract a solution curve (represented by the red curve in Figure 1(a)). This solution curve should not contain the equivalent solutions from the manifold, except one representative solution is included in this desired solution curve. In other words, for each set of the equivalent solutions, only one representative solution should be tracked by the continuation method, which subsequently forms the desired solution curve. It is worth noting that, even if a target computational domain is not radially symmetric, similar numerical difficulty may still occur when, for example, a radially symmetric trap potential is applied and the solution is confined therein.

In the following section, we briefly outline the main ideas of continuation methods. In Section 2, we propose the rotational quotient procedure that overcomes the previously mentioned numerical difficulty. In Section 3, by taking a time-independent nonlinear Schrödinger (NLS) equation on a disk domain as an example, we demonstrate how the proposed method can track the desired solution curves effectively. We conclude the article in Section 4.

1.1 A Framework of Continuation Methods

Continuation methods are numerical schemes aiming to compute approximate solutions of a system of parameterized nonlinear equations. We give a brief account of the main ideas below; the detailed description of the methods can be found, for example, in [1,4–6].

In general, a parameterized nonlinear equation system can be denoted as

\[ \mathbf{G}(\mathbf{u}, p) = 0, \]

where \( \mathbf{G} : \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N \) is a smooth mapping, \( \mathbf{u} \in \mathbb{R}^N \) and \( p \in \mathbb{R} \) is a
parameter. Parameterizing via arc-length \( s \), a solution curve of (1) can be defined as

\[
\mathcal{C} = \left\{ y(s) = (u(s)^\top, p(s))^\top | \text{G}(y(s)) = 0, \ s \in \mathbb{R} \right\}.
\]

(2)

To follow the solution curve (2), a continuation method usually takes a prediction-correction approach. In particular, starting from the point \( y_i = y(s_i) = (u(s_i)^\top, p(s_i))^\top \in \mathbb{R}^{N+1} \) is a solution point lying (approximately) on a solution curve \( \mathcal{C} \), the prediction and correction steps are described as follows.

- In the prediction step, the Euler predictor

\[
y_{i+1,1} = y_i + h_i(\dot{y}_i / \|\dot{y}_i\|)
\]

is computed. Here, \( h_i > 0 \) is a suitable step length and \( \dot{y}_i \equiv (\dot{u}_i^\top, \dot{p}_i)^\top \) is the tangent vector of the solution curve at \( y_i \). To compute \( \dot{y}_i \), we solve the linear system

\[
\mathcal{D}\text{G}(y(s_i))\dot{y}_i = 0,
\]

which is obtained by differentiating (1) with respect to \( s \). Note that

\[
\mathcal{D}\text{G}(y(s_i)) = [G_u(y(s_i)), G_p(y(s_i))] \in \mathbb{R}^{N \times (N+1)}
\]

denotes the Jacobian matrix of \( \text{G} \) at \( y(s_i) \).

- In the correction step, Newton’s method is usually used to to solve the nonlinear equation

\[
\begin{cases}
\text{G}(u, p) = 0, \\
\dot{u}_i^\top u + \dot{p}_i p = u_{i+1,1}^\top u_{i+1,1} + \dot{p}_i p_{i+1,1},
\end{cases}
\]

(4)

with initial guess \( y_{i+1,1} = (u_{i+1,1}^\top, p_{i+1,1})^\top \). That is, for the correction vector \( \delta_i \), the iteration \( y_{i+1,l+1} = y_{i+1,l} + \delta_i \) is computed for \( l = 1, 2, \ldots \) until a convergence criterion is satisfied for \( l = l_\infty \). Finally, \( y_{i+1} = y_{i+1,l_\infty} \) is taken as a new approximate solution on the solution curve \( \mathcal{C} \).

2 Rotational Quotient Procedure

We consider a boundary value problem of a time-independent PDE on a radially symmetric domain and assume that some steady-state solutions process the rotation invariant property - there are arbitrary many equivalent solutions that can be generated by rotating a non-radially symmetric solution through any given angle. Without loss of generality, let

\[
\Omega = \{(r, \theta) : 0 \leq r \leq r_0, \ -\pi \leq \theta < \pi \}
\]
be a two dimensional disk domain defined on the polar coordinates. A certain solution \( u(r, \theta) \) is rotation invariant provided \( u(r, \theta + \phi) \) is also a solution of the PDE for any \( \phi \in [-\pi, \pi] \).

Let \( p \in \mathbb{R} \) be the changeable continuation parameter and \( u_*(r, \theta) \) be a solution of the PDE at \( p = p_* \). We can observe the following facts. First, let \( u_*(r, \theta) \) be a non-radially symmetric solution that \( u_*(r, \theta) \neq u_*(r, 0) \) for some \( (r, \theta) \in \Omega \).

A solution curve
\[
\begin{align*}
u_\phi(r, \theta) := u_*(r, \theta + \phi)
\end{align*}
\] (5)
for \( \phi \in [-\pi, \pi] \) can be understood conceptually as the blue-dashed circle in Figure 1. The tangent vector of \( u_\phi \) at \( \phi = 0 \) satisfies
\[
\begin{align*}
\frac{\partial u_\phi}{\partial \phi} \bigg|_{\phi=0} = \frac{\partial u_*(r, \theta)}{\partial \theta}.
\end{align*}
\] (6)

Second, if \( u_*(r, \theta) \) is radially symmetric, the solution curve \( u_\phi(r, \theta) \) in (5) becomes an isolated solution and the tangent vector (6) at \( \phi = 0 \) is a zero function.

In addition, we define some notations to be used later. Suppose the PDE is discretized, for example, by a finite difference scheme that results in a parameterized nonlinear equation. Let \( u \in \mathbb{R}^N \) be the approximation of a steady-state solution \( u(r, \theta) \). Then the equation can be rewritten as in (1). We also define the solution set \( \mathcal{M} \) of (1) as
\[
\begin{align*}
\mathcal{M} = \{(u, p) : G(u, p) = 0\}.
\end{align*}
\]

Now, we develop a new continuation method to track the desired solution curves. To avoid being trapped by the undesired solution curves, our main idea is to consider a quotient solution set by applying an additional constraint on the system. First, we define the quotient solution curve \( C \) is parameterized by the arc length parameter \( s \):
\[
\begin{align*}
C \equiv \mathcal{M}/[-\pi, \pi] = \{y(s) = (u(s), p(s)) : G(y(s)) = 0, \ s \in \mathbb{R}\}.
\end{align*}
\] (7)

Unlike standard continuation methods that simply track solution curves by solving a system of parameterized nonlinear equations \( G(u(s), p(s)) = 0 \) defined in (1), we propose a rotational quotient procedure (RQP) that is comprised of a standard and a modified continuation methods. To switch between the two methods, the RQP monitors the characteristic of the current solution \( y_i \), where \( y_i \equiv (u_i, p_i) = (u(s_i), p(s_i)) \in C \). In particular, the RQP tracks the curve \( C \) defined in (7) by using one of the following methods appropriately.

1. **Radially symmetric tracker (RST).** If \( u_i \) is a radially symmetric solution, the change of \( u_i \) along the angle direction is zero. That is, by
letting

\[ a_\theta = D_\theta u_i, \]  

where \( D_\theta \in \mathbb{R}^{N \times N} \) is the discretization matrix of the differential operator \( \frac{\partial}{\partial \theta} \), we have \( a_\theta = 0 \) provided \( u_i \) is radially symmetric. In this case, we can use a standard continuation method to track the solution curve \( C \) without any problem.

(2) **Non-Radially symmetric tracker (NRST).** If \( u_i \) is a non-radially symmetric solution (i.e. \( a_\theta \neq 0 \)), then we use a modified continuation method with an additional constraint to track the solution curve \( C \) as follows.

- In the prediction step, a standard continuation method requires that the tangent vector \( \dot{y}_i = (\dot{u}_i, \dot{p}_i) \) of \( C \) should satisfy \( DG(y_i)\dot{y}_i = 0 \), where \( DG(y_i) \) is the Jacobian of \( G \). Here, we further apply another constraint that the vector \( \dot{u}_i \) should be orthogonal to the tangent vector \( a_\theta \). That is, the tangent vector \( \dot{y}_i \) should satisfy

\[
\begin{bmatrix}
DG(y_i) \\
a_\theta^\top 0
\end{bmatrix} \dot{y}_i = 0.
\]

(9)

Note that the row vector \([a_\theta^\top 0]\) in the coefficient matrix in (9) makes it full row-ranked. Furthermore, the Euler predictor is given by (3).

- In the correction step, let \( y_{i+1,1} = (u_{i+1,1}, p_{i+1,1}) \) be the Euler predictor (3). With initial guess \( y_{i+1,1} \), we then use Newton’s method to compute the solution of equations

\[
\begin{aligned}
G(u, p) &= 0, \\
\dot{u}_i^\top u + \dot{p}_i p &= \dot{u}_i^\top u_{i+1,1} + \dot{p}_i p_{i+1,1}, \\
a_\theta^\top u &= a_\theta^\top u_{i+1,1}.
\end{aligned}
\]

(10)

Note that the third equation of (10) is an additional constraint that involves the normal vector \( a_\theta \).

We have developed a numerical scheme for computing the radially and non-radially symmetric steady-state solutions of a PDE that satisfies the rotation invariant property. The proposed RQP can be applied to higher dimensional problems with suitable modifications. For example, if the domain \( \Omega \) is a three dimensional ball, two constraints corresponding to the inclination and azimuth directions must be applied to (9) and (10). We conclude this section by summarizing the RQP in the flowchart shown in Figure 2.
3 Numerical Results

In this section, we present the numerical results for solving a time-independent nonlinear Schrödinger (NLS) equation on a two dimensional disk domain that models a system of Bose-Einstein condensates (BEC) [7–10]. In particular, we consider the exploration of quantized vortex states and their connections with superfluidity. We assume that a rotating laser beam with angular velocity \( \omega \) is applied to the magnetic trap to create a harmonic and anisotropic potential. In such circumstances, vortex lattices [11], vortex nucleation [12], and vortex arrays [13] have also been observed.

The target time-independent NLS equation that describes a BEC with an external driven field in the rotating frame [9,14,15] can be written as

\[
-\frac{1}{2} \nabla^2 \psi(x) + V(x)\psi(x) + \alpha|\psi|^2\psi(x) + \omega \partial_\theta \psi(x) = \lambda \psi(x),
\]

for \( x \in \Omega = \{ x \in \mathbb{R}^2 : \|x\|_2 \leq r_0 \} \) with

\[
\int_\Omega |\psi(x)|^2 \, dx = 1. \tag{11b}
\]

Here \( \psi(x) \) is a complex function representing the wave function of the BEC, \( \iota = \sqrt{-1} \), \( V(x) \geq 0 \) is a magnetic trapping potential, \( \partial_\theta \) is the angular momentum, \( \omega \) is the angular velocity of the rotating laser beam, \( \alpha \) denotes the intra-component scattering length, and \( \lambda \) is the chemical potential.

To use the RQP developed in Section 2 to compute the steady-states of the rotating BEC, we first denote the approximation of the complex wave function \( \psi(x) \) in (11) as \( v_1 + \iota v_2 \), where \( v_1, v_2 \in \mathbb{R}^N \). Let \( u = (v_1^T, v_2^T, \lambda)^T \in \mathbb{R}^{2N+1} \). Then the discretized version of (11) is the parameterized nonlinear equation

\[
G(u, \omega) = 0. \tag{12}
\]

In particular, \( G = (G_1, G_2, g) : \mathbb{R}^{2N+1} \times \mathbb{R} \to \mathbb{R}^{2N+1} \) and

\[
G_1(u, \omega) = Av_1 + \alpha[\text{diag}(v_1^\odot) + \text{diag}(v_2^\odot)]v_1 - \omega \partial_\theta v_2 - \lambda v_1,
\]

\[
G_2(u, \omega) = Av_2 + \alpha[\text{diag}(v_1^\odot) + \text{diag}(v_2^\odot)]v_2 + \omega \partial_\theta v_1 - \lambda v_2,
\]

\[
g(u) = c^T(v_1^\odot + v_2^\odot) - 1,
\]

where \( v_1^\odot = (v_{1,1}^2, v_{1,2}^2, \ldots, v_{1,N}^2)^T \) and \( v_2^\odot = (v_{2,1}^2, v_{2,2}^2, \ldots, v_{2,N}^2)^T \). In addition, \( A \in \mathbb{R}^{N \times N} \) is the the discretization matrix of the operator \( -\frac{1}{2} \nabla^2 + V(x) \) and \( D_\theta = -D_\theta^T \in \mathbb{R}^{N \times N} \) is the the discretization matrix of \( \partial_\theta \). The vector \( c \in \mathbb{R}^N \) is a constant vector such that \( c^T(v_1^\odot + v_2^\odot) \) represents the
approximation of $\int_\Omega |\psi(x)|^2 dx$. Now, by denoting $u_i = (v_{1,i}^T, v_{2,i}^T, \lambda_i)^T$ and rewriting the vector $a_\theta$ corresponding to (12) as $a_\theta = \text{diag}\{D_{\theta}', D_{\theta}, 0\} u_i = [(D_{\theta}v_{1,i})^T, (D_{\theta}v_{2,i})^T, 0]^T \in \mathbb{R}^{2N+1}$, the RQP produces each solution curve of (12) by tracking $y_i = (u_i^T, \omega_i)^T$, for $i = 1, 2, 3, \ldots$. 

In our numerical experiments, we assume that $r_0 = 6$, $V(x) = \|x\|^2_2$, $\alpha = 100$ and take $\omega \in [0, 0.8]$ as the continuation parameter. We use the RQP to track the solution curves starting from point A ($\omega = 0$). The results are shown in Figure 3. In the figure, we plot the conceptual solution curves of $G(u, \omega) = 0$ for $\omega \in [0, 0.8]$. The corresponding nodal domains of the density $|v_{1,i} + \omega v_{2,i}|^2$ are attached near the solution curves. Here, the green and red curves indicate the corresponding solutions that are computed by RST and NRST, respectively.

As the solutions are radially symmetric along the primal stalk, the RST is used until the first bifurcation point is identified at B ($\omega = 0.596$). The RST can be used to track the primal stalk further to C and beyond. To track another solution curves from B to D ($\omega = 0.593$), we need to use the NRST. Otherwise, a standard continuation method may fail to track the solution curves from B to D and other solution curves in red. Such undesirable behavior is due to these solutions are non-radially symmetric and the corresponding Jacobian matrices of (4) are singular. Consequently, Newton’s method cannot converge in the correction steps within a standard continuation method. In contrast, the NRST successfully tracks the solution curves between points B-D, D-E, D-F, and G-H. In these particular solution curves plotted in red, the corresponding solutions are non-radially symmetric and the the corresponding Jacobian matrices of (10) are non-singular, thanks to the additional constraints involving non-zero $a_\theta$'s.

4 Conclusion

To overcome the numerical difficulties that regular continuation methods may encounter due to radially symmetric domains, we have proposed a rotational quotient procedure that an additional constraint is applied. By suitably choosing between RST and NRST, the RQP successfully tracks the solution curves composed by radially symmetric and non-radially symmetric solutions without being interfered by the rational invariant solutions. We have solved a time-independent nonlinear Schrödinger equation that models BEC on a disk domain to demonstrate the feasibility of the RQP.

Finally, we make the following two remarks.

• With some modifications, the proposed RQP can be generalized to solve coupled PDE systems. Taking multi-component BEC model [1,10,16] as
an example, we can analogously apply a similar hyperplane constraint described in the NRST, in which the corresponding $D_\theta$ defined in (8) becomes a block diagonal matrix. The number of blocks is the number of components.

- It is of general interest to explore the behavior when the angular velocity $\omega$ approaches to its physical maximum. Actually, when $\omega$ is getting larger, the bifurcation diagram becomes more complicated as more bifurcation points and more vertexes appear. In such cases, larger computational domains with finer discretizations are necessary. Although the proposed method can be applied straightforwardly for the increasing $\omega$’s (possibly with high numerical complexity), we expect a novel and efficient method will be more appropriate.

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References


Fig. 1. (a) Relations of a two-dimensional solution manifold, an equivalent solution curve (in blue-dashed), and a meaningful solution curve (in red) are shown conceptually. (b) Four examples of solutions on the equivalent solution curve.

Fig. 2. The flowchart of the rotational quotient procedure.
Fig. 3. A bifurcation diagram of solution curve $C$ of (12). The green and red curves indicate the corresponding solutions that are computed by RST and NRST, respectively. The corresponding nodal domains, with a density of $|v_1 + iv_2|^2$ are attached near the solution curves.