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Short note

Leveraging Anderson Acceleration for improved convergence of iterative solutions to transport systems

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ABSTRACT

In this note we demonstrate that using Anderson Acceleration (AA) in place of a standard Picard iteration can not only increase the convergence rate but also make the iteration more robust for two transport applications. We also compare the convergence acceleration provided by AA to that provided by moment-based acceleration methods. Additionally, we demonstrate that those two acceleration methods can be used together in a nested fashion. We begin by describing the AA algorithm. At this point, we will describe two application problems, one from neutronics and one from plasma physics, on which we will apply AA. We provide computational results which highlight the benefits of using AA, namely that we can compute solutions using fewer function evaluations, larger time-steps, and achieve a more robust iteration.

1. Introduction

Originally conceived in 1965, Anderson Acceleration (AA) was designed to accelerate iterative methods for solving nonlinear integral equations [1]. Recent work by Toth and Kelley [4] and Calef [5] has demonstrated the effectiveness of Anderson Acceleration, or the closely related Nonlinear Krylov Acceleration (NKA). Similarly, the authors of [6] have shown that AA can provide an algorithmic speed-up when coupling fluid and solid heat-transfer problems. Others have shown that AA is closely related to unrestarted GMRES, which requires only finite storage [7,8]. In Ref. [4], Toth and Kelley have developed some of the first convergence theory for nonlinear problems. These results suggest that for appropriate problems, AA can yield computational improvements over a standard Picard Iteration.[1]

In the past, we have utilized moment-based acceleration (MBA) techniques to accelerate the standard Picard iteration for a variety of transport problems [10,13,14]. These MBA techniques yield the same high-quality solution as the unaccelerated iteration, however at a small fraction of the original cost. We propose AA, not as a replacement to MBA technique, but as an additional level of acceleration to enhance the performance of the MBAs. In the context of neutron transport we use an MBA method often referred to as nonlinear diffusion acceleration (NDA) [10], while in the context of plasma physics we will use an algorithm called moment-accelerated Vlasov–Ampère (MAVA) [13]. These techniques are very similar in nature and both yield accurate, consistent solutions for a reduced computational cost.

In this work, we will give a brief overview of the Anderson Acceleration algorithm and describe how it can be used to aid in the solution of the fixed-source neutron transport equation and the Vlasov–Ampère equations. We also review the moment-based acceleration methods for both application areas. For the fixed-source neutron transport equation, we will

[1] Anderson Acceleration, as described in [1], is closely related to nonlinear GMRES, introduced later in both [2] and [3].

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demonstrate that Anderson Acceleration can achieve faster convergence than Picard iteration and may allow convergence in some cases where a standard Picard iteration does not converge. We also show that the moment-based acceleration method can be much more efficient, but also potentially less robust, as compared to an unaccelerated solution technique. Finally, we show that the combination of the two acceleration methods results in the best combination of efficiency and robustness. Within the plasma physics domain, we find that AA allows us to take larger time-steps, in addition to faster convergence of each time-step solution and again we find that an MBA technique in conjunction with AA is the most efficient combination.

2. Anderson Acceleration

Suppose we wish to compute the nonlinear fixed-point,

$$x^* = G(x^*). \tag{1}$$

If G is a contraction mapping in a neighborhood of the solution and x_0 is some initial approximation to x^* within that neighborhood, then the iteration produced via successive substitution will converge, potentially very slowly, to the solution [9]. We define this successive substitution, or Picard Iteration, formally in Algorithm 1.

Algorithm 1 (PI).

Picard Iteration

Input function G, initial iterate x_0, convergence tolerance τ
Set $z = 0$.
while $\|x_{z+1} - x_z\| > \tau$ **do**
  Set $x_{z+1} = G(x_z)$
  Increment $z = z + 1$.
end while

It is important to note that this nonlinear iteration is guaranteed to converge only when G is a contraction mapping. Furthermore, this iteration may converge unacceptably slowly to the solution. Several other approaches have been considered for this problem including recasting the problem as a nonlinear equation $F(x) = 0$. In this case, one can use a Newton-based method to potentially achieve quadratic convergence. In this paper, we will leave the problem in its original fixed-point form and apply either an MBA method or Anderson Acceleration to improve convergence. Anderson Acceleration applies an update formula at each iteration which takes into account a (generally) limited history of old residuals. We describe Anderson Acceleration (as presented in [7]) in Algorithm 2.

Algorithm 2 (AA).

Anderson Acceleration(m)

Given x_0 and $m \geq 1$.
Compute $x_1 = G(x_0)$.
for $z = 1, 2, \ldots$ **do**
  Set $m_z = \min\{m, z\}$.
  Set $F_z = (f_{k-m_z}, \ldots, f_z)$, where $f_i = G(x_i) - x_i$.
  Compute $\alpha^{(z)} = (\alpha_0^{(z)}, \ldots, \alpha_{m_z}^{(z)})^T$ where

$$\alpha^{(z)} = \arg\min_{\alpha} \|F_z \alpha\|_2 \quad \text{s.t.} \quad \sum_{i=0}^{m_z} \alpha_i = 1 \tag{2}$$

  Set $x_{z+1} = \sum_{i=0}^{m_z} \alpha_i^{(z)} G(x_{z-m_z+i})$
end for

We see that we must solve a constrained minimization problem at each iteration. In most references, the minimization in Eq. (2) is recast as an unconstrained minimization problem. We generally keep the number of vectors, m, in the Anderson history small so as to ensure we have sufficient storage and so as to make the optimization problem less ill-conditioned. From here we seek to demonstrate applications of the Anderson Acceleration algorithm (see [8,7,4]) and we leave the reader to explore any additional theory independently.

3. Neutron transport

In this section we are interested in solving the neutron transport equation with isotropic scattering. This equation is given by

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, \hat{\Omega}) = \frac{1}{4\pi}\left[\Sigma_s \phi(\vec{r}) + q(\vec{r})\right], \tag{3}$$