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The Effect of Anderson Acceleration on Superlinear and Sublinear Convergence

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Abstract

This paper considers the effect of Anderson acceleration (AA) on the convergence order of nonlinear solvers in fixed point form $x_{k+1} = g(x_k)$, that are looking for a fixed point x^* of g. While recent work has answered the fundamental question of how AA affects the convergence rate of linearly converging fixed point iterations (at a single step), no analytical results exist (until now) for how AA affects the convergence order of solvers that do not converge linearly. We first consider AA applied to general methods with convergence order r, and show that $m = 1$ AA changes the convergence order to (at least) $\frac{r+1}{2}$; a more complicated expression for the order is found for the case of larger m. This result is valid for superlinearly converging methods and also locally for sublinearly converging methods where $r < 1$ locally but $r \to 1$ as the iteration converges, revealing that AA slows convergence for superlinearly converging methods but (locally) accelerates it for sublinearly converging methods. We then consider AA-Newton, and find that it is a special case that fits in the framework of the recent theory for linearly converging methods which allows us to deduce that depth level m reduces the asymptotic convergence order from 2 to the largest positive real root of $\alpha^{m+1} - \alpha^m - 1 = 0$ (i.e. with $m = 1$ the order is 1.618, and decreases as m increases). Several numerical tests illustrate our theoretical results.

Keywords Anderson acceleration · Newton's method · Superlinear convergence · Sublinear convergence · Bingham equations

1 Introduction

Anderson acceleration (AA) has recently gained considerable interest as an extrapolation technique that can improve convergence properties of a fixed point algorithm, typically with

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little additional cost. It was developed in 1965 by D.G. Anderson [4], and although it has been used since then to solve various application problems, its use has exploded since the paper of Walker and Ni in 2011 [38] where they showed how effective it could be on a wide range of problems. AA has now been used to solve a large variety of problems across the spectrum of science and engineering, including flow problems [22, 30, 32], geometry optimization [25], accelerating Douglas-Rachford splitting convergence [16], radiation diffusion and nuclear physics [3, 36], seismic inversion [42], and many others e.g. [16, 19–22, 38, 40]. An excellent review of the literature up to 2018 is given in a review paper by C.T. Kelley in [20].

The fundamental question of *how* AA speeds up convergence in linearly converging fixed point iterations was finally resolved in a series of three papers from 2019-2022 [14, 27, 29], details of which are given below. Essentially, they showed that the linear convergence rate of the underlying fixed point method is scaled by the gain of the AA optimization problem (which is at most 1, but often less than 1 and sometimes much less than 1). While these papers provided critical results that resolved a 55 year old open problem about how AA affects the *rate* of linearly converging methods, there remains classes of solvers these results do not address, such as ones converging superlinearly or sublinearly. However, AA has been applied to such methods in recent literature, including applying AA to Newton in [14, 26, 31, 41] and applying AA to a (seemingly) sublinearly converging iteration for viscoplastic flow in [28]. The purpose of this paper is thus to analytically and numerically study the convergence of Anderson accelerated methods that converge with order $r \neq 1$. Our results still apply to the $r = 1$ case and find that AA does not change the order, which is already well known.

Our main results are the following. First, for general methods of order r we prove that the convergence order for the associated $m = 1$ AA method has order (at least) $\frac{r+1}{2}$; for larger m the expression is more complicated and is given in Sect. 3. These new theoretical results show that AA slows asymptotic convergence for superlinearly converging methods. However, for sublinearly converging methods where locally $r < 1$ even though asymptotically $r \to 1$, AA will improve convergence. Second, we find that AA-Newton is a special case of superlinearly converging methods that fits in the analysis framework of [27]. For the depth $m = 1$ case, we reduce the problem of convergence order determination to that of the classical theory of secant method convergence (e.g. from [7]), and find that convergence order is approximately 1.618, which is an improvement over the general theory which only predicts (at least) order 1.5. While the numerical tests of the general theory were sharp for AA-Secant and AA-Chebyshev and AA applied to sublinearly converging methods, AA-Newton was better than the $\frac{r+1}{2}$ predicted convergence order as its order was 1.618 for $m = 1$, as our AA-Newton theory predicts. Convergence rates for higher m with AA-Newton can be determined in a similar way, noting that an increase in m leads to a decrease in the convergence order (although it always remains superlinear). Numerical results illustrate these results for simple 1D tests, nonlinear Helmholtz, regularized Bingham equations, and the Boussinesq equations.

While there are many numerical results for AA, there are relatively few analytical results in the literature. The first proof of convergence appeared in 2015 in [37], is sharpened in [20], and proves that for contractive iterations AA at least does no harm. The work in [29] showed how AA improves the convergence rate for steady Navier–Stokes Picard iterations by proving the linear convergence rate of Picard is scaled by the ratio gain of the AA optimization problem. This result was extended to general contractive iterations in [14], and was subsequently sharpened and generalized in [27]. We note these works provided one step analyses, and the gain of the optimization problem can vary from step to step. Analytical results that partially address the question of AA asymptotic linear convergence for the general case are found in [33–35] and for application to ADMM in [39]. Very recently there are also some analytical results for the case of nonsmooth fixed point problems [11, 12]. Some convergence results for stabilized AA are given in [13], and these authors also give some new interpretations of AA. To our knowledge, no analytical results exist (until this paper) for how AA affects convergence order for general solvers that do not converge linearly, although one paper of author Mengying Xiao considers the specific case of AA-Newton for NSE [41] and the papers [26, 31] contribute to the understanding of AA-Newton and AA's effect on convergence radius. We note that this paper considers only asymptotic convergence order of AA applied to various iterations and solvers. While we find that AA reduces the asymptotic convergence order of superlinearly converging methods, we do not address the question of how AA might affect the behavior when the iterate is not very close to the root (work in [26, 31] suggests AA helps here), nor do we address how AA affects the convergence radius of a method. These remain important open questions in the understanding of AA applied to solvers that do not converge linearly.

This paper is arranged as follows. In Sect. 2, convergence order of fixed-point iterations and AA background are given, including the algorithm and known convergence results. Section 3 considers how AA affects general methods' convergence order and gives results of a test for superlinearly converging methods and a sublinearly converging method. Section 4 discusses AA-Newton, and gives results for convergence order for any m along with results of numerical tests. Finally, conclusions are drawn in the final section.

2 Mathematical Preliminaries

We give now some definitions, notation and preliminaries to make for a smoother discussion to follow.

2.1 Fixed Point and Convergence Order Preliminaries

Our interest in this paper is solving the equation

$$g(x) = x,$$

for $g : X \to X$ with X a Hilbert space and $\|\cdot\|$ the associated norm. A solution x^* to this equation is called a fixed point of the function g, i.e. $g(x^*) = x^*$. We refer to g as the fixed point function.

The fixed point iteration is defined by

$$x_{k+1} = g(x_k),$$

together with an initial guess x_0.

We refer to the order r of convergence as follows. Suppose for k sufficiently large, the iterates satisfy for $\rho > 0$,

$$\|x_{k+1} - x^*\| \le \rho \|x_k - x^*\|^r. \tag{2.1}$$

If $r > 1$, the order of convergence is called superlinear, and if $r = 1$ and $\rho < 1$ the convergence is called linear [6, 17].

There are two ways to describe a sublinearly convergent iteration, one from convergence rate ρ in Eq. (2.1), whereas the other one from convergence order r. If the iteration satisfies

$$\|x_{k+1} - x^*\| \le \rho_k \|x_k - x^*\|,$$

and ρ_k converges to 1, then the convergence is called sublinear [17]. Clearly, it can be viewed as a linearly convergent iteration if only a single iteration is considered, and it is studied in [14, 27] for how AA affects the convergence rate ρ of a fixed point iteration for such a case, see (2.5), (2.7) in Sect. 2.2. In this work, we focus on how AA affects the sublinear convergent iteration from the convergence order aspect, where the sublinearly convergent iteration is defined by a converging sequence satisfying

$$\|x_{k+1} - x^*\| \le L_k \|x_k - x^*\|^{r_k},$$

with $r_k \le 1$, $L_k \le 1$ and $r_k \to 1$. Herein, we consider a single step (i.e. local) analysis of convergence order, and in a local setting this is a more precise description of a sublinearly converging method. Hence for a single step, based on the above, we can discuss the local convergence order r to satisfy (2.1) even if $r < 1$. If $r \ge 1$, then the local order and usual order are the same.

2.2 Anderson Acceleration

We state now the Anderson acceleration algorithm, which is used to improve convergence properties of the fixed point iteration.

For a fixed point function $g : X \to X$ with X a Hilbert space and $\|\cdot\|$ the associated norm, the depth $m \ge 0$ Anderson acceleration algorithm with damping parameters $0 < \beta_{k+1} \le 1$ is given by:

Step 0: Choose $x_0 \in X$.
Step 1: Find $w_1 \in X$ such that $w_1 = g(x_0) - x_0$. Set $x_1 = x_0 + w_1$.
Step $k+1$: For $k = 1, 2, 3, \ldots$ Set $m_k = \min\{k, m\}$.

[a.] Find $w_{k+1} = g(x_k) - x_k$.
[b.] Solve the minimization problem for $\{\alpha_j^{k+1}\}_{k-m_k}^{k}$

$$\min_{\sum_{j=k-m_k}^{k} \alpha_j^{k+1}=1} \left\| \sum_{j=k-m_k}^{k} \alpha_j^{k+1} w_{j+1} \right\| \tag{2.2}$$

[c.] For damping factor $0 < \beta_{k+1} \le 1$, set

$$x_{k+1} = \sum_{j=k-m_k}^{k} \alpha_j^{k+1} x_j + \beta_{k+1} \sum_{j=k-m_k}^{k} \alpha_j^{k+1} w_{j+1}, \tag{2.3}$$

where $w_{k+1} := g(x_k) - x_k$ is the stage k residual. We note this is an unconstrained minimization problem and can be solved via a simple $m_k \times (m_k - 1)$ linear least squares problem.

Remark 2.1 We assume the α_j^{k+1} are uniformly bounded. As discussed in [27], this is equivalent to assuming full column rank of the matrix with columns $(w_{j+1} - w_j)_{j=k,k-1,\ldots k-m}$ and so can be controlled by reducing m if needed.

Remark 2.2 For simplicity, we will assume throughout this paper that $k \ge m$, so that $m_k = m$.

A key idea of [29] in understanding how AA improves convergence was to define the gain of the optimization problem by

$$\theta_k := \frac{\left\| \sum_{j=k-m_k}^{k} \alpha_j^{k+1} w_{j+1} \right\|}{\|w_k\|}. \tag{2.4}$$

This is considered the gain because the numerator represents the minimum value of the sum using the optimal parameters, and the denominator represents the value of the sum if the usual fixed point method (i.e. no AA) was used (i.e. when $\alpha_k^{k+1} = 1$ and $\alpha_{k-1}^{k+1} = \alpha_{k-2}^{k+1} = \ldots = \alpha_{k-m_k}^{k+1} = 0$). With this tool in hand, the fundamental question of *how* AA speeds up convergence in linearly converging fixed point iterations was finally resolved in a series of three papers from 2019-2022 [14, 27, 29] that prove AA improves the linear convergence rate by scaling it by the gain factor θ_k of the underlying AA optimization problem. For AA depth $m = 1$, the result from Theorem 4.1 in [27] reads

$$\|w_{k+1}\| \leq \|w_k\| \left\{ \theta_k\big((1-\beta_k) + \kappa_g \beta_k\big) + \hat{\kappa}_g \sigma^{-1}\sqrt{1-\theta_k^2} \times \left(\|w_k\| \left(\sigma^{-1}\sqrt{1-\theta_k^2} + \beta_k\theta_k\right) + \|w_{k-1}\| \left(\sigma^{-1}\sqrt{1-\theta_{k-1}^2} + \beta_{k-1}\theta_{k-1}\right)\right)\right\}, \tag{2.5}$$

where κ_g is the linear convergence rate of the usual fixed point iteration (the Lipschitz constant of g in some subset of X which contains the iterates), $\hat{\kappa}_g$ is the Lipschitz constant of g', and $\sigma > 0$ satisfies

$$\|w_{k+1} - w_k\| \geq \sigma \|x_k - x_{k-1}\|, \tag{2.6}$$

noting that if g is contractive then $\sigma = 1 - \kappa_g$ ([27] discusses the case when g is not contractive). The above result assumes $\sigma > 0\ \forall k$ and g is Lipschitz continuously differentiable. The result for general m is analogous, and from Theorem 5.3 of [27] we have that

$$\|w_{k+1}\| \leq \|w_k\| \left\{ \theta_k((1-\beta_k) + \kappa_g\beta_k) + C\hat{\kappa}_g \sum_{n=k-m_{k-1}}^{k} \|w_n\| \right\}, \tag{2.7}$$

where C depends on σ^{-1}, relaxation and gain parameters, as well as the degree to which the past m differences $w_{j+1} - w_j$ are linearly independent (note this can be controlled by reducing m if needed [27]). We note that Theorem 5.3 of [27] gives a more precise result, but (2.7) is sufficient for our analysis herein.

3 Anderson Acceleration for General Order Convergent Fixed Point Methods

We now study how Anderson acceleration would affect the convergence order for fixed-point iterations of the form $x_{k+1} = g(x_k)$, with g satisfying certain properties described below. We denote by x^* a fixed point of g.

Assumption 3.1 Let $g : D \subset X \to X$, with X a Hilbert space and $\|\cdot\|$ the associated norm, be a fixed-point iteration on a bounded convex set D containing x^* and satisfying

1. One of the following must hold:
   (a) there are constants $r > 1$ and $L_0 > 0$ with
   $$\|g(x+h) - g(x)\| \leq L_0\|h\|^r$$
   (b) g is Lipschitz continuous: $\|g(x+h) - g(x)\| \leq C_0\|h\|$, and there exists a continuous function $r : [0, \infty) \to (0, 1]$ satisfying $r(0) = 1$ and constant $L_0 \leq 1$ satisfying
   $$\|g(x+h) - g(x)\| \leq L_0\|h\|^{r(x-x^*)}$$

2. g is Fréchet differentiable, and its derivative $g' : D \times D \to X$ satisfies $\|g'(x; s)\| \leq C_1\|x\|\|s\|$.
3. g' is Lipschitz continuous $\|g'(x+h; s) - g'(x; s)\| \leq L_1\|h\|\|s\|$.

where the constants $C_1, C_0, L_1, L_0 > 0$ are independent of $x, h, s \in X$.

Remark 3.2 The assumptions for the linearly convergent case in [14, 27] are Lipschitz continuity together with Assumptions 2 and 3, and we note that Assumption 1 above implies Lipschitz continuity in either case. While the inequality $\|g(x+h) - g(x)\| \leq L_0\|h\|^{r(x-x^*)}$ is assumed on D, as our analysis to follow is for a single step of a fixed point method, we will consider a fixed $r < 1$ to be the local (sublinear) convergence order.

It is known that $\left\|g(x+h) - g(x) - g'(x; h)\right\|$ is a higher order term of $\|h\|$ as $\|h\| \to 0$, since g is Fréchet differentiable. Now we specify that it is second order in $\|h\|$ as $\|h\| \to 0$ under Assumption 3.1. This result will be used frequently in the analysis to follow.

Lemma 3.3 *Under Assumption 3.1, for any $x, x+h \in D$ the following inequality is satisfied*

$$\|g(x+h) - g(x) - g'(x; h)\| \leq \frac{L_1}{2}\|h\|^2. \tag{3.1}$$

Proof By the integral mean value theorem, for any $x, x+h \in D$ we have

$$g(x+h) - g(x) = \int_0^1 g'(x+th; h)\, dt.$$

Taking norms on both sides gives

$$\begin{aligned}\|g(x+h) - g(x) - g'(x; h)\| &= \left\|\int_0^1 \left(g'(x+th; h) - g'(x; h)\right)\, dt\right\| \\ &\leq \int_0^1 \|g'(x+th; h) - g'(x; h)\|\, dt \\ &\leq \int_0^1 L_1\|th\|\|h\|\, dt = \frac{L_1}{2}\|h\|^2,\end{aligned}$$

due to the Lipschitz continuity of g'. □

With Lemma 3.3, we will now prove results for how Anderson acceleration affects the convergence order of g.

3.1 Anderson Acceleration with Depth $m = 1$

Our analysis begins with the $m = 1$ AA case, and then extends to larger depths m in the next subsection. In this subsection, we will show that the convergence order of g is $\frac{r+1}{2}$ for a nonlinear solver satisfying Assumption 3.1.

When $m = 1$, the minimization step in Anderson algorithm (2.2) is reduced to

$$\alpha^{k+1} = \text{argmin}_\alpha\|(1-\alpha)w_{k+1} + \alpha w_k\|.$$

For notational simplicity, we define

$$\begin{aligned} e_j &= x_j - x_{j-1}, \quad \tilde{e}_j = g(x_j) - g(x_{j-1}), \\ w_{j+1} &= g(x_j) - x_j, \quad w_{j+1}^\alpha = (1-\alpha^{j+1})w_{j+1} + \alpha^{j+1}w_j. \end{aligned} \tag{3.2}$$

Also, from (2.4) and (2.2) we have equation (see e.g. [27]):

$$|\alpha^{j+1}|\|w_{j+1}-w_j\| = \sqrt{1-\theta_j^2}\|w_{j+1}\|. \tag{3.3}$$

This leads to two important inequalities that will allow us to bound the difference between successive iterations by the residual w_j

Lemma 3.4 *The following inequalities hold for any positive integer j*

$$\|e_{j-1}\| \le \frac{1}{\sigma|\alpha^j|}\sqrt{1-\theta_{j-1}^2}\|w_j\|, \tag{3.4}$$

$$\|e_j\| \le \left(\theta_{j-1} + \frac{1}{\sigma}\sqrt{1+\theta_{j-1}^2}\right)\|w_j\|. \tag{3.5}$$

Equation (3.4) can be derived directly from (2.6) and (3.3), while Eq. (3.5) is obtained from

$$\|e_j\| = \|w_j^\alpha - \alpha^j e_{j-1}\| \le \theta_{j-1}\|w_j\| + |\alpha^j|\|e_{j-1}\|,$$

thanks to $w_{j+1}^\alpha = e_{j+1} + \alpha^{j+1}e_j$, and the triangle inequality.

Now we give the result for $m = 1$ Anderson acceleration convergence order for general nonlinear solvers.

Theorem 3.5 (Convergence order for $m = 1$) *Consider AA applied to the fixed point iteration defined by $x_{k+1} = g(x_k)$ satisfying Assumption 3.1, with the previous two iterates sufficiently close to the fixed point. We have the one-step bound for the residual w_{k+1}:*

$$\|w_{k+1}\| \le C(\|w_k\|^{\frac{r+1}{2}} + \|w_k\|^2), \tag{3.6}$$

where C is a positive constant depending on $\alpha^k, C_1, L_0, L_1, \theta_{k-1}, \sigma, x^*$.

Remark 3.6 We thus observe that $m = 1$ AA reduces the convergence order of superlinearly converging methods, but increases the (local) order for sublinearly converging methods. This result is also consistent with what is already known for linearly convergent methods, i.e. AA does not affect the order of linearly converging methods but improves the rate.

Proof From the polarization identity, we have

$$\begin{aligned}
&2(w_{k+1}, g'(x_{k-1}; e_k) + \alpha^k g'(x_{k-2}; e_{k-1})) \\
&\quad = \|w_{k+1}\|^2 + \left\|g'(x_{k-1}; e_k) + \alpha^k g'(x_{k-2}; e_{k-1})\right\|^2 \\
&\qquad - \left\|w_{k+1} - g'(x_{k-1}; e_k) - \alpha^k g'(x_{k-2}; e_{k-1})\right\|^2,
\end{aligned}$$

which immediately leads to

$$\begin{aligned}
\|w_{k+1}\|^2 \le &\left\|w_{k+1} - g'(x_{k-1}; e_k) - \alpha^k g'(x_{k-2}; e_{k-1})\right\|^2 \\
&+2(w_{k+1}, g'(x_{k-1}; e_k) + \alpha^k g'(x_{k-2}; e_{k-1})),
\end{aligned}$$

by dropping the nonnegative term $\|g'(x_{k-1}; e_k) + \alpha^k g'(x_{k-2}; e_{k-1})\|^2$. Now we bound the right hand side term by term. To keep the analysis clean, we denote

$$\psi_j = g(x_j) - g(x_{j-1}) - g'(x_{j-1}; e_j).$$

From the triangle inequality, Lemma 3.3 and inequalities (3.4)–(3.5) we obtain

$$\begin{aligned}\|w_{k+1} - g'(x_{k-1}; e_k) - \alpha^k g'(x_{k-2}; e_{k-1})\|^2 &= \|\psi_k + \alpha^k \psi_{k-1}\|^2 \\ &\leq 2\|\psi_k\|^2 + 2|\alpha^k|^2 \|\psi_{k-1}\|^2 \\ &\leq \frac{L_1^2}{2}\|e_k\|^4 + |\alpha^k|^2 \frac{L_1^2}{2}\|e_{k-1}\|^4 \\ &\leq C\|w_k\|^4,\end{aligned}$$

where C is a constant depending on $\alpha^k, L_1, \theta_{k-1}, \sigma$. Utilizing Assumption 3.1 that g' is bounded, we have

$$\begin{aligned}\|g'(x_{k-1}; e_k) + \alpha^k g'(x_{k-2}; e_{k-1})\| &\leq \|g'(x_{k-1}; e_k)\| + |\alpha^k| \|g'(x_{k-2}; e_{k-1})\| \\ &\leq C_1\|x_{k-1}\|\|e_k\| + |\alpha^k| C_1 \|x_{k-2}\|\|e_{k-1}\| \leq C\|w_k\|,\end{aligned}$$

since the previous two iterates are assumed close to the fixed point.

On the other hand, from Cauchy-Schwarz inequality and the identity $w_{k+1} = \tilde{e}_k + \alpha^k \tilde{e}_{k-1}$, we get

$$\begin{aligned}&(w_{k+1}, g'(x_{k-1}; e_k) + \alpha_k g'(x_{k-2}; e_{k-1})) \\ &\quad = (\tilde{e}_k + \alpha^k \tilde{e}_{k-1}, g'(x_{k-1}; e_k) + \alpha_k g'(x_{k-2}; e_{k-1})) \\ &\quad \leq \|\tilde{e}_k + \alpha^k \tilde{e}_{k-1}\| \|g'(x_{k-1}; e_k) + \alpha_k g'(x_{k-2}; e_{k-1})\| \\ &\quad \leq \left(L_0\|e_k\|^r + |\alpha^k| L_0 \|e_{k-1}\|^r\right) C\|w_k\| \leq C\|w_k\|^{1+r},\end{aligned}$$

thanks to Assumption 3.1 for the convergence order of g, and (3.4)–(3.5). Combining the inequalities above, we get

$$\begin{aligned}\|w_{k+1}\|^2 &\leq 2(w_{k+1}, g'(x_{k-1}; e_k) + \alpha_k g'(x_{k-2}; e_{k-1})) \\ &\quad + \|w_{k+1} - g'(x_{k-1}; e_k) - \alpha_k g'(x_{k-2}; e_{k-1})\|^2 \\ &\leq C\left(\|w_k\|^{r+1} + \|w_k\|^4\right).\end{aligned}$$

Taking square-roots on both sides finishes the proof. □

3.2 Anderson Acceleration with $m > 1$

We consider now the case of depth $m > 1$ and prove a result for how AA affects the convergence order in this case. With $m = 2$, the minimization step in (2.2) reduces to

$$(\alpha_1^{k+1}, \alpha_2^{k+1}) = \text{argmin}_{\alpha_1,\alpha_2} \|(1 - \alpha_1 - \alpha_2)w_{k+1} + \alpha_1 w_k + \alpha_2 w_{k-1}\|.$$

We reuse the notation defined in (3.2) except for w_{k+1}^α. For the case of $m = 2$,

$$w_{k+1}^\alpha = (1 - \alpha_1^{k+1} - \alpha_2^{k+1})w_{k+1} + \alpha_1^{k+1} w_k + \alpha_2^{k+1} w_{k-1}.$$

Without loss of generality, we assume $\alpha_2^{k+1} \neq 0$, otherwise, the minimization step is back to the AA with $m = 1$ case. Now we list two inequalities related to residuals which are proven in [14, 27, 41]:

$$\|w_j - w_{j-1}\| \le \|w_j\| + \|w_{j-1}\|, \tag{3.7}$$

$$|\alpha_2^{j+1}|\|w_{j-1} - w_{j-2}\| \le \left(\sqrt{1-\theta_j^2} + \left|\alpha_1^{j+1} + \alpha_2^{j+1}\right|\right)\|w_j\| + \left|\alpha_1^{j+1} + \alpha_2^{j+1}\right|\|w_{j-1}\|. \tag{3.8}$$

Next, we bounds the difference between successive iterations by residuals using the two inequalities above.

Lemma 3.7 *For any step with $\alpha_2^{j+1} \neq 0$, we have*

$$\|e_{j-2}\|, \|e_{j-1}\|, \|e_j\| \le C\left(\|w_j\| + \|w_{j-1}\|\right), \tag{3.9}$$

where C is a positive constant depending on $\alpha_1^j, \alpha_2^j, \theta_{j-1}, \sigma$.

Proof From (2.6) and (3.7)–(3.8), we immediately have the estimates

$$\begin{aligned}\|e_{j-1}\| &\le \frac{1}{\sigma}\|w_j - w_{j-1}\| \le \frac{1}{\sigma}\left(\|w_j\| + \|w_{j-1}\|\right),\\ \|e_{j-2}\| &\le \frac{1}{\sigma}\|w_{j-1} - w_{j-2}\| \le \frac{1}{\sigma|\alpha_2^{j+1}|}\\ &\quad \left((1 + |\alpha_1^{j+1} + \alpha_2^{j+1}|)\|w_j\| + |\alpha_1^{j+1} + \alpha_2^{j+1}|\|w_{j-1}\|\right).\end{aligned}$$

Utilizing the identity $w_j^\alpha = e_j + (\alpha_1^j + \alpha_2^j)e_{j-1} + \alpha_2^j e_{j-2}$, we get

$$\|e_j\| \le \theta_{j-1}\|w_j\| + |\alpha_1^j + \alpha_2^j|\|e_{j-1}\| + |\alpha_2^j|\|e_{j-2}\|.$$

Combining these inequalities finishes the proof. □

We can now present and prove the convergence order result for AA $m = 2$.

Theorem 3.8 (Convergence order for $m = 2$) *Assuming $\alpha_2^{k+1} \neq 0$, we have the following one-step bound of the residual w_{k+1}:*

$$\|w_{k+1}\| \le C\left((\|w_k\| + \|w_{k-1}\|)^{\frac{r+1}{2}} + (\|w_k\| + \|w_{k-1}\|)^2\right), \tag{3.10}$$

where C is a positive constant depending on $\alpha_1^k, \alpha_2^k, L_0, L_1, \theta_{k-1}, \sigma$.

Proof From the polarization identity, we have the equality

$$\begin{aligned}&2(w_{k+1}, g'(x_{k-1}; e_k) + (\alpha_1^k + \alpha_2^k)g'(x_{k-2}; e_{k-1}) + \alpha_2^k g'(x_{k-3}; e_{k-2}))\\ &\quad = \|w_{k+1}\|^2 + \left\|g'(x_{k-1}; e_k) + (\alpha_1^k + \alpha_2^k)g'(x_{k-2}; e_{k-1}) + \alpha_2^k g'(x_{k-3}; e_{k-2})\right\|^2\\ &\quad - \left\|w_{k+1} - g'(x_{k-1}; e_k) - (\alpha_1^k + \alpha_2^k)g'(x_{k-2}; e_{k-1}) - \alpha_2^k g'(x_{k-3}; e_{k-2}))\right\|^2,\end{aligned}$$

which after rearranging and dropping a positive term from the right hand side of the equation leads to the inequality

$$\begin{aligned}\|w_{k+1}\|^2 &\le 2(w_{k+1}, g'(x_{k-1}; e_k) + (\alpha_k^1 + \alpha_k^2)g'(x_{k-2}; e_{k-1}) + \alpha_k^2 g'(x_{k-3}; e_{k-2}))\\ &\quad + \left\|w_{k+1} - g'(x_{k-1}; e_k) - (\alpha_k^1 + \alpha_k^2)g'(x_{k-2}; e_{k-1})\right.\\ &\quad \left. - \alpha_k^2 g'(x_{k-3}; e_{k-2}))\right\|^2.\end{aligned} \tag{3.11}$$

To estimate the last term on the right hand side of (3.11) we use the identity $w_{k+1} = \tilde{e}_k + (\alpha_1^k + \alpha_2^k)\tilde{e}_{k-1} + \alpha_2^k \tilde{e}_{k-2}$, the triangle inequality and Lemma 3.3 to obtain

$$\begin{aligned}
&\|w_{k+1} - g'(x_{k-1}; e_k) - (\alpha_1^k + \alpha_2^k) g'(x_{k-2}; e_{k-1}) - \alpha_2^k g'(x_{k-3}; e_{k-2}))\|^2 \\
&\quad = \|\psi_k + (\alpha_1^k + \alpha_2^k)\psi_{k-1} + \alpha_2^k \psi_{k-2}\|^2 \\
&\quad \le 2\|\psi_k\|^2 + 2|\alpha_1^k + \alpha_2^k|^2 \|\psi_{k-1}\|^2 + 2|\alpha_2^k|^2 \|\psi_{k-2}\|^2 \\
&\quad \le \frac{L_1^2}{2}\|e_k\|^4 + |\alpha_1^k + \alpha_2^k|^2 \frac{L_1^2}{2}\|e_{k-1}\|^4 + |\alpha_2^k|^2 \frac{L_1^2}{2}\|e_{k-2}\|^4,
\end{aligned}$$

where $\psi_j = g(x_j) - g(x_{j-1}) - g'(x_{j-1}; e_j)$. From Lemma 3.7 this reduces to

$$\begin{aligned}
&\|w_{k+1} - g'(x_{k-1}; e_k) - (\alpha_1^k + \alpha_2^k) g'(x_{k-2}; e_{k-1}) - \alpha_2^k g'(x_{k-3}; e_{k-2}))\|^2 \\
&\quad \le C\left(\|w_k\| + \|w_{k-1}\|\right)^4,
\end{aligned}$$

where C depends on $\alpha_1^k, \alpha_2^k, \sigma, \theta_{k-1}, L_1$. Similarly, we have

$$\|g'(x_{k-1}; e_k) + (\alpha_1^k + \alpha_2^k) g'(x_{k-2}; e_{k-1}) + \alpha_2^k g'(x_{k-3}; e_{k-2})\| \le C\left(\|w_k\| + \|w_{k-1}\|\right), \tag{3.12}$$

thanks to Assumption 3.1. Next, we bound the first term on the right hand side of (3.11). Applying Cauchy-Schwarz inequality, (3.12), the triangle inequality and Lemma 3.7 yields

$$\begin{aligned}
&(w_{k+1}, g'(x_{k-1}; e_k) + (\alpha_1^k + \alpha_2^k) g'(x_{k-2}; e_{k-1}) + \alpha_2^k g'(x_{k-3}; e_{k-2})) \\
&\quad \le \|w_{k+1}\| \|g'(x_{k-1}; e_k) + (\alpha_1^k + \alpha_2^k) g'(x_{k-2}; e_{k-1}) + \alpha_2^k g'(x_{k-3}; e_{k-2})\| \\
&\quad \le \left(\|\tilde{e}_k\| + |\alpha_1^k + \alpha_2^k| \|\tilde{e}_{k-1}\| + |\alpha_2^k| \|\tilde{e}_{k-2}\|\right) C\left(\|w_k\| + \|w_{k-1}\|\right) \\
&\quad \le \left(L_0\|e_k\|^r + |\alpha_1^k + \alpha_2^k| L_0 \|e_{k-1}\|^r + |\alpha_2^k| L_0 \|e_{k-2}\|^r\right) C\left(\|w_k\| + \|w_{k-1}\|\right) \\
&\quad \le C\left(\|w_k\| + \|w_{k-1}\|\right)^{r+1}.
\end{aligned}$$

Combining the inequalities above produces

$$\|w_{k+1}\|^2 \le C\left(\left(\|w_k\| + \|w_{k-1}\|\right)^{r+1} + \left(\|w_k\| + \|w_{k-1}\|\right)^4\right),$$

and taking square root finishes the proof. □

The $m = 1$ and $m = 2$ results can be extended to any positive integer m by a similar proof process. Therefore we have the following convergence order result for general depth m.

Theorem 3.9 (Convergence order for general $m \ge 1$) *Assuming $\alpha_k^{k-m_k} \ne 0$, we have one-step bound of residual w_{k+1} for general depth $m \ge 1$ AA:*

$$\begin{aligned}
\|w_{k+1}\| \le C\Big(&\left(\|w_k\| + \|w_{k-1}\| + \cdots + \|w_{k-m_k}\|\right)^{\frac{r+1}{2}} \\
&+ \left(\|w_k\| + \|w_{k-1}\| + \cdots + \|w_{k-m_k}\|\right)^2\Big),
\end{aligned} \tag{3.13}$$

where C is a constant depending on problem data.

3.3 Numerical Experiments

We perform two tests to illustrate the theoretical results above. The first test is for a 1D problem, to show methods converging superlinearly with order r are reduced with $m = 1$ AA to order $\frac{r+1}{2}$, although we find that AA-Newton is slightly better (and show in the next section that it should be). Second, we consider another 1D test, now to test sublinear convergence, again observing local order r convergence is improved to local order $\frac{r+1}{2}$. Our third test is for the regularized Bingham model of viscoplastic flow. The Picard iteration for this system is known from numerical tests in [5, 28] to converge sublinearly, and here we show that the convergence order is increased by AA, just as the theory above suggests.

3.3.1 1D Test for Superlinearly Converging Method

For our first experiment in this section we consider finding the root $x^* = 2$ for $f(x) = x^2 - x - 2$. We compute with fixed point iterations corresponding to the Newton iteration, Chebyshev iteration, Secant iteration, AA-Newton, AA-Chebyshev and AA-secant. Only $m = 1$ was used for AA, since the optimization problem is already solved exactly when $m = 1$ so higher m would not change anything. We used an initial guess of $x_0 = 10$, and computed until the residual for the fixed point problem was less than 10^{-10}. We recall from that the Chebyshev iteration to find a zero of a C^2 function f is defined by [1, 2, 18]

$$x_{n+1} = g(x_n) = x_n - \left(1 + \frac{1}{2}\frac{f(x_n)f''(x_n)}{(f'(x_n))^2}\right)\frac{f(x_n)}{f'(x_n)},$$

and is known to be cubically convergent.

Results are shown in Table 1 and Fig. 1. Table 1 shows the convergence orders calculated from the standard formula at each iteration, and we observe that Chebyshev is consistent with third order, Newton is consistent with second order, and Secant is consistent with 1.618, i.e. they are all consistent with their well known convergence orders. For AA-Chebyshev, the orders from successive iterates is inconclusive, however from Fig. 1 we see the convergence curve follows that of Newton which is second order; this is consistent with our theory that $r = 3$ convergence order is reduced by $m = 1$ AA to $\min\{\frac{3+1}{2}, 2\} = 2$. Finally, for AA-secant the theory predicts $\frac{1.618+1}{2} = 1.309$, and both Table 1 and Fig. 1 are consistent with this order. AA-Newton, on the other hand, has order approximately 1.62 which is greater than $\frac{2+1}{2} = 1.5$. While this is still consistent with the theory (since the converge order results are a lower bound), the fact that our analytical results appear sharp for AA-Secant and AA-Chebyshev but not for AA-Newton led us to consider AA-Newton in more detail in the next section; indeed, we do find AA-Newton is a special case and show in the next section that for $m = 1$ one should expect order 1.618.

3.3.2 1D Test for Sublinearly Converging Method

Next, we study how AA affects the convergence order of a sublinearly converging fixed-point iteration corresponding to the fixed point function $g(x) = \frac{x}{x+1}$, with initial guess $x_0 = 10$, and tolerance 10^{-10}. We consider g defined on $x \geq 0$, and note that for any positive x_0, the fixed point iteration will remain positive. From Fig. 2, we observe sublinear convergence for this 1D test, and almost linear convergence when AA is applied; AA clearly improves the convergence speed for the sublinear convergent iteration, which matches our expectation from Theorem 3.5.

Table 1 Shown above are calculated approximate convergence orders for the 1D test, using the calculation conv order $\approx \log(w_{k+1}/w_k)/\log(w_k/w_{k-1})$ where $w_k = |g(u_k) - u_k|$ is the residual at step k and g is the fixed point operator

Conv order $\approx \log(w_{k+1}/w_k)/\log(w_k/w_{k-1})$						
Iteration	Chebyshev	AA-Chebyshev	Newton	AA-Newton	Secant	AA-Secant
3	1.5599	1.3048	1.1892	0.6549	0.1810	0.4835
4	2.3641	1.4737	1.5269	1.5509	3.4982	0.3985
5	2.9024	0.4669	1.8928	1.3138	1.1463	8.9389
6	–	7.7745	1.9952	1.6119	1.7139	0.1049
7	–	1.2122	2.0000	1.5942	1.6315	7.4716
8	–	–	–	1.6152	1.6509	1.8849
9	–	–	–	1.6187	1.6187	1.3223
10	–	–	–	–	1.6193	1.3461
11	–	–	–	–	–	1.5703

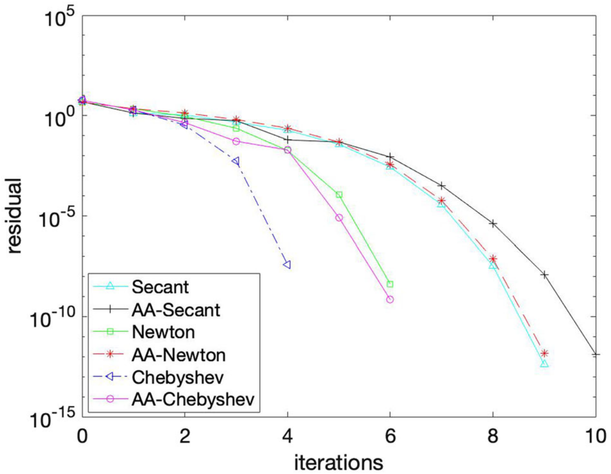

Fig. 1 Shown above are convergence plots for the 1D tests on the Secant method, Newton's method and Chebyshev method, with and without Anderson acceleration

In order to discuss how AA affects the convergence order locally (our theory predicts local order $r < 1$ is improved to at least local order $\frac{r+1}{2}$) for this iteration, we divide the convergence plot using the magnitude of residuals w_k, so that each piece is approximately linearly convergent. We color plot black, blue, red, green and magenta when w_k belongs to the intervals $[0.1, +\infty)$, $[0.01, 0.1)$, $[10^{-3}, 0.01)$, $[10^{-4}, 10^{-3})$, $(-\infty, 10^{-4})$ respectively, compute the average convergence order using formula $\log(w_{k+1}/w_k)/\log(w_k/w_{k-1})$ for each piece, and then summarize results in Table 2. By comparing the convergence orders in Table 2, we find that the local convergence order of iteration with AA is always greater than $(1 + r)/2$, and close to this value for $w_k \leq 10^{-3}$, which is consistent with Theorem 3.5.

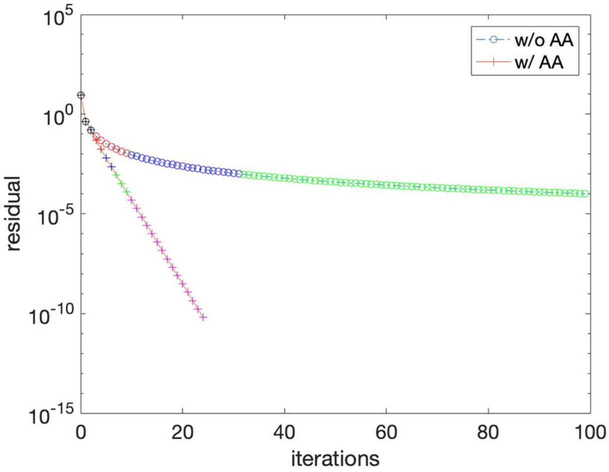

Fig. 2 Shown above are convergence plot for the 1D sublinear convergence test, with and without Anderson acceleration, the corresponding convergence order are summarized in Table 2

Table 2 Shown above are the average convergence order for the 1D sublinear convergence, on differential intervals of residuals, with and without Anderson acceleration

conv order $\approx \log(w_{k+1}/w_k)/\log(w_k/w_{k-1})$		
Residual interval	w/o AA	w/ AA
$10^{-2} \le w_k < 10^{-1}$	0.8060	1.0492
$10^{-3} \le w_k < 10^{-2}$	0.9457	0.9877
$10^{-4} \le w_k < 10^{-3}$	0.9831	0.9939
$w_k < 10^{-4}$	–	0.9995

3.3.3 Regularized Bingham

We consider for our second test simulation of the regularized Bingham equations, which are used to model viscoplastic flow. The system we consider is given by [10]

$$\begin{aligned} -\nabla \cdot \left(2\mu + \frac{\tau_s}{(|Du|^2+\epsilon^2)^{1/2}}\right) Du + \nabla p = f, \\ \nabla \cdot u = 0, \end{aligned} \tag{3.14}$$

where $\tau_s > 0$ is the yield stress, $\mu > 0$ is the plastic viscsoity, u is velocity, f is an external forcing, Du is the deformation tensor of u, ϵ is the regularization parameter, and the unknowns are the pressure p and velocity u.

We consider the Picard iteration for this system considered in [5, 28] which takes the form

$$\begin{aligned} -\nabla \cdot \left(2\mu + \frac{\tau_s}{(|Du_k|^2+\epsilon^2)^{1/2}}\right) Du_{k+1} + \nabla p_{k+1} = f, \\ \nabla \cdot u_{k+1} = 0. \end{aligned} \tag{3.15}$$

This linearization is known to be well-posed for any $\epsilon > 0$ under homogeneous Dirichlet boundary conditions [5]. For a fixed point iteration, we define our fixed point function g to be the solution operator to (3.15) equipped with a standard inf-sup stable mixed finite element discretization such as what is used in [5, 28].

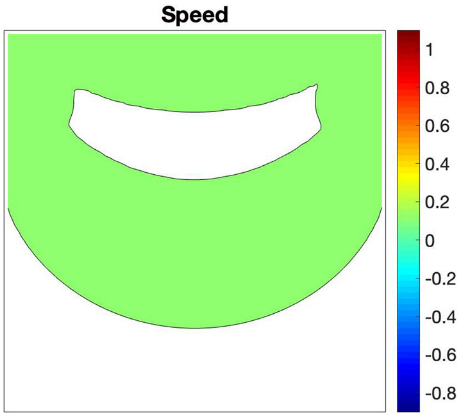

Fig. 3 Shown above are growth of the rigid region (white) for lid-driven flow by $\tau_s = 5$ when $h = 1/64$

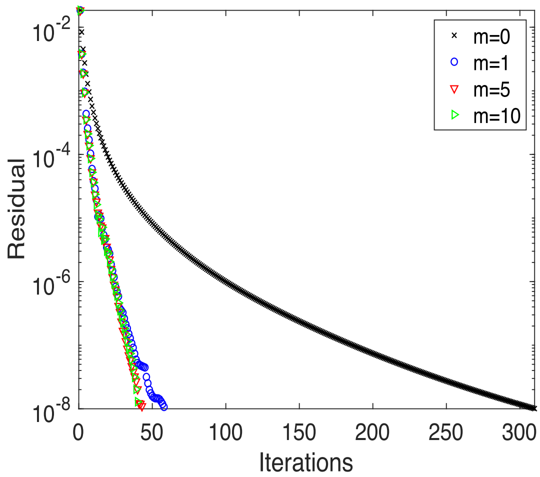

Fig. 4 Shown above are convergence plots for the regularized Bingham tests with varying m

The test problem we consider is the 2D driven cavity on the unit square $\Omega = (0, 1)^2$ also studied in [5, 10, 23, 24, 28]. Our spatial discretization uses (P_2, P_1) Taylor-Hood elements on a $\frac{1}{32}$ uniform mesh, enforcing strongly the Dirichlet boundary conditions $u|_{y=1} = (1, 0)^T$ and $u = 0$ on the other walls. We choose parameters $\tau_s = 5$, $f = 0$ and $\epsilon = 10^{-7}$, choose 0 as the initial guess, and compute until the L^2 velocity residual falls below 10^{-8}. We compute with varying m, but no relaxation since as discussed in [28] relaxation will slow the iteration down for these parameter choices. Figure 3 shows the growth of rigid region (white) for lid-driven flow with these parameter choices, they are well agree with the literature [5, 28].

Convergence plots for $m = 0$, $m = 1,\ 5,\ 10$ are shown in Fig. 4. The Picard iteration appears to converge sublinearly, and from the plot data we find the convergence order for Picard begins near 0.8 and then slowly increases to nearly 1 once the residual is less than 10^{-6}. The AA-Picard plots are also seen to be sublinear, and begin with convergence order calculated to be approximately 0.9 and then increase to near 1, and there is little difference in convergence for any $m > 0$. These results are consistent with our theory for changing local order r convergence to local order $\frac{r+1}{2}$.

4 AA-Newton Convergence

As shown in the previous section, AA-Newton's convergence order appears numerically to be better than the order 1.5 that our theory predicts (noting that our theory gives a lower bound on convergence order, but appears sharp for multiple methods in the previous section). Thus, we consider now the case of AA-Newton convergence order, now denoting $g(x) = x - f'(x)^{-1}f(x)$ for some given function $f : X \to X$ for which a root x^* is desired, and $f'(x)^{-1}$ is defined appropriately. We will assume $f'(x^*) \neq 0$, i.e. x^* is not a multiple root, and that g is Lipschitz continuously differentiable. The multiple root case for AA-Newton is discussed in [26], and it is found that in this case Newton converges linearly and so the convergence results in Sect. 2 (from [27]) apply directly with θ_k improving the linear convergence rate. We also assume that the initial guess of the algorithm is sufficiently good, which for asymptotic analysis is equivalent to assuming the last m iterates are close to the root.

The key observance for determining AA-Newton convergence order is to notice that Newton is a single step fixed point iteration with $g'(x^*) = 0$, and so the convergence results of [27] from Sect. 2 apply, but now with $\kappa_g = 0$. Hence from (2.7) we obtain that the AA-Newton residuals satisfy

$$\|w_{k+1}\| \leq \theta_k(1-\beta_k)\,\|w_k\| + C\hat{\kappa}_g\,\|w_k\| \sum_{n=k-m}^{k} \|w_n\|\,. \tag{4.1}$$

4.1 No Relaxation

If very close to the root, in general one would not use relaxation since the method is already contractive/converging and relaxation will only slow down superlinear convergence. Assuming $\beta_k = 1$, we obtain the estimate

$$\|w_{k+1}\| \leq C\hat{\kappa}_g\,\|w_k\| \sum_{n=k-m_{k-1}}^{k} \|w_n\| = C\hat{\kappa}_g\left(\|w_k\|^2 + \|w_k\|\|w_{k-1}\| + \cdots \|w_k\|\|w_{k-m}\|\right).$$

In a converging method the last term on the right hand side is dominant, and so in the asymptotic range this reduces to

$$\|w_{k+1}\| \overset{\sim}{\leq} C\hat{\kappa}_g\|w_k\|\|w_{k-m}\|.$$

From here, one can follow theory similar to that for proving convergence of the secant method (see e.g. [7]) to find that the order of such a method will be (at least) the largest positive real root of

$$\alpha^{m+1} - \alpha^m - 1 = 0.$$

These expected convergence orders for AA-Newton are given in Table 3 for varying m. It is no coincidence that AA-Newton with $m = 1$ has the same order as the secant method, since $\|w_{k+1}\| \leq c\|w_k\|\|w_{k-1}\|$ is a key estimate in the Secant method convergence proof from which the convergence order is directly determined to be 1.618 [7]. This result explains the AA-Newton convergence behavior in the previous section.

Table 3 Shown above are expected convergence orders for AA-Newton with varying m

m	Conv order for AA-Newton
0	2
1	1.618
2	1.466
3	1.380
4	1.325
14	1.147

4.2 With Relaxation

The case of Newton with relaxation is important as well. It is often the case the Newton is used with relaxation, especially at early iterations, and once the direction is found the relaxation parameter may be determined with a line search that minimizes a residual. Since the Newton direction is a descent direction for small enough step size, the line search Newton method can improve robustness especially when not very close to a root (when a full step size should be used to obtain quadratic convergence).

For a single step, the convergence of relaxed (with parameter β) Newton is given by

$$\|x_{k+1} - x^*\| \le (1-\beta)\|x_k - x^*\| + \beta C_{g''}\|x_k - x^*\|^2.$$

Meanwhile, the estimate for $m = 1$ AA-Newton convergence with parameter β is

$$\|w_{k+1}\| \le \theta_k(1-\beta)\,\|w_k\| + C\hat{\kappa}_g\,\|w_k\| \sum_{n=k-m}^{k} \|w_n\|\,. \tag{4.2}$$

Assuming the $(k-m)^{th}$ iterate is sufficiently close to the root, we have for both of these estimates that the higher order terms are negligible, leaving

$$\text{Newton error: } \|x_{k+1} - x^*\| \lesssim (1-\beta)\|x_k - x^*\|,$$

$$\text{AA-Newton residual: } \|w_{k+1}\| \lesssim \theta_k(1-\beta)\,\|w_k\|\,.$$

Hence we observe the advantage of AA-Newton, as the $\theta_k < 1$ will scale the linear convergence rate, making AA-Newton convergence faster. AA-Newton does assume the prior m iterates are sufficiently close to the root, so this result may break down for AA-Newton for m too large. But for smaller m the advantage of AA for relaxed Newton is clear.

4.3 Numerical Tests for AA-Newton

To illustrate the theory above for AA-Newton, we give results for tests on two application problems: the nonlinear Helmholtz (NLH) equation from optics, and the Boussinesq model for non-isothermal flow. Our tests show convergence (approximately) follows the rates of the table for unrelaxed Newton, and that AA improves convergence in relaxed Newton.

4.3.1 AA-Newton Test 1: Convergence Order for Nonlinear Helmholtz Equation

For our first test of AA-Newton we consider solving the nonlinear Helmholtz (NLH) equation from optics. The interest here is in the propagation of continuous-wave laser beams through

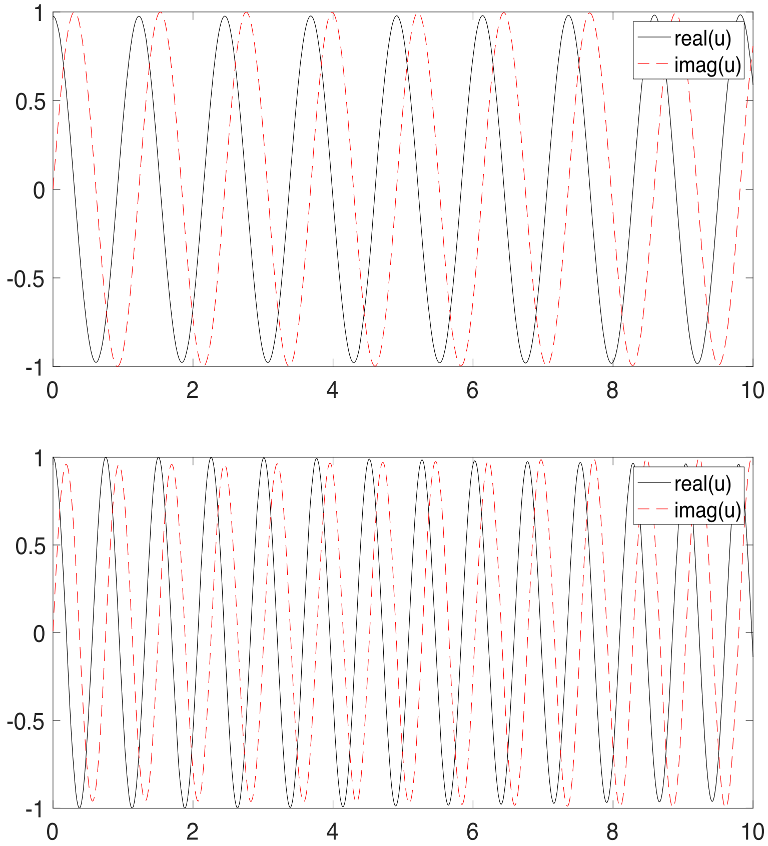

Fig. 5 Shown above are solutions to NLH for $k_0 = 5,\ \epsilon = 0.05$ (top) and $k_0 = 8,\ \epsilon = 0.09$ (bottom), which are used in numerical tests in Sects. 4.3.1 and 4.3.3

transparent dielectrics. The 1D NLH system is written as: Find $u : [0, 10] \to \mathbb{C}$ satisfying

$$u_{xx} + k_0^2 \left(1 + \epsilon(x)|u|^2\right) u = 0, \quad 0 < x < 10,$$

where $u = u(x)$ denotes the (complex) scalar electric field, k_0 is the linear wavenumber, and $\epsilon(x)$ is a normalized quantity involving the linear index of refraction and the Kerr coefficient. The physically consistent two-way boundary condition is given by [9, 15]:

$$u_x + ik_0 u = 2ik_0 \text{ at } x = 0, \quad u_x - ik_0 u = 0 \text{ at } x = 10.$$

Despite being 1D, NLH can be quite challenging for nonlinear solvers due to its cubic nonlinearity [8, 9].

The Newton iteration for this system takes the form

$$\begin{aligned}
&u_{j+1_{xx}} + k_0^2 u_{j+1} + k_0^2 \epsilon(x) \left(u_{j+1} * u_j u_j + u_j^* u_{j+1} u_j + u_j^* u_j u_{j+1} - 2u_j^* u_j u_j\right) = 0,\\
&\qquad 0 < x < 10,\\
&u_{j+1_x} + ik_0 u_{j+1} = 2ik_0, \quad x = 0,\\
&u_{j+1_x} - ik_0 u_{j+1} = 0, \quad x = 10.
\end{aligned}$$

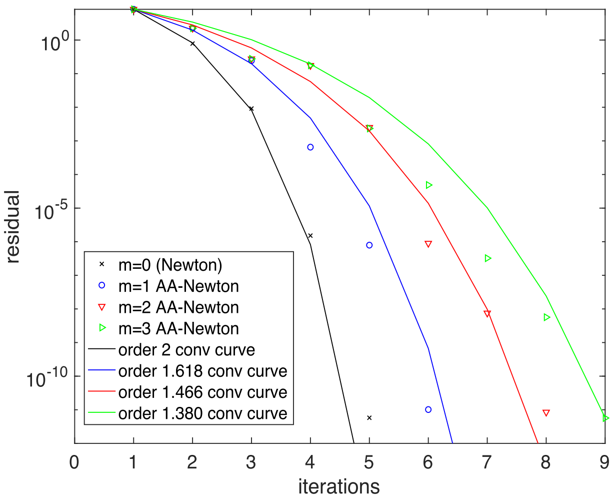

Fig. 6 Shown above is convergence data for NLH along with predicted convergence order curves

We discretize in space using a second order centered finite difference with $N = 2001$ equally spaced nodes, and with this discretization we obtain a Newton fixed point iteration we denote by $u^h_{j+1} = g(u^h_j)$. For an initial guess we use the linear interpolant of the linear Helmholtz equation solution, $u^h_0 = I^h(\cos(k_0 x) + i\sin(k_0 x))$. We consider parameters $k_0 = 5$ and constant $\epsilon = 0.05$, and run the algorithm using $m = 0$ (usual Newton), along with $m = 1, 2, 3$, all with no relaxation ($\beta = 1$). A plot of the solution is shown in Fig. 5. The AA optimization problem uses the $L^2(a, b)$ norm, and the iterations were run until the residual satisfied $\|u^h_{j+1} - u^h_j\|_{L^2(a,b)} < 10^{-10}$. Results are shown in Fig. 6 as convergence plots together with curves representing order 2, 1.618, 1.466 and 1.380 convergence (convergence table do not give conclusive evidence for this problem, as the volatility of the convergence can be seen in the plot for $m \geq 2$). We observe the convergence data is in general agreement with the convergence curves with orders from Table 3.

4.3.2 Differentially Heated Complex Domain

Next, we present results from a Boussinesq problem modeling non-isothermal flow, which typically are flows driven by buoyancy in problems such as ventilation, solar collectors, window insulation and many others. The steady Boussinesq system takes the following form in a domain $\Omega \subset \mathbb{R}^d$ (d=2 or 3):

$$(u \cdot \nabla)u - \nu\Delta u + \nabla p = Ri\langle 0, \theta\rangle^T + f,$$
$$\nabla \cdot u = 0,$$
$$(u \cdot \nabla)\theta - \kappa\Delta\theta = \gamma, \tag{4.3}$$

with u representing the velocity, p the pressure, θ the temperature (or density), and f and γ are the external momentum forcing and thermal sources. The kinematic viscosity $\nu > 0$ is defined as the inverse of the Reynolds number ($Re = \nu^{-1}$), and the thermal conductivity $\kappa = Re^{-1}Pr^{-1}$ where Pr is the Prandtl number and Ri is the Richardson number. Appropriate boundary conditions are required to determine the system. The Rayleigh number is defined

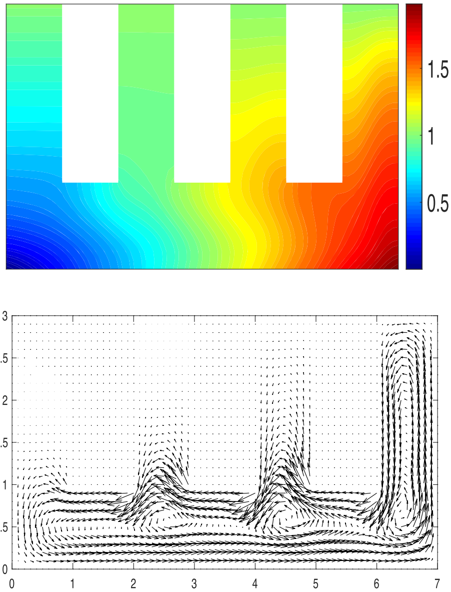

Fig. 7 Plots above show the temperature (top) and velocity (bottom) of the Boussinesq solution $Ra = 2100$

by $Ra = Ri \cdot Re^2 \cdot Pr$, and higher Ra leads to more complex physics as well as more difficulties in numerically solving the system.

The Newton iteration for this system takes the form

$$(u_{k-1} \cdot \nabla)u_k + (u_k \cdot \nabla)u_{k-1} - (u_{k-1} \cdot \nabla)u_{k-1} - \nu\Delta u_k + \nabla p_k = Ri\langle 0, \theta_k\rangle^T + f, \quad (4.4)$$

$$\nabla \cdot u_k = 0, \quad (4.5)$$

$$(u_{k-1} \cdot \nabla)\theta_k + (u_k \cdot \nabla)\theta_{k-1} - (u_{k-1} \cdot \nabla)\theta_{k-1} - \kappa\Delta\theta_k = \gamma, \quad (4.6)$$

together with appropriate boundary conditions.

We consider a test problem from [30] which is on a complex domain, enforces temperature boundary conditions $T(x, 1) = 1, T(x, 0) = \frac{2x}{7}$, and $\nabla T \cdot n = 0$ on all other boundaries, and no-slip velocity. We use a barycenter refined triangulation with (P_2, P_1^{disc}) Scott-Vogelius elements, and P_2 for temperature, which provides 30,705 total degrees of freedom. Solution plots for $Ra = 2100$ are shown in Fig. 7. We selected parameters $\nu = 0.01$, $\kappa = 0.01$ and Richardson number $Ri = 0.21$ to create Rayleigh number $Ra = 2100$. We computed with AA-Newton using $m = 0, 1, 2, 5$ and no relaxation, and results are shown in Fig. 8. Here we observe that the convergence data agrees well with the predicted convergence order curves, once the residuals are sufficiently small.

4.3.3 Improving Relaxed Newton Convergence with AA

We consider again the NLH test from above, now with parameters $k_0 = 8$ and $\epsilon = 0.09$ (a plot of the solution is shown in Fig. 5), and for varying relaxation parameter $\beta = 1, 0.5$ and adaptive β ($\beta = 0.5$ until the residual is reduced to below 10^{-2} and then $\beta = 1$). Results are shown in Fig. 9, and we observe immediately that Newton ($m = 0$, $\beta = 1$) fails to converge, at least not in the first 200 iterations. Interestingly, each of $m = 1, 2, 3$ do achieve convergence without $\beta = 1$. As expected from our theory above, for the $\beta = 1$ case, convergence deteriorated as m was increased from 1 to 2 to 3.

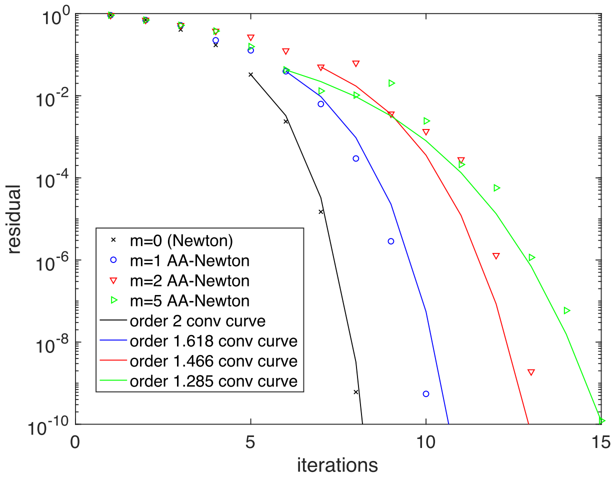

Fig. 8 Shown above are convergence plots of AA-Newton for varying m

For relaxed Newton ($m = 0$), we observe that $\beta = 0.5$ allows for convergence, and as expected the convergence is linear (see Fig. 9 at the center). As predicted by the theory, we also observe that relaxed AA-Newton improves on Newton in its linear convergence rate. Of course, for large enough m, the higher order terms created will eventually dominate the linear term at earlier iterations and this will slow the convergence; this seems to be the effect on early iterates for $m = 3$ although it was still able to recover and provide the fastest convergence of those tested.

Since relaxation provided convergence but this convergence is only linear, we did a final test where $\beta = 0.5$ until the residual is reduced to below 10^{-2} and then we set $\beta = 1$. Results are shown in Fig. 9 at the right, and we observe good convergence for each of $m = 0, 1, 2, 3$, although $m = 1$ performed best. This is explained by $m = 1$ reaching the 10^{-2} level first and then superlinear convergence taking over and winning before the quadratic convergence for $m = 0$ even gets started.

5 Conclusions

We have investigated the convergence order of AA applied to various fixed point iteration solvers. For superlinearly converging methods of order r, we prove a new convergence theory that shows such methods converge with order (at least) $\min\{2, \frac{r+1}{2}\}$ for $m = 1$, and derived expressions for convergence order for $m > 1$; these theories also hold for local order $r < 1$ sublinear convergence. These theories suggest slower convergence for superlinearly converging methods as m is increased. We showed numerically this was a sharp bound for AA-Chebyshev and AA-Secant, as well as for a sublinearly converging 1D test problem and sublinearly converging Picard iteration for a regularized Bingham problem. For AA-Newton, we show analytically and numerically that in the asymptotic range, AA reduces the convergence order from 2 to the largest positive root of $\alpha^{m+1} - \alpha^m - 1$ (1.618 for $m = 1$, 1.466 for $m = 2$ and so on).

The results herein are a new contribution to the theory of AA, which is quickly becoming a widely used method but for which there are very few analytical results. The results for

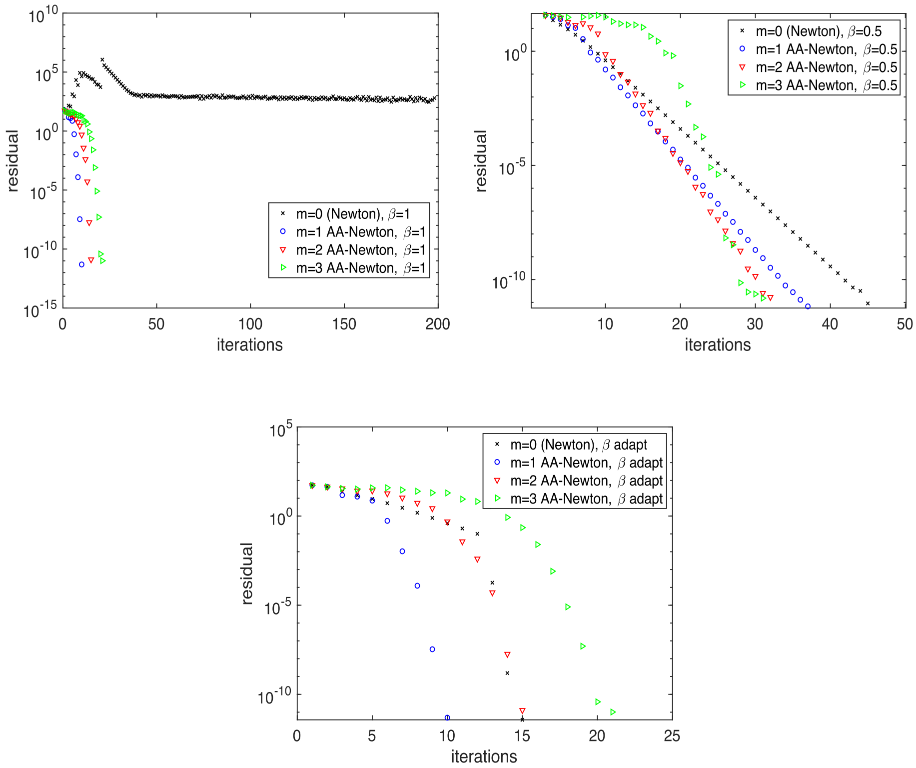

Fig. 9 Shown above are convergence plots for AA-Newton with $k_0 = 8$ and constant $\epsilon = 0.09$, for $\beta = 1$ (top left), $\beta = 0.5$ (top right) and adaptive β (bottom)

sublinearly converging iterations, on the other hand, were both positive and surprising (at least to us), with AA significantly helping such iterations. On the other hand, our results turn out to be negative for superlinearly converging methods, with the asymptotic convergence worsening as m increases; still these results are an important contribution to AA theory. However, it is important to note that the results are asymptotic, and so they do *not* suggest anything about how AA may or may not expand the convergence radius when applied to a particular superlinearly converging solver. This remains an important an open problem which the authors hope to study in the near future.

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Availability of Data and Materials The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Code Availability The code for the current study is available from the corresponding author on reasonable request.

Declarations

Conflict of interest The authors have no conflicts of interest to declare that are relevant to the content of this article. The authors have no relevant financial or non-financial interests to disclose.

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