Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **13**, No. 5, pp. 1096-1125

DOI: 10.4208/aamm.OA-2020-0270
October 2021

Anderson Acceleration of Nonlinear Solvers for the Stationary Gross-Pitaevskii Equation

Dominique Forbes, Leo G. Rebholz[1,*] and Fei Xue

School of Mathematical and Statistical Sciences, Clemson University, Clemson, SC 29634, USA

Received 26 August 2020; Accepted (in revised version) 2 February 2021

Abstract. We consider Anderson acceleration (AA) applied to two nonlinear solvers for the stationary Gross-Pitaevskii equation: a Picard type nonlinear iterative solver and a normalized gradient flow method. We formulate the solvers as fixed point problems and show that they both fit into the recently developed AA analysis framework. This allows us to prove that both methods' linear convergence rates are improved by a factor (less than one) from the gain of the AA optimization problem at each step. Numerical tests for finding ground state solutions in 1D and 2D show that AA significantly improves convergence behavior in both solvers, and additionally some comparisons between the solvers are drawn. A local convergence analysis for both methods are also provided.

AMS subject classifications: 65J15, 65B05, 65N30

Key words: Gross-Pitaevskii, Anderson acceleration, convergence analysis.

1 Introduction

We consider numerical solvers for the following nonlinear eigenvalue problem,

$$\mu\phi(x) = -\frac{1}{2}\Delta\phi(x) + V(x)\phi(x) + \beta|\phi(x)|^2\phi(x), \qquad x \in \Omega, \tag{1.1a}$$

$$\phi(x) = 0, \qquad x \in \partial\Omega, \tag{1.1b}$$

$$\int_\Omega |\phi(x)|^2\, dx = 1, \tag{1.1c}$$

where V is a given trapping potential of the form

$$V(x) = \frac{1}{2}(\gamma_1^2 x_1^2 + \cdots + \gamma_d^2 x_d^2)$$

*Corresponding author.
Emails: dforbes@clemson.edu (D. Forbes), rebholz@clemson.edu (L. G. Rebholz), fxue@clemson.edu (F. Xue)

with $\gamma_i > 0$, $\forall i$, real parameter β, with ϕ being the unknown and the eigenvalue μ can be calculated as

$$\mu = \int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + V|\phi|^2 + \beta|\phi|^4 \right) dx. \tag{1.2}$$

This system describes stationary solutions of the nonlinear Schrödinger (NLS) equation, which is also known as the the non-rotational Gross-Pitaevskii equation (GPE) in the context of Bose-Einstein condensates (BEC) [7, 25, 27]; in the GPE setting ϕ represents the macroscopic wave function of the condensate. The parameter β being positive/negative represents defocusing/focusing in NLS, and attraction/repulsion of the condensate atoms in GPE. Following [7, 9], we will assume $\beta \geq 0$ for simplicity, although a more technical analysis would allow for our results to hold with β taking small negative values. Herein we assume a solution $\phi \in H_0^1(\Omega)$ exists to (1.1a)-(1.1c) that is locally unique; see [9] for more on this assumption and conditions for its validity.

Solutions of (1.1a)-(1.1c) represent local minima of the Gross-Pitaevskii energy

$$E_\beta(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla\phi|^2 + V|\phi|^2 + \frac{\beta}{2}|\phi|^4 \right) dx,$$

and are used to numerically create initial conditions for real time dynamics of BEC, and to consider experimentally observed physical features through direct investigation [36]. Solutions to (1.1a)-(1.1c) that globally minimize energy are called ground state solutions, and it is stated in 2004 in [7] that "One of the fundamental problems in numerical simulation of BEC lies in computing the ground state solution". Existing methods include the normalized gradient flow (or gradient flow with discrete normalization) [3, 6, 7], which is most well-known, optimization methods such as steepest descent (without preconditioning) [36], preconditioned steepest descent (PSD, which is also effective in related problems [11, 14–16, 23]) and conjugate gradient (PCG) [4], and regularized Newton's method [33], as well as specialized non-optimization methods such as nonlinear inverse iterations [20], self-consistent field iteration [5], and implicit algorithms based on inexact Newton's method [21]. While normalized gradient flow methods have been widely used in the literature to find solutions of (1.1a)-(1.1c), improving the convergence and robustness of these methods remains an important problem and is the purpose of this paper.

We consider herein Anderson acceleration (AA) applied to two nonlinear solvers for (1.1a)-(1.1c). AA was originally developed in 1965 by D.G Anderson [2] as an extrapolation technique which forms the next iterate in a nonlinear fixed point iteration from an (in a sense) optimal linear combination of previous iterates. AA has increased in popularity since the work of [37], which showed how to implement it efficiently as a post-processor for a fixed point iteration and that it could be used successfully on a variety of application problems. Theoretical justification for how AA works was proved in [12], building on the theory from [13, 24, 34], and then sharpened and generalized to the case of noncontractive operators in [30]. AA has been used in a wide variety of applications including e.g., computing nearest correlation matrices in [19], geometry optimization [26], electronic