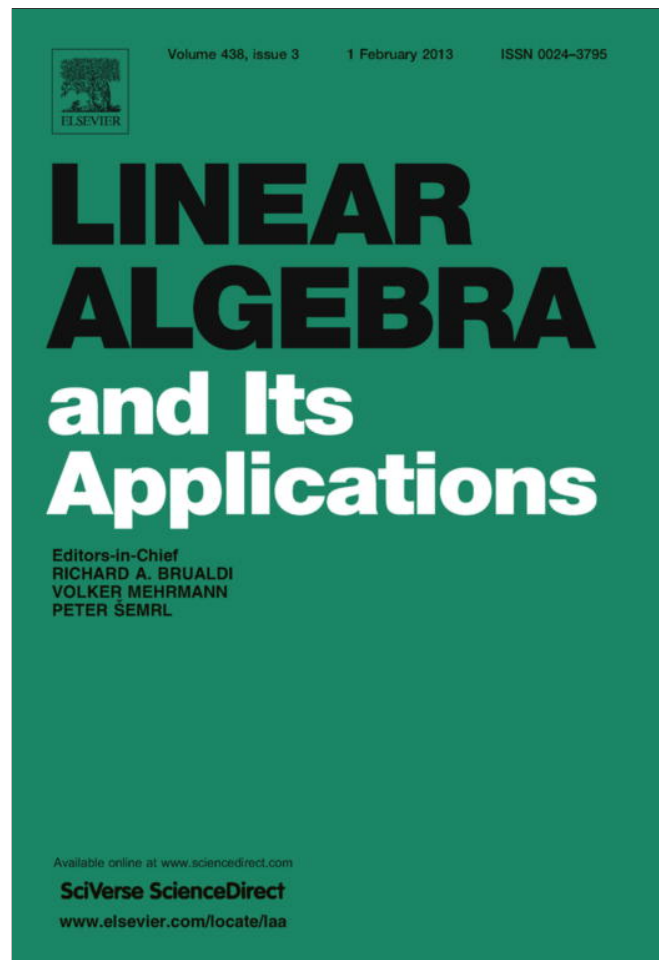


Provided for non-commercial research and education use.
Not for reproduction, distribution or commercial use.



This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

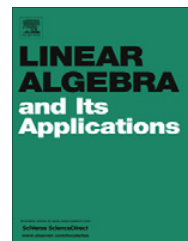
In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

<http://www.elsevier.com/copyright>



Contents lists available at SciVerse ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

A characterization of the behavior of the Anderson acceleration on linear problems

Florian A. Potra^{a,*}, Hans Engler^b

^a Department of Mathematics & Statistics, University of Maryland, Baltimore County, 1000 Hilltop Circle, Baltimore, MD 21250, USA

^b Department of Mathematics, Georgetown University, Box 571233, Washington, DC 20057, USA

ARTICLE INFO

Article history:

Received 12 February 2011

Accepted 25 June 2012

Available online 5 November 2012

Submitted by V. Mehrmann

Keywords:

Anderson acceleration

Anderson mixing

GMRES

ABSTRACT

We give a complete characterization of the behavior of the Anderson acceleration (with arbitrary nonzero mixing parameters) on linear problems. Let ν be the grade of the residual at the starting point with respect to the matrix defining the linear problem. We show that if Anderson acceleration does not stagnate (that is, produces different iterates) up to ν , then the sequence of its iterates converges to the exact solution of the linear problem. Otherwise, the Anderson acceleration converges to a point that is not a solution. Anderson acceleration and GMRES are essentially equivalent up to the index where the iterates of Anderson acceleration begin to stagnate. This result holds also for an optimized version of Anderson acceleration, where at each step the mixing parameter is chosen so that it minimizes the residual of the current iterate.

© 2012 Elsevier Inc. All rights reserved.

1. Introduction

The Anderson acceleration, or Anderson mixing, was initially developed in 1965 by Donald Anderson [1] as an iterative procedure for solving some nonlinear integral equations arising in physics. It turns out that the Anderson acceleration is very efficient for solving other types of nonlinear equations as well, see [2,6], and the literature cited therein. In [6] it was shown that for linear problems written in fixed point form, the Anderson acceleration, with all mixing parameters equal to 1, and GMRES are “essentially equivalent”. In the present paper we extend the results of [6] for linear problems to allow general nonzero mixing parameters. By introducing the notion of index of the Anderson acceleration, $\mu(A, x_0)$, we manage to give a complete characterization of the behavior

* Corresponding author. Tel.: +1 410 455 2429; fax: +1 410 455 1066.

E-mail addresses: potra@umbc.edu (F.A. Potra), engler@georgetown.edu (H. Engler).

¹ Research supported in part by the National Science Foundation under Grant 0728878.

of the Anderson acceleration with infinite history on linear problems. We show that the index of the Anderson acceleration is the same for any choice of nonzero mixing parameters, and that it can be expressed in terms of the stagnation index of the GMRES method. The main result of the paper shows that if the index of the Anderson acceleration coincides with the grade of the residual at the starting point with respect to the matrix defining the linear problem, $\nu(A, r_0)$ [7, p. 37], then the Anderson acceleration converges to the exact solution of the linear problem in either $\nu(A, r_0)$ or $\nu(A, r_0) + 1$ steps. If $\mu(A, x_0) < \nu(A, r_0)$, then the Anderson acceleration converges to a point that is not a solution. We also investigate the optimal Anderson acceleration, where at each step the mixing parameter is chosen so that it minimizes the residual of the current iterate. We show that the performance of the optimal Anderson acceleration is not essentially better than the performance of the Anderson acceleration with arbitrary nonzero mixing parameters.

2. Simple mixing

Consider the linear equation

$$Ax + b = 0 \tag{1}$$

where A is a nonsingular $N \times N$ matrix and b is a given N vector. We wish to solve (1) with various iterative methods that produce sequences $x_n^{[M]}$ where the superscript $[M]$ indicates the method that is being used. Let $x^* = -A^{-1}b$ be the exact solution of this problem. Since the exact solution is usually not known, the errors $x_n^{[M]} - x^*$ are difficult to estimate, so that the performance of the method is assessed by analyzing the residuals $Ax_n^{[M]} + b$. All methods use the same starting point $x_0^{[M]} = x_0$ at which the residual is $r_0 = Ax_0 + b$.

Consider now the simple fixed point iteration

$$x_{n+1} = x_n + Ax_n + b = Mx_n + b \tag{2}$$

where $M = I + A$. Of course this scheme need not converge, and an improvement consists in iterating

$$x_{n+1}^S = (1 - \beta)x_n^S + \beta (Mx_n^S + b) = x_n^S + \beta (Ax_n^S + b) \tag{3}$$

where β is a suitably chosen parameter. The method averages or “mixes” the previous iterate and the new fixed point iterate. Following [2], we shall call this iteration *simple mixing*. It will be indicated with the superscript S .

3. GMRES and Anderson mixing (Anderson acceleration)

The GMRES method for the equation $Ax + b = 0$ determines x_n^G as

$$x_n^G = x_0 + z_n, \quad \text{where } z_n = \operatorname{argmin}_{z \in \mathcal{K}_n} \{ \|A(x_0 + z) + b\| : z \in \mathcal{K}_n \}. \tag{4}$$

Here \mathcal{K}_n is the Krylov space

$$\mathcal{K}_n = \mathcal{K}_n(A, r_0) = \operatorname{Span} \{r_0, Ar_0, \dots, A^{n-1}r_0\}. \tag{5}$$

Note that since $r_0 = Ax_0 + b$, x_1^G is given by $x_1^G = x_0 + \beta^*(Ax_0 + b)$, where

$$\beta^* = \operatorname{argmin}_\beta \|r_0 + \beta Ar_0\| = -\frac{r_0^T Ar_0}{\|Ar_0\|^2}, \tag{6}$$

that is, the first step of GMRES is a simple mixing step with a mixing parameter β that minimizes the residual of the result.

Let K_n denote the projection onto the subspace $A\mathcal{K}_n$ of \mathbb{R}^N . From (4) it follows that

$$A(x_n^G - x_0) = Az_n = -K_n(Ax_0 + b) = -K_nr_0. \tag{7}$$

Therefore we can write

$$x_n^G - x^* = x_0 - x^* - A^{-1}K_n r_0 = A^{-1}(I - K_n)r_0, \tag{8}$$

which is equivalent to

$$Ax_n^G + b = (I - K_n)r_0. \tag{9}$$

We also note that

$$\mathcal{K}_n = \mathcal{K}_{n+1} \Leftrightarrow (I - K_n)A^{n+1}r_0 = 0, \tag{10}$$

$$x_n^G = x_{n+1}^G \Leftrightarrow K_n r_0 = K_{n+1} r_0 \Leftrightarrow r_0^T (I - K_n)A^{n+1}r_0 = 0. \tag{11}$$

Following Wilkinson [7, pp. 37], the *grade* of $r_0 \neq 0$ with respect to A is defined as

$$\nu(A, r_0) = \max \{n : \dim \mathcal{K}_n = n\}. \tag{12}$$

Thus $\nu(A, r_0)$ is the smallest integer n for which there is a non-zero polynomial $p(z)$ of degree n such that $p(A)r_0 = 0$, i.e.,

$$\nu(A, r_0) = \min \{n \in \mathbb{N} : r_0, Ar_0, \dots, A^n r_0 \text{ are linearly dependent}\}. \tag{13}$$

Then clearly $\nu(A, r_0) \leq N$, and $p(z)$ divides the minimal polynomial of A . Also, $\mathcal{K}_n = \mathcal{K}_\nu(A, r_0)$, $\forall n \geq \nu = \nu(A, r_0)$. The following result is given in [5]. For the reader's convenience, we give a proof that uses the notation introduced above.

Proposition 1. *The GMRES method (4) converges in exactly $\nu(A, r_0)$ steps, i.e.,*

$$x_n^G \neq x^*, \text{ for } n < \nu(A, r_0), \text{ and } x_n^G = x^*, \text{ for } n \geq \nu(A, r_0).$$

Proof. If $n = \nu(A, r_0)$, then from (13) it follows that there are numbers ξ_0, \dots, ξ_n such that $\sum_{i=0}^n \xi_i A^i r_0 = 0$. It is easily seen that we must have $\xi_0 \neq 0$ and $\xi_n \neq 0$, because otherwise the minimality of n is contradicted. Since $\xi_0 \neq 0$, we deduce that $r_0 \in AK_n$. According to (8) we have therefore $x_n^G = x^*$. If $n < \nu(A, r_0)$, then the vectors $r_0, Ar_0, \dots, A^{n-1}r_0$ are linearly independent, so that $r_0 \notin AK_n$, which means that $x_n^G \neq x^*$. \square

We next summarize Anderson mixing, for the nonlinear equation $f(x) = 0$.

Anderson mixing. Given a nonlinear operator f on \mathbb{R}^N , an initial point $x_0 \in \mathbb{R}^N$, a sequence β_0, β_1, \dots in $\mathbb{R} \setminus \{0\}$, and an integer m :

0. Set

$$f_0 = f(x_0), \quad x_1 = x_0 + \beta_0 f_0.$$

1. For $k = 1, 2, \dots$, set

$$m_k = \min\{m, k\}, \quad r_k = k - m_k, \quad f_k = f(x_k),$$

$$(\alpha_{0,k}, \dots, \alpha_{m_k,k}) = \operatorname{argmin}_{(\alpha_0, \dots, \alpha_{m_k})} \left\{ \left\| \sum_{i=0}^{m_k} \alpha_i f_{r_k+i} \right\|^2 : \sum_{i=0}^{m_k} \alpha_i = 1 \right\},$$

$$x_{k+1} = \sum_{i=0}^{m_k} \alpha_{i,k} x_{r_k+i} + \beta_k \sum_{i=0}^{m_k} \alpha_{i,k} f_{r_k+i} = \sum_{i=0}^{m_k} \alpha_{i,k} (x_{r_k+i} + \beta_k f_{r_k+i}).$$

For $\beta_i \equiv 1$ and $f(x) = g(x) - x$, this algorithm reduces to Algorithm AA from [6]. The version given here was proposed in [1]. There is also an equivalent (in exact arithmetic) version of this algorithm in terms of difference vectors $x_k - x_{k-1}$ and $f(x_k) - f(x_{k-1})$. It is presented in [2] in order to reveal its

connection to multiseant and Broyden type methods for solving nonlinear operator equations, but it obscures the “mixing” idea. We therefore do not give that version here.

The constrained optimization problem from this algorithm may be solved with the substitution method, e.g., by setting $\alpha_0 = 1 - \sum_{i=1}^{m_k} \alpha_i$ and solving the corresponding unconstrained optimization problem for $\alpha_1, \dots, \alpha_{m_k}$,

$$\min_{\alpha_1, \dots, \alpha_{m_k}} \|f_{r_k} + \alpha_1(f_{r_{k+1}} - f_{r_k}) + \alpha_2(f_{r_{k+2}} - f_{r_k}) + \dots + \alpha_{m_k}(f_k - f_{r_k})\|. \tag{14}$$

While the differencing may lead to loss of significance in the case of ill-conditioned problems, other solution methods may well experience similar difficulties in this case. The authors of [6] follow [2] in suggesting that the unconstrained version (14) be solved and report that solving the constrained version with a Lagrange multiplier approach leads to much worse condition numbers. Other methods for solving the constrained optimization problem are discussed in [4].

4. Convergence analysis in the linear case

In what follows we will investigate the relationship between the Anderson mixing and GMRES, for linear systems of the form (1). We use the notation x_n^G for the sequence generated by the GMRES method as described in the previous section, and x_n^A for the sequence generated by Anderson mixing with $m = \infty$ and $f(x) = Ax + b$, i.e.,

$$x_{n+1}^A = \sum_{i=0}^n \alpha_{i,n} x_i^A + \beta_n \sum_{i=0}^n \alpha_{i,n} (Ax_i^A + b) = \bar{x}_{n+1}^A + \beta_n (A\bar{x}_{n+1}^A + b), \tag{15}$$

$$(\alpha_{0,n}, \dots, \alpha_{n,n}) = \operatorname{argmin}_{(\alpha_0, \dots, \alpha_n)} \left\{ \left\| b + A \sum_{i=0}^n \alpha_i x_i^A \right\| : \sum_{i=0}^n \alpha_i = 1 \right\}.$$

Here

$$\bar{x}_{n+1}^A = \sum_{i=0}^n \alpha_{i,n} x_i^A \tag{16}$$

may be viewed as a prediction of the next iterate, a linear combination of all previous iterates. Using $\sum_{i=0}^n \alpha_i = 1$, we deduce that

$$\bar{x}_{n+1}^A = \left(1 - \sum_{i=1}^k \alpha_{i,n} \right) x_0 + \sum_{i=1}^n \alpha_{i,n} x_i^A = x_0 + \sum_{i=1}^n \alpha_{i,n} (x_i^A - x_0). \tag{17}$$

Therefore (15) can be written as

$$x_{n+1}^A = x_0 + \sum_{i=1}^n \alpha_{i,n} (x_i^A - x_0) + \beta_n \left(b + A \left(x_0 + \sum_{i=1}^n \alpha_{i,n} (x_i^A - x_0) \right) \right), \tag{18}$$

$$(\alpha_{1,n}, \dots, \alpha_{n,n}) = \operatorname{argmin}_{(\alpha_1, \dots, \alpha_n)} \left\| b + A \left(x_0 + \sum_{i=1}^n \alpha_i (x_i^A - x_0) \right) \right\|. \tag{19}$$

The coefficient $(\alpha_{1,n}, \dots, \alpha_{n,n})$ are uniquely defined as long as the vectors $x_i^A - x_0$ are linearly dependent for $i = 1, \dots, n$. The least squares problem (19) becomes rank deficient when these vectors are linearly dependent. However, the \bar{x}_n^A and hence also the x_n^A are well defined even after this rank deficiency occurs, and they can be found with one of the usual methods for rank deficient least squares problems. To see this, consider the linear subspaces

$$\mathcal{L}_n = \operatorname{Span} \{x_1^A - x_0, \dots, x_n^A - x_0\}, \tag{20}$$

and denote by L_n the projection onto $A\mathcal{L}_n$. With this notation we have

$$A(\bar{x}_{n+1}^A - x_0) = -L_n(Ax_0 + b) = -L_nr_0, \tag{21}$$

which is equivalent to

$$\bar{x}_{n+1}^A = x_0 - A^{-1}L_nr_0 = x^* + A^{-1}r_0 - A^{-1}L_nr_0 = x^* + A^{-1}(I - L_n)r_0. \tag{22}$$

Therefore,

$$A\bar{x}_{n+1}^A + b = (I - L_n)r_0, \tag{23}$$

$$x_{n+1}^A - x^* = (I + \beta_n A)A^{-1}(I - L_n)r_0 = (I + \beta_n A)(\bar{x}_{n+1}^A - x^*), \tag{24}$$

$$Ax_{n+1}^A + b = (I + \beta_n A)(I - L_n)r_0 = (I + \beta_n A)(A\bar{x}_{n+1}^A + b), \tag{25}$$

$$A(x_{n+1}^A - x_0) = -L_nr_0 + \beta_n A(I - L_n)r_0 = \beta_n Ar_0 - L_nr_0 - \beta_n AL_nr_0. \tag{26}$$

Definition 4.1. The index of the Anderson acceleration (18) is defined as

$$\mu(A, x_0) = \max \left\{ n \in \mathbb{N} : x_1^A - x_0, x_2^A - x_0, \dots, x_n^A - x_0 \text{ are linearly independent} \right\}. \tag{27}$$

The stagnation index of the GMRES method (4) is defined as

$$\eta^G = \min \left\{ n \in \{0, 1, \dots\} : x_n^G = x_{n+1}^G \right\}. \tag{28}$$

The index $\mu(A, x_0)$ allows for a complete description of the convergence properties of the Anderson acceleration for linear problems, for arbitrary sequences of relaxation parameters β_n . For the case $\beta_n = 1$ for all n , the formulae in (a) and (b) are given in [6].

Proposition 2. The index $\mu(A, x_0)$ is always less than or equal than the grade $\nu(A, r_0)$, and the sequences generated by the two methods satisfy the following properties:

(a) $x_{n+1}^A = x_n^G + \beta_n (Ax_n^G + b), n = 0, 1, \dots, \mu(A, x_0);$

(b) $\bar{x}_{n+1}^A = x_n^G, n = 0, 1, \dots, \mu(A, x_0).$

Proof. Let us first prove by induction that $\mathcal{L}_n \subset \mathcal{K}_n$. Since $x_1^A - x_0 = \beta_0 r_0$ this is readily verified for $n = 1$. Assume that $\mathcal{L}_n \subset \mathcal{K}_n$. Then from (18) it follows that

$$x_{n+1}^A - x_0 = \beta_n r_0 + (I + \beta_n A) \sum_{i=1}^n \alpha_{i,n} (x_i^A - x_0) \in \mathcal{K}_n + A\mathcal{K}_n = \mathcal{K}_{n+1}, \tag{29}$$

which completes the induction step. Since $\mathcal{L}_n \subset \mathcal{K}_n$, the linear independence of $x_1^A - x_0, \dots, x_n^A - x_0$ always implies the linear independence of $r_0, \dots, A^{n-1}r_0$. This implies that $\mu(A, x_0) \leq \nu(A, r_0)$. It also implies that

$$\mathcal{L}_n = \mathcal{K}_n, \text{ and } \dim(\mathcal{K}_n) = n, \text{ for } n = 1, \dots, \mu(A, x_0). \tag{30}$$

Point (a) of our proposition follows from (8) and (24), while point (b) follows from (8) and (22). \square

The result shows that varying the sequence of relaxation parameters β_k does not change the behavior of the sequence x_k^A in a significant way for linear problems, if exact arithmetic is used and as long as $k \leq m$. However, for nonlinear problems, the convergence behavior can be quite sensitive to

the “right” choice of the β_k ; see e.g., [3]. Also, the choice of the β_n does matter for large n if m is finite, as is shown by numerical experience.

It is instructive to observe what exactly happens at the step $\mu(A, x_0)$. Of course, if $\mu(A, x_0) = \nu(A, r_0)$, the Anderson mixing has converged to the solution. In the case where $\mu(A, x_0) < \nu(A, r_0)$, we have the following characterization.

Proposition 3. *If $n < \mu(A, x_0) < \nu(A, r_0)$, then*

- (a) $\alpha_{n,n} \neq 0$ in (17),
- (b) $\|Ax_{n-1}^G + b\| > \|Ax_n^G + b\|$.

If $n = \mu(A, x_0) < \nu(A, r_0)$, then

- (c) $\alpha_{n,n} = 0$ in (17),
- (d) $(A\bar{x}_n^A + b)^T A (x_n^A - x_0) = 0$,
- (e) $x_{n-1}^G = \bar{x}_n^A = \bar{x}_{n+1}^A = x_n^G = \bar{x}_{n+2}^A$,
- (f) $\|Ax_{n-1}^G + b\| = \|Ax_n^G + b\|$.

Proof. Using (30) we can write

$$x_n^A - x_0 = \sum_{i=1}^n \xi_{i,n} A^{i-1} r_0, \quad \text{with } \xi_{i,n} \neq 0, \quad n = 1, \dots, \mu(A, x_0) \tag{31}$$

for some uniquely determined scalars $\xi_{1,n}, \dots, \xi_{n,n}$. Using (18) we obtain

$$\begin{aligned} x_{n+1}^A - x_0 &= \beta_n r_0 + \sum_{i=1}^n \alpha_{i,n} (x_i^A - x_0) + \beta_n A \sum_{i=1}^{n-1} \alpha_{i,n} (x_i^A - x_0) + \beta_n \alpha_{n,n} A (x_n^A - x_0) \\ &= y_n + \beta_n \alpha_{n,n} \xi_{n,n} A^n r_0, \quad \text{with } y_n \in \mathcal{L}_n = \mathcal{K}_n, \quad n = 1, \dots, \mu(A, x_0). \end{aligned}$$

If $n < \mu(A, x_0)$, then $\mathcal{L}_{n+1} \neq \mathcal{L}_n$, so that we must have $\alpha_{n,n} \neq 0$. This proves part (a). On the other hand, if $n = \mu(A, x_0) < \nu(A, r_0)$, then $\mathcal{L}_{n+1} = \mathcal{L}_n = \mathcal{K}_n \neq \mathcal{K}_{n+1}$. This implies $\alpha_{n,n} = 0$, which shows the validity of part (c). If $\alpha_{n,n} = 0$, then from (18) and (17) we have $\bar{x}_n^A = \bar{x}_{n+1}^A$, which, in view of Proposition 2, implies $x_{n-1}^G = \bar{x}_n^A = \bar{x}_{n+1}^A = x_n^G$. Since $\mathcal{L}_{n+1} = \mathcal{L}_n$ we also have $\bar{x}_{n+1}^A = \bar{x}_{n+2}^A$, which completes the proof of part (e). Part (f) follows trivially.

To prove (d), observe that the normal equations from (18) can be written as

$$(A\bar{x}_{n+1}^A + b)^T A (x_i^A - x_0) = 0, \quad i = 1, \dots, n.$$

Geometrically, the above relation follows immediately, since according to (23), $A\bar{x}_{n+1}^A + b \in (A\mathcal{L}_n)^\perp$. In case $n = \mu(A, x_0)$, according to (e), we have $\bar{x}_{n+1}^A = \bar{x}_n^A$. For $i = n$ we get part (d).

To prove part (b), note that by (4), $\|Ax_n^G + b\| \leq \|Ax_{n-1}^G + b\|$. Suppose there is equality, then from (9) $\|(I - K_n)r_0\| = \|(I - K_{n-1})r_0\|$. Since these are orthogonal projections, this implies in turn $K_n r_0 = K_{n-1} r_0$, and therefore by Proposition 2, (8), and (22), we should have $\bar{x}_{n+1}^A = x_n^G = x_{n-1}^G = \bar{x}_n^A$.

But this is impossible, since $\bar{x}_n^A - x_0 \in \mathcal{L}_{n-1}$, but $\bar{x}_{n+1}^A - x_0 \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$, due to $\alpha_{n,n} \neq 0$. Therefore, $\|Ax_n^G + b\| < \|Ax_{n-1}^G + b\|$. \square

Using Propositions 1–3, we obtain the following theorem, which represents the main result of our paper.

Theorem 1. Assume that A is an invertible $N \times N$ -matrix. Consider the GMRES method (4), and the Anderson acceleration method (18) for finding the solution x^* of the linear equation (1), with arbitrary nonzero mixing parameters β_0, β_1, \dots . For any starting point x_0 , consider also the grade $\nu(A, r_0)$, defined in (13), and the index $\mu(A, x_0)$, defined in (27).

(i) $\mu(A, x_0) = \nu(A, r_0) = \nu$ if and only if

$$\|Ax_0 + b\| > \|Ax_1^G + b\| > \dots > \|Ax_{\nu-1}^G + b\| > \|Ax_\nu^G + b\| = 0. \tag{32}$$

Moreover, in this case the sequence produced by the Anderson acceleration satisfies

$$x_{n+1}^A = \begin{cases} x_n^G + \beta_n (Ax_n^G + b), & \text{if } n < \nu \\ x^*, & \text{if } n \geq \nu \end{cases}, \tag{33}$$

$$\bar{x}_{n+1}^A = x_n^G, \quad n = 0, 1, \dots \tag{34}$$

(ii) $\mu = \mu(A, x_0) < \nu(A, r_0)$ if and only if

$$\|Ax_0 + b\| > \|Ax_1^G + b\| > \dots > \|Ax_{\mu-1}^G + b\| = \|Ax_\mu^G + b\| > 0. \tag{35}$$

Moreover, in this case $\mu(A, x_0) = \eta^G + 1$, and the sequence produced by the Anderson acceleration satisfies

$$x_{n+1}^A = \begin{cases} x_n^G + \beta_n (Ax_n^G + b), & \text{if } n \leq \mu \\ x_{\mu-1}^G + \beta_n (Ax_{\mu-1}^G + b), & \text{if } n \geq \mu \end{cases}, \tag{36}$$

$$\bar{x}_{n+1}^A = \begin{cases} x_n^G, & \text{if } n \leq \mu \\ x_{\mu-1}^G, & \text{if } n \geq \mu \end{cases}. \tag{37}$$

Proof. The fact that $\mu(A, x_0) = \nu(A, r_0) = \nu$ implies (32), (33), and (34) follows from Propositions 1, 2 and 3.

In order to prove that $\mu = \mu(A, x_0) < \nu(A, r_0)$ implies (35), we first prove by induction that $\mathcal{L}_n = \mathcal{L}_\mu = \mathcal{K}_\mu$ for all $n > \mu$. This is certainly true for $n = \mu + 1$ from Definition 4.1. Suppose that our statement is true for an $n > \mu$. Then, according to (8), (22), and point (e) of Proposition 3, we have $\bar{x}_{n+1}^A = x_\mu^G = x_{\mu-1}^G$. This proves $x_{n+1}^A = x_{\mu-1}^G + \beta_n (Ax_{\mu-1}^G + b)$. To complete the induction step, we note that from (7) and (9) it follows that

$$A(x_{n+1}^A - x_0) = A(x_{\mu-1}^G - x_0) + \beta_n A(Ax_{\mu-1}^G + b) = \beta_n Ar_0 - (I + \beta_n A)K_{\mu-1}r_0.$$

Since $AK_{\mu-1}r_0 \in A^2\mathcal{K}_{\mu-1} \subset \mathcal{K}_{\mu+1}$, we deduce that $x_{n+1}^A - x_0 \in \mathcal{K}_\mu$, which shows that $\mathcal{L}_{n+1} = \mathcal{K}_\mu$. The fact $\mu = \mu(A, x_0) < \nu(A, r_0)$ implies (36) and (37) and that $\mu(A, x_0) = \eta^G$ in this case follows from Propositions 2 and 3.

Assume now that (32) holds, but $\mu(A, x_0) \neq \nu(A, r_0) = \nu$. Since $\mu(A, x_0) \leq \nu(A, r_0)$, this implies $\mu = \mu(A, x_0) < \nu(A, r_0)$, which in turn, as seen above implies (35), so that (32) cannot be true. Hence, (32) is equivalent to $\mu(A, x_0) = \nu(A, r_0) = \nu$.

Similarly if $\mu = \mu(A, x_0) < \nu(A, r_0)$ is not true, we must have $\mu = \mu(A, x_0) = \nu(A, r_0)$, which, as seen above, implies (32) so that (35) is not true. Therefore (35) is equivalent to $\mu = \mu(A, x_0) < \nu(A, r_0)$. \square

Theorem 1 gives a complete characterization of the behavior of the Anderson acceleration on linear problems. If $\mu(A, x_0) = \nu(A, r_0)$, then the Anderson acceleration converges to x^* . If $\mu(A, x_0) < \nu(A, r_0)$, then $\mu(A, x_0)$ is precisely the first index for which GMRES stagnates (i.e., produces two identical successive iterates). If this ever happens, GMRES continues to generate larger Krylov spaces, and it will eventually converge to x^* , while Anderson mixing will then stagnate forever. An extreme example is given by $A = P_N$, where P_N is the permutation matrix for the cycle $(123 \dots N)$, with minimal polynomial $q(z) = 1 - z^N$. Then if b is any standard basis vector e_k , Anderson mixing will immediately stagnate (i.e., $\mu(A, x_0) = 1$), while GMRES will converge in $\nu(A, b) = N$ steps, stagnating at the initial value until the very last step.

Corollary 1. *The Anderson acceleration for linear problems converges in at most $\mu(A, x_0) + 1$ steps, but not necessarily to the solution of the linear problem. If $\mu(A, x_0) = \nu(A, r_0)$, the Anderson acceleration converges to the exact solution of the linear problem in either $\nu(A, r_0)$ or $\nu(A, r_0) + 1$ steps.*

Proof. The first part of the corollary follows directly from Theorem 1. We note that if $n < \mu(A, x_0)$, then $x_{n+1}^A - x^* = x_n^G - x^* + \beta_n (Ax_n^G + b) = x_n^G - x^* + \beta_n A (x_n^G - x^*)$. Therefore $x_{n+1}^A - x^*$ if and only if $x_n^G - x^*$ is an eigenvector of A with eigenvalue $-1/\beta_n$, but in this case we have $\|Ax_{n+1}^G + b\| \leq \|Ax_{n+1}^A + b\| = 0$, so that $x_{n+1}^G = x^*$, and therefore $n + 1 = \nu(A, r_0)$. \square

Corollary 2. *We have $\eta^G = 0$, $\mu(A, x_0) = 1$ if and only if the quantity β^* defined in (6) vanishes.*

Proof. If $\beta^* = 0$, then (as noted in the remarks following (6)), $x_1^G = x_0 + \beta^*(Ax_0 + b) = x_0$, and hence $\eta^G = \mu(A, x_0) - 1 = 0$. \square

5. Anderson acceleration with optimized mixing parameters

The Anderson acceleration for the linear problem (1) defined in (18) depends on a sequence of mixing parameters β_0, β_1, \dots . In this section we consider a variant of the Anderson acceleration, where at each step β_n is chosen so that the residual at x_{n+1}^A is minimal. More precisely we consider the following algorithm:

Optimized Anderson acceleration for linear problems.

Set $\bar{x}_1^{A*} = x_0$ and $x_1^{A*} = x_0 + \beta_0^*(Ax_0 + b)$, with β^* defined in (6);

For $n = 1, 2, \dots$

 Compute

$$(\alpha_{1,n}^*, \dots, \alpha_{n,n}^*) = \operatorname{argmin}_{(\alpha_1, \dots, \alpha_n)} \left\| b + A \left(x_0 + \sum_{i=1}^n \alpha_i (x_i^{A*} - x^0) \right) \right\|;$$

 Compute

$$\bar{x}_{n+1}^{A*} = x_0 + \sum_{i=1}^n \alpha_{i,n}^* (x_i^{A*} - x^0)$$

 If $A\bar{x}_{n+1}^{A*} + b = 0$, set $\beta_n^* = 0$. Otherwise set

$$\beta_n^* = - \frac{(A\bar{x}_{n+1}^{A*} + b)^T A (A\bar{x}_{n+1}^{A*} + b)}{\|A (A\bar{x}_{n+1}^{A*} + b)\|^2};$$

 Set $x_{n+1}^{A*} = \bar{x}_{n+1}^{A*} + \beta_n^* (A\bar{x}_{n+1}^{A*} + b)$.

We note that Theorem 1 implies that $\mu(A, x_0)$ is the same for any choice of nonzero mixing parameters β_0, β_1, \dots and that the sequence \bar{x}_n^A is independent of this choice. Also, once $\beta_n^* = 0$, then clearly $\beta_r^* = 0$ for all $r > n$. Therefore, if $\beta_n^* \neq 0$ for some $n \geq 0$, then

$$\beta_r^* \neq 0, \quad \bar{x}_{r+1}^A = \bar{x}_{r+1}^{A*}$$

for all $r \leq n$. However, it seems possible that the β_n^* become zero for some $n < \mu(A, x_0)$ and that optimized Anderson acceleration stagnates before a general Anderson acceleration scheme stagnates (in which $\beta_n \neq 0$ for all n is enforced). We now show that this can never happen and that β_n^* becomes zero precisely for $n > \mu(A, x_0)$.

Theorem 2. Assume that A is an invertible $N \times N$ -matrix. Consider the GMRES method (4), the Anderson acceleration method (18), with arbitrary nonzero mixing parameters β_0, β_1, \dots , and the optimized Anderson acceleration for linear problems described above. Then for all n , $\beta_n^* \neq 0$ if and only if $n \leq \mu(A, x_0) = \eta^G + 1$. Also for all n ,

$$x_{n+1}^{A*} = \begin{cases} x_n^G + \beta_n^* (Ax_n^G + b), & \text{if } n < \eta^G \\ x_{\eta^G}^G, & \text{if } n \geq \eta^G \end{cases}, \tag{38}$$

$$\bar{x}_{n+1}^{A*} = \bar{x}_{n+1}^A = \begin{cases} x_n^G, & \text{if } n < \eta^G \\ x_{\eta^G}^G, & \text{if } n \geq \eta^G \end{cases}, \tag{39}$$

$$\|Ax_{n+1}^G + b\| \leq \|Ax_{n+1}^{A*} + b\| < \|Ax_n^G + b\|, \quad \text{if } n < \eta^G \tag{40}$$

$$\|Ax_{n+1}^{A*} + b\|^2 = \|A\bar{x}_{n+1}^{A*} + b\|^2 - \beta_n^{*2} \|A(A\bar{x}_{n+1}^{A*} + b)\|^2 \tag{41}$$

$$\leq \|Ax_n^{A*} + b\|^2 - \beta_n^{*2} \|A(A\bar{x}_{n+1}^{A*} + b)\|^2 \tag{42}$$

Proof. We begin by observing that (41) and (42) follow from the construction of the x_n^{A*} for all n . Let

$$R = \max\{n \mid \beta_n^* \neq 0\}. \tag{43}$$

Then $\beta_n^* \neq 0$ for all $n < R$, since otherwise $x_n^{A*} = x_{n+1}^{A*}$ for some $n < R$ and hence $\beta_k^* = 0$ for all $k \geq n$. Then an induction argument and the results in Theorem 1 show that (38)–(40) hold for $n \leq R$. Clearly, $R \leq \mu(A, x_0)$. It remains to show that $R \geq \mu(A, x_0)$.

Let therefore $n = R + 1$, and assume that $n \leq \mu(A, x_0)$. We may also assume that $n \leq \nu(A, r_0)$, since otherwise there is nothing to prove. We want to show that

$$\bar{x}_{n+1}^A = \bar{x}_{n+2}^A \tag{44}$$

which will imply the direct contradiction $n = R + 1 > \mu(A, x_0)$. Now the equation $A\bar{x}_{n+1}^A - Ax_0 = -L_n r_0$ (see (21)), where L_n is the orthogonal projection on $AL_n = AL_n$, is equivalent to

$$\xi^T (A\bar{x}_{n+1}^A + b) = 0 \tag{45}$$

for all $\xi \in AL_n$. Showing (44) is now equivalent to proving (45) for all $\xi \in AL_{n+1}$, since then $A\bar{x}_{n+1}^A - Ax_0 = -L_{n+1} r_0 = A\bar{x}_{n+2}^A - Ax_0$ and hence (44) holds. To show (45) for all $\xi \in AL_{n+1}$, it suffices to show (45) for a single $\xi \in AL_{n+1} \setminus AL_n$. Now use the assumption $\beta_n^* = 0$, which is equivalent to

$$(A(A\bar{x}_{n+1}^A + b))^T (A\bar{x}_{n+1}^A + b) = 0.$$

We wish to show that

$$\xi = (A(A\bar{x}_{n+1}^A + b)) \in AL_{n+1} - AL_n \tag{46}$$

which will prove (45) for all $\xi \in A\mathcal{L}_{n+1}$ and complete the proof of the theorem.

We know that $\bar{x}_{n+1}^A - x_0 \in \mathcal{L}_n$. But $\bar{x}_{n+1}^A - x_0 \notin \mathcal{L}_{n-1} = \mathcal{L}_R$, since otherwise

$$A\bar{x}_{n+1}^A - Ax_0 = L_{n-1} \left(A\bar{x}_{n+1}^A - Ax_0 \right) = -L_{n-1}L_n r_0 = -L_{n-1}r_0$$

and therefore already $\bar{x}_R^A = \bar{x}_{R+1}^A$, contradicting $R < \mu(A, x_0)$. Therefore we can write

$$\bar{x}_{n+1}^A - x_0 = \sum_{j=0}^{n-1} \lambda_j A^j r_0 \in \mathcal{L}_n$$

and $\lambda_{n-1} \neq 0$. Consequently

$$A\bar{x}_{n+1}^A + b = r_0 + \sum_{j=0}^{n-1} \lambda_j A^{j+1} r_0 \in \mathcal{L}_{n+1}$$

But if $A\bar{x}_{n+1}^A + b \in \mathcal{L}_n$, then a calculation shows that $A\bar{x}_{n+1}^A - Ax_0 \in A\mathcal{L}_{n-1}$ and hence $\bar{x}_{n+1}^A - x_0 \in \mathcal{L}_{n-1}$, which was ruled out above. Consequently

$$A\bar{x}_{n+1}^A + b \in \mathcal{L}_{n+1} \setminus \mathcal{L}_n.$$

This implies (46) and therefore (45) for all $\xi \in A\mathcal{L}_{n+1}$. Then $\bar{x}_{n+2}^A = \bar{x}_{n+1}^A$, and all conclusions of the theorem follow. \square

The theorem shows that optimized Anderson acceleration enjoys the descent property

$$\|Ax_{n+1}^{A*} + b\| < \|A\bar{x}_{n+1}^{A*} + b\| \leq \|Ax_n^{A*} + b\|$$

for all $n < \mu(A, x_0)$, but that it does not accelerate convergence otherwise when compared to Anderson acceleration with arbitrary $\beta_n \neq 0$.

Acknowledgement

The authors would like to thank the referee for several very useful suggestions.

References

- [1] D.G. Anderson, Iterative procedures for nonlinear integral equations, *J. Assoc. Comput. Mach.* 12 (1965) 547–560.
- [2] H. Fang, Y. Saad, Two classes of multiseant methods for nonlinear acceleration, *Numer. Linear Algebra Appl.* 16 (3) (2009) 197–221.
- [3] L.D. Marks, D.R. Luke, Robust mixing for ab initio quantum mechanical calculations, *Phys. Rev. B* 78 (7) (2008)
- [4] P. Ni, Anderson Acceleration of Fixed-point Iteration with Applications to Electronic Structure Computations, Ph.D. thesis, Worcester Polytechnic Institute, 2009.
- [5] Y. Saad, M.H. Schultz, GMRES: a generalized minimal residual method for solving nonsymmetric linear systems, *SIAM J. Sci. Stat. Comput.* 7 (3) (1986) 856–869.
- [6] H. Walker, P. Ni, Anderson acceleration for fixed-point iterations, *SIAM J. Numer. Anal.* 49 (4) (2011) 1715–1735.
- [7] J.H. Wilkinson, *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, 1965.