Shanks and Anderson-type acceleration techniques for systems of nonlinear equations

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Abstract

This paper examines a number of extrapolation and acceleration methods, and introduces a few modifications of the standard Shanks transformation that deal with general sequences. One of the goals of the paper is to lay out a general framework that encompasses most of the known acceleration strategies. The paper also considers the Anderson Acceleration method under a new light and exploits a connection with quasi-Newton methods, in order to establish local linear convergence results of a stabilized version of Anderson Acceleration method. The methods are tested on a number of problems, including a few that arise from nonlinear Partial Differential Equations.

Keywords: extrapolation methods, Anderson acceleration, quasi-Newton methods, Krylov subspace methods, regularization, nonlinear Poisson problems, Navier-Stokes equation.

1 Introduction

In numerical analysis and in applied mathematics, many applications lead to sequences of numbers, vectors, matrices or even tensors. When the sequence is slowly converging, or even diverging, and when one has only access to the sequence and nothing else (i.e., when it is produced by a "black box"), it is possible to transform it, by a *sequence transformation*, into a new sequence, which, under some assumptions, converges faster than the original one to the same limit. It was necessary to develop a variety of such sequence transformations since, in fact, it was proved by Delahaye and Germain-Bonne [26] that a universal sequence transformation able to accelerate all sequences, or even all monotonically converging scalar ones, cannot exist. For a review, see, for example, [12, 15, 16, 25, 58, 65, 66].

One way to transform a sequence into a faster converging one is to resort to *extrapolation*. Here, the transformation is built so that it yields the exact limit of all sequences satisfying a certain

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algebraic relation. The set of these sequences is called the *kernel* of the transformation. Among these, this paper focuses on *Shanks transformation* [55] and a number of its generalizations. As we will see, this well-established method transforms a sequence (\mathbf{s}_n) into a set of sequences $\{(\mathbf{t}_n^{(k)})\}$. Introduced by Shanks for scalar sequences [55], it has been extensively studied, and extended, in various ways, to sequences of vectors, matrices, and tensors. Here, we only consider the vector case.

All these extensions to vectors of the scalar Shanks transformation share the property that, for a fixed value of k, $\mathbf{t}_n^{(k)} = \mathbf{s}$ for all n if the sequence (\mathbf{s}_n) of elements of \mathbb{R}^p or \mathbb{C}^p satisfies, for all n, the following linear difference equation of order k

$$\alpha_0(\mathbf{s}_n - \mathbf{s}) + \dots + \alpha_k(\mathbf{s}_{n+k} - \mathbf{s}) = 0, \tag{1}$$

where **s** is the limit of (\mathbf{s}_n) if it converges, and is called its *antilimit* otherwise. The numbers α_i are independent of n, and it is assumed that $\alpha_0 \alpha_k \neq 0$, so that the difference equation has the order k exactly, and $\alpha_0 + \cdots + \alpha_k \neq 0$, so that **s** be uniquely defined. Thus, these conditions imply that k cannot be replaced by a smaller value. It does not restrict the generality to assume that $\alpha_0 + \cdots + \alpha_k \neq 0$, so that \mathbf{s} be uniquely defined. Thus, these conditions imply that k cannot be replaced by a smaller value. It does not restrict the generality to assume that $\alpha_0 + \cdots + \alpha_k = 1$. The set of sequences satisfying (1) is called the *Shanks kernel*. Among sequences in this kernel are those produced by the iterations $\mathbf{s}_{n+1} = M\mathbf{s}_n + \mathbf{b}$, thus providing a link with Krylov subspace and Lanczos methods; see, in particular, [7, 9, 56, 59].

Besides their use in a number of different applications, extrapolation techniques have recently been promoted as an effective tool also for problems related to the emerging field of Data Science [22,23,54,67]. But since there is often some confusion in the literature about the terminology used, we would like clarify it – using a high level of generality. Specifically, we would like to draw a distinction between *extrapolation methods*, *sequence transformations*, and *convergence acceleration methods*. This distinction will help the reader to better understand the approaches described in Section 2 for building our sequence transformations.

Let (\mathbf{s}_n) be a sequence of elements of a vector space E on \mathbb{C} . A common problem encountered in numerical analysis is to estimate the limit of this sequence from a certain number of its terms. The problem can be solved by an *extrapolation method* as follows [6, 17]. Let

$$\boldsymbol{\varphi}: \mathbb{N} \times D \longmapsto E, \qquad D \subseteq \mathbb{C}^k,$$

be such that

$$\forall \mathbf{b} \in D, \quad \lim_{n \to \infty} \boldsymbol{\varphi}(n, \mathbf{b}) = 0.$$

Let V_{φ} be the linear variety of sequences of elements of E such that

$$\forall n, \quad \mathbf{s}_n = \mathbf{s} + \boldsymbol{\varphi}(n, \mathbf{b}),$$

with $\mathbf{s} \in E$. Obviously $\lim_{n\to\infty} \mathbf{s}_n = \mathbf{s}$.

By definition, if $(\mathbf{s}_n) \in V_{\varphi}$, then, $\forall n, \mathbf{s} = \mathbf{s}_n - \varphi(n, \mathbf{b})$. Now, if $(\mathbf{s}_n) \notin V_{\varphi}$, let us consider a sequence $(\mathbf{t}_n = \mathbf{t} + \varphi(n, \beta)) \in V_{\varphi}$, and impose that it satisfies the *interpolation conditions* $\mathbf{t}_{n+i} = \mathbf{s}_{n+i}$ for $i = 0, \ldots, k$. The vector $\beta \in D$ can be computed, assuming that it exists and is unique, in different ways as the solution of a system of k scalar equations that can be obtained as follows. Let E^* be the algebraic dual vector space of E, that is the vector space of linear functionals on E. Let $\mathbf{y}, \mathbf{y}_1, \ldots, \mathbf{y}_k \in E^*$, and let $\langle \cdot, \cdot \rangle$ denote the duality product between E^* and E. The first strategy consists in computing the vector $\boldsymbol{\beta}$ as the solution of the system

$$\langle \mathbf{y}_i, \mathbf{s}_{n+1} - \mathbf{s}_n \rangle = \langle \mathbf{y}_i, \boldsymbol{\varphi}(n+1, \boldsymbol{\beta}) - \boldsymbol{\varphi}(n, \boldsymbol{\beta}) \rangle, \quad i = 1, \dots, k.$$

In the particular case of Shanks transformation, writing this system in matrix form, leads to a relation having the same structure as *Approach 3* in the *minimal residual approach* of Section 2.1.3, but with different indexes.

In the second strategy, the vector $\boldsymbol{\beta}$ is the solution of the system

$$\langle \mathbf{y}, \mathbf{s}_{n+i+1} - \mathbf{s}_{n+i} \rangle = \langle \mathbf{y}, \boldsymbol{\varphi}(n+i+1, \boldsymbol{\beta}) - \boldsymbol{\varphi}(n+i, \boldsymbol{\beta}) \rangle, \quad i = 0, \dots, k-1.$$

For Shanks transformation, this approach corresponds, in matrix form, to something similar to *Approach 6* in the *topological approach* of Section 2.2.3.

Then, in both cases, we set $\mathbf{t} = \mathbf{s}_n - \boldsymbol{\varphi}(n, \boldsymbol{\beta})$. Since $\mathbf{t} = \lim_{n\to\infty} \mathbf{t}_n$, it is an approximation of \mathbf{s} , and it has been obtained by extrapolation. Obviously \mathbf{t} depends on n and k, and we will now denote it by $\mathbf{t}_n^{(p_k)}$ where $p_k + 1$ denotes the number of elements of the initial sequence used in the process. Thus, when n and p_k vary, the sequence (\mathbf{s}_n) has been transformed into the set of sequences $\{(\mathbf{t}_n^{(p_k)})\}$. This procedure is named an extrapolation method. An important remark to be made is that it is a purely algebraic procedure. Richardson's and Romberg's methods, and Aitken's Δ^2 process are such well known scalar extrapolation methods. Thus, an extrapolation method results in a sequence transformation $T : (\mathbf{s}_n) \mapsto (\mathbf{t}_n^{(p_k)})$ when either p_k or n is fixed, and the other index tends to infinity. Conversely, most sequence transformations can be interpreted as extrapolation methods. The variety V_{φ} is usually named the kernel of the transformation T, and it is denoted \mathcal{K}_T . If, when n or p_k tends to infinity, the sequence $(\mathbf{t}_n^{(p_k)})$ converges to \mathbf{s} faster than the sequence (\mathbf{s}_n) , the denomination convergence acceleration method is also used. Let us mention that extrapolation methods can also be applied to diverging sequences. They are often used for accelerating fixed point iterations, sometimes coupled with a restarting strategy.

In this paper, instead of building Skanks transformation by computing the coefficients in (1) as the solution of a linear system in the usual way, we propose a new optimization approach, based on minimization. This allows to easily introduce, for sequences not belonging to the Shanks kernel, a unified framework that includes also regularized and preconditioned techniques.

Anderson Acceleration (AA) [2,3], also called Anderson mixing, Pulay mixing or Direct Inversion in the Iterative Subspace (DIIS) [51], in the computational physics and chemistry communities, has been widely used and applied to the solution of various fixed point problems over the last decades. The literature on this method is too broad to allow for an exhaustive discussion but it suffices to search recent citations to this work to understand the truly exceptional renewed interest in Anderson Acceleration across many disciplines. A few of the classical citations include the papers by Walker and Ni [64], Higham and Strabić [40], Toth and Kelley [63], and by Fang and Saad [31], and a few papers that describe applications are [4, 32, 42, 44, 47, 49, 67].

However, it is important here to stress that AA is not an extrapolation method in the exact sense defined above since it does not start from an arbitrary given sequence and transforms it into a new sequence. Instead it builds its own sequence step by step. Anderson acceleration is in fact more akin to quasi-Newton techniques than to extrapolation. It was viewed as a form of secant method in the classic book by Ortega and Rheinboldt [46, pp. 204-205]. Its relations to secant type methods, specifically 'multi-secant methods' was unraveled by Eyert [30], and later exploited in [31] and also in [32]. In short, Anderson-Pulay mixing is a second order method whose goal is to accelerate a fixed point iteration. If we were to allow the number of preview iterates used in the process to increase indefinitely we would get something rather similar to a standard quasi-Newton method whose convergence would be superlinear at the limit. This is not done in practice because of cost and numerical stability considerations. However, a certain relation with the RRE method, which is an extrapolation method, exists, and AA can be recovered by using the Coupled Shanks transformations, as explained in [18]. Due to this connection, we gave, in Section 5, new procedures in the style of Anderson acceleration, that are called Anderson-Type Mixing (ATM in short). Stabilized and regularized versions of AA will be also proposed.

The outline of the paper is the following

- In Section 2, we present an overview of transformation techniques for sequences belonging to the Shanks kernel, and show how their limit or antilimit can be obtained exactly from these transformations. Four out of six of these techniques are presented in a new way that comes out from an optimization problem. Coupled sequences used in Section 5 are also described.
- In Section 3, we present transformations based on the Shanks kernel. We show how to adapt and extend the idea proposed in [54] to our approaches. These modifications are specifically designed to accelerate general/nonlinear sequences which do not belong to the Shanks kernel.
- In Section 4, we present the *Restarted* and the *Continuous-Updating* methods for exploiting the Shanks-based transformations presented in the previous section. In this way we are able to introduce a unified framework able to encompass simultaneously the newly introduced transformations and many of transformations already present in the literature.
- In Section 5, we present new Anderson-Type Mixing methods. We show how the classical AA fits into them. Then, we introduce preconditioning and a regularization strategies. Moreover, exploiting the connection with quasi-Newton methods, we prove the local linear convergence of a stabilized version of the classical AA, which allows us to substantiate theoretically the regularization strategy encompassed in the Anderson-type techniques previously presented in this section.
- In Section 6, we perform a comparative experimental study of some of the techniques proposed using, among other tests, a set of nonlinear problems arising from Partial Differential Equations (PDEs).

Let us explain our notation. Given a sequence (\mathbf{s}_n) , we set $S_i^{(j)} = [\mathbf{s}_i, \dots, \mathbf{s}_{i+j-1}] \in \mathbb{R}^{p \times j}$. Thus, the superscript j corresponds to the number of columns formed by the p-dimensional vectors of the sequence (\mathbf{s}_n) , and the lower index i is the index of the first of these vectors in the sequence. Whenever it is used, the forward difference operator Δ is applied to the lower index, that is $\Delta S_i^{(j)} = S_{i+1}^{(j)} - S_i^{(j)} = [\Delta \mathbf{s}_i, \dots, \Delta \mathbf{s}_{i+j-1}]$, and similarly for Δ^2 . For a fixed value of k, we denote by $\overline{S}_i^{(j)}$ the $kp \times j$ matrix formed by stacking the k matrices $S_i^{(j)}, \dots, S_{i+k-1}^{(j)}$ of dimension $p \times j$. When not explicitly indicated, the norm used is the Euclidean norm. Throughout the paper, if not explicitly indicated, all matrices whose inverse is needed are assumed to be nonsingular. If it is not the case, the pseudo-inverse may be used.

2 Transformations for sequences in the Shanks kernel

Let (\mathbf{s}_n) be a sequence of vectors in \mathbb{R}^p or \mathbb{C}^p such that (1) holds for a fixed value of k and for all n. Assuming, without loss of generality, that $\sum_{i=0}^k \alpha_i = 1$, then we get from (1)

$$\alpha_0 \mathbf{s}_n + \dots + \alpha_k \mathbf{s}_{n+k} = \mathbf{s}, \qquad \text{for all } n \ge 0.$$

Alternatively, we can write

$$\mathbf{s}_{n+k} - \sum_{j=0}^{k-1} \beta_j \Delta \mathbf{s}_{n+j} = \mathbf{s},\tag{3}$$

with $\beta_j = \sum_{i=0}^{j} \alpha_i$ for $j = 0, \dots, k-1$ (note that the β_i 's are defined in a slightly different way than in [18, Sect. 3.1.3]).

In Sections 2.1 and 2.2, we show that when (\mathbf{s}_n) belongs to the Shanks kernel for a fixed value of k, it is possible to compute exactly the limit or the antilimit of the sequence from a certain number ℓ_k (which depends on k and on the transformation used) of consecutive vectors of the sequence, where $\ell_k = k + 2$ (for the Minimal residual approaches) or $\ell_k = 2k + 1$ (for the Topological approaches). For this purpose, we present six different strategies for computing the coefficients $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_k)^T$ or $\boldsymbol{\beta} = (\beta_0, \dots, \beta_{k-1})^T$. It should be reminded that $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are not dependent on n if (\mathbf{s}_n) satisfies (1), or (2), or (3). Four of these strategies (Approaches 1, 2, 4 and 5 below) are presented as the solution of a minimization problem. Approaches 1 and 4 proceed in what appears to be a new way, not considered before in the literature devoted to Shanks sequence transformations. Approaches 2 and 5 can be considered as particular cases of the Least-squares strategy evoked in [18, Sect. 3.1.3. These four strategies will be useful for the generalization presented in Section 3. Two of these strategies (Approaches 3 and 6 below) are already known since they enter into the framework of extrapolation methods as explained in Section 1, and are derived in Section 2.1 and 2.2 by a purely algebraic process as the solution of a linear system and they can be easily obtained by a modification of the Approaches 2 and 5. Moreover, as will be explained in Section 3, these two strategies could also be included into the framework of the minimization by changing the metric of the norm. Approaches 3 and 6 will be used in Section 2.3, where the notion of *coupled sequence*, defined in [18], is invoked.

Let us explain the idea behind the minimization used for finding the vector $\boldsymbol{\alpha}$ (since $\boldsymbol{\beta}$ is related to $\boldsymbol{\alpha}$, the idea is similar). This idea was introduced in [54], but it was not related to Shanks transformations. In Section 4 and the following ones, our transformations are used to solve the fixed point problem $\mathbf{s} = G(\mathbf{s})$ from iterates of the form $\mathbf{s}_{n+1} = G(\mathbf{s}_n)$. Under some assumptions, it holds that $\mathbf{s}_n - \mathbf{s} = (G'(\mathbf{s}))^n (\mathbf{s}_0 - \mathbf{s}) + \mathcal{O}(||\mathbf{s}_0 - \mathbf{s}||^2)$. Thus, neglecting the terms of second order,

$$\sum_{i=0}^{k} \alpha_i \mathbf{s}_{n+i} - \mathbf{s} \approx (G'(\mathbf{s}))^n \sum_{i=0}^{k} \alpha_i (G'(\mathbf{s}))^i (\mathbf{s}_0 - \mathbf{s}).$$

The idea is to minimize this error term. But $\Delta \mathbf{s}_n \approx (G'(\mathbf{s}) - I)(\mathbf{s}_n - \mathbf{s})$, and thus

$$\sum_{i=0}^{k} \alpha_i \Delta \mathbf{s}_{n+i} \approx (G'(\mathbf{s}) - I)(G'(\mathbf{s}))^n \sum_{i=0}^{k} \alpha_i (G'(\mathbf{s}))^i (\mathbf{s}_0 - \mathbf{s}),$$

which is similar to the expressions minimized for obtaining the vector $\boldsymbol{\alpha}$ in Approaches 1 and 4 below.

When α or β has been computed, in any one of the ways described below, the vector **s** is directly obtained by (2) or (3) as

$$\mathbf{s} = [\mathbf{s}_{n+i}, \dots, \mathbf{s}_{n+i+k}] \boldsymbol{\alpha} = S_{n+i}^{(k+1)} \boldsymbol{\alpha}, \quad \text{for all } i,$$
(4)

or

$$\mathbf{s} = \mathbf{s}_{n+i+k} - [\Delta \mathbf{s}_{n+i}, \dots, \Delta \mathbf{s}_{n+i+k-1}]\boldsymbol{\beta} = \mathbf{s}_{n+i+k} - \Delta S_{n+i}^{(k)}\boldsymbol{\beta}, \quad \text{for all } i.$$
(5)

Remark 1 As can be seen, (5) has the form of a Schur complement

$$\mathbf{u} = \mathbf{u}_0 - [\mathbf{u}_1, \dots, \mathbf{u}_k] A^{-1} \mathbf{v},$$

where $\mathbf{u}, \mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{u}_k \in \mathbb{R}^p$, $\mathbf{v} \in \mathbb{R}^k$, and $A \in \mathbb{R}^{k \times k}$. Several other expression in the sequel have the same form.

From the extended Schur determinantal formula [10], **u** can be expressed as a ratio of two determinants

$$\mathbf{u} = \frac{\begin{vmatrix} \mathbf{u}_0 & \mathbf{u}_1 \cdots \mathbf{u}_k \\ \mathbf{v} & A \end{vmatrix}}{|A|}.$$

The determinant in the numerator is to be understood as the linear combination of the elements of its first row by applying the classical rules for expanding a determinant with respect its first row. It is exactly through this connection that all the transformations given in [18] (Least-Squares strategy apart) have been defined.

2.1 Minimal residual approaches

All the Minimal residual approaches described in this Section for computing α or β require the knowledge of the k + 2 vectors $\mathbf{s}_n, \ldots, \mathbf{s}_{n+k+1}$.

2.1.1 Approach 1

Writing (2) for the indices n and n+1 and subtracting, we obtain

$$\alpha_0 \Delta \mathbf{s}_n + \dots + \alpha_k \Delta \mathbf{s}_{n+k} = 0.$$

Then, one way to compute $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_k)^T$ is to solve the problem

$$\boldsymbol{\alpha} = \underset{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^T \boldsymbol{\gamma} = 1}{\arg\min} \|\Delta S_n^{(k+1)} \boldsymbol{\gamma}\|^2$$
(6)

where **e** is the vector of all ones. This is exactly the same relation introduced in [54], but obtained from a different starting point and without regularization. The original paper by Pulay [51] also solves the least squares problem with the same constraint that the sum of the α_i equal to 1 by using Lagrange multipliers. Observe that equation (2) and the minimality of k ensure that dim ker $(\Delta S_n^{(k+1)}) = 1$. Hence, the solution of problem (6) can be obtained by normalizing the unique vector in the kernel; alternatively, it can also be obtained as follows (which leads to the SVD-MPE approach, see [57])

$$\boldsymbol{\alpha} = \frac{\overline{\boldsymbol{\alpha}}}{\mathbf{e}^T \overline{\boldsymbol{\alpha}}} \quad \text{where} \quad \overline{\boldsymbol{\alpha}} = \underset{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \|\boldsymbol{\gamma}\|^2 = 1}{\arg\min} \|\Delta S_n^{(k+1)} \boldsymbol{\gamma}\|^2.$$
(7)

2.1.2 Approach 2

Writing (3) for the indices n and n+1 and subtracting, we have

$$\Delta \mathbf{s}_{n+k} - \sum_{j=0}^{k-1} \beta_j [\Delta \mathbf{s}_{n+1+j} - \Delta \mathbf{s}_{n+j}] = \mathbf{0},$$

i.e., in compact form,

$$\Delta \mathbf{s}_{n+k} - \Delta^2 S_n^{(k)} \boldsymbol{\beta} = \mathbf{0},\tag{8}$$

where $\Delta^2 S_n^{(k)} = [\Delta^2 \mathbf{s}_n, \dots, \Delta^2 \mathbf{s}_{n+k-1}].$

The vector $\boldsymbol{\beta}$ is solution of the problem

$$\boldsymbol{\beta} = \underset{\boldsymbol{\eta} \in \mathbb{R}^k}{\arg\min} \|\Delta \mathbf{s}_{n+k} - \Delta^2 S_n^{(k)} \boldsymbol{\eta}\|^2,$$
(9)

and therefore it can be obtained by solving the normal equations:

$$(\Delta^2 S_n^{(k)})^T \Delta^2 S_n^{(k)} \boldsymbol{\beta} = (\Delta^2 S_n^{(k)})^T \Delta \mathbf{s}_{n+k},$$
(10)

which leads to the strategy of the Reduced Rank Extrapolation (RRE) due to Eddy [27] and Mesina [45].

2.1.3 Approach 3

This approach generalizes the one seen in the preceding Section. We consider a matrix $Y \in \mathbb{R}^{p \times k}$, where p is the dimension of the vectors of the sequence. If we multiply (8) by Y^T , it is possible to obtain the β_i by solving the following system that generalizes (10) which is obtained when $Y = \Delta^2 S_n^{(k)}$

$$Y^T \Delta^2 S_n^{(k)} \boldsymbol{\beta} = Y^T \Delta \mathbf{s}_{n+k},\tag{11}$$

assuming that rank $(Y^T \Delta^2 S_n^{(k)}) = k$.

The best choice of the matrix Y is a difficult problem which has not been studied yet. However, some experimental results show that an appropriate choice of it can improve the convergence. As shown, for example, in [18], particular choices of Y yield several existing extrapolation methods. Thus, the choice $Y = [\mathbf{y}_1, \ldots, \mathbf{y}_k]$, where the \mathbf{y}_i 's are k linear independent vectors, corresponds to the MMPE of Brezinski [8] and Pugachev [50] which can be recursively implemented by the $S\beta$ -algorithm of Jbilou [41]. The choice $\mathbf{y}_i = \Delta \mathbf{s}_{n+i-1}$ leads to the MPE of Cabay and Jackson [20], and the RRE of Mešina [45] and Eddy [27] is recovered with $\mathbf{y}_i = \Delta^2 \mathbf{s}_{n+i-1}$.

2.2 Topological approaches

These approaches differ from those presented in Section 2.1 in that the algebraic equations for computing the coefficients α_i or β_i require more vectors of the sequence (\mathbf{s}_n) , namely they now need to utilize the 2k + 1 vectors $\mathbf{s}_n, \ldots, \mathbf{s}_{n+2k}$.

2.2.1 Approach 4

Writing (2) for the indices $n, \ldots, n+k$, and subtracting, we have

$$\alpha_0 \Delta \mathbf{s}_{n+i} + \dots + \alpha_k \Delta \mathbf{s}_{n+k+i} = 0, \quad \text{for } i = 0, \dots, k-1,$$

and the coefficients α_i are obtained by solving

$$\boldsymbol{\alpha} = \underset{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^T \boldsymbol{\gamma} = 1}{\arg\min} \|\Delta \overline{S}_n^{(k+1)} \boldsymbol{\gamma}\|^2$$
(12)

where

$$\Delta \overline{S}_{n}^{(k+1)} = \begin{pmatrix} \Delta \mathbf{s}_{n} & \Delta \mathbf{s}_{n+1} & \cdots & \Delta \mathbf{s}_{n+k} \\ \Delta \mathbf{s}_{n+1} & \Delta \mathbf{s}_{n+2} & \cdots & \Delta \mathbf{s}_{n+k+1} \\ \vdots & \vdots & & \vdots \\ \Delta \mathbf{s}_{n+k-1} & \Delta \mathbf{s}_{n+k} & \cdots & \Delta \mathbf{s}_{n+2k-1} \end{pmatrix} = \begin{pmatrix} \Delta S_{n}^{(k+1)} \\ \Delta S_{n+1}^{(k+1)} \\ \vdots \\ \Delta S_{n+k-1}^{(k+1)} \end{pmatrix} \in \mathbb{R}^{kp \times (k+1)}.$$

2.2.2 Approach 5

The β_i 's can be computed by writing (3) for the indices $n + k, \ldots, n + 2k$, and subtracting. We have

$$\Delta \mathbf{s}_{n+k+i} - \sum_{j=0}^{k-1} \beta_j \Delta^2 \mathbf{s}_{n+i+j} = \mathbf{0}, \qquad \text{for } i = 0, \dots, k-1.$$

The coefficients β_i are solution of the problem

$$\boldsymbol{\beta} = \underset{\boldsymbol{\eta} \in \mathbb{R}^k}{\operatorname{arg\,min}} \|\Delta \overline{S}_{n+k}^{(1)} - \Delta^2 \overline{S}_n^{(k)} \boldsymbol{\eta}\|^2$$
(13)

where

$$\Delta \overline{S}_{n+k}^{(1)} = \begin{pmatrix} \Delta \mathbf{s}_{n+k} \\ \vdots \\ \Delta \mathbf{s}_{n+2k-1} \end{pmatrix} \in \mathbb{R}^{kp}, \ \Delta^2 \overline{S}_n^{(k)} = \begin{pmatrix} \Delta^2 \mathbf{s}_n & \Delta^2 \mathbf{s}_{n+1} \cdots & \Delta^2 \mathbf{s}_{n+k-1} \\ \Delta^2 \mathbf{s}_{n+1} & \Delta^2 \mathbf{s}_{n+2} \cdots & \Delta^2 \mathbf{s}_{n+k} \\ \vdots & \vdots & \vdots \\ \Delta^2 \mathbf{s}_{n+k-1} & \Delta^2 \mathbf{s}_{n+k} \cdots & \Delta^2 \mathbf{s}_{n+2k-2} \end{pmatrix} \in \mathbb{R}^{kp \times k},$$

that is

$$\boldsymbol{\beta} = ((\Delta^2 \overline{S}_n^{(k)})^T \Delta^2 \overline{S}_n^{(k)})^{-1} (\Delta^2 \overline{S}_n^{(k)})^T \Delta \overline{S}_{n+k}^{(1)}.$$

2.2.3 Approach 6

As in Approach 3, choosing $Y \in \mathbb{R}^{kp \times k}$, we can alternatively solve

$$Y^T \Delta^2 \overline{S}_n^{(k)} \boldsymbol{\beta} = Y^T \Delta \overline{S}_{n+k}^{(1)} \tag{14}$$

 $\text{if } \operatorname{rank}(Y^T\Delta^2\overline{S}_n^{(2k-2)})=k.$

When $Y = I_k \otimes \mathbf{y}$, for some $\mathbf{y} \in \mathbb{R}^p$, we recover the so called *Topological Shanks transformation* that can be implemented recursively by the topological ε -algorithms of Brezinski [8] (in short TEA) or, more economically, by the simplified topological ε -algorithms (in short STEA) [13, 14].

2.3 Coupled transformations

We now recall the concept of *Coupled Sequences* introduced in [18] since, by using this extension, it is possible to link Anderson acceleration to the transformations based on the Shanks kernel.

Given a sequence (\mathbf{s}_n) belonging to the Shanks kernel, a coupled sequence (\mathbf{c}_n) is a sequence which satisfies, for all n

$$\alpha_0 \mathbf{c}_n + \dots + \alpha_k \mathbf{c}_{n+k} = 0$$

where the coefficients α_i are the same as in (2), or, equivalently a sequence satisfying

$$\mathbf{c}_{n+k} - \sum_{j=0}^{k-1} \beta_j \Delta \mathbf{c}_{n+j} = \mathbf{0}, \quad \text{ for all } n$$

with the same coefficients β_j as in (3). For example, the sequence $(\mathbf{c}_n = \Delta^m \mathbf{s}_n)$ is a sequence coupled to (\mathbf{s}_n) for any $m \ge 1$.

By using a known coupled sequence, we can build additional generalizations of the Approaches 3 and 6, which are recovered if we take $(\mathbf{c}_n = \Delta \mathbf{s}_n)$, and compute $\boldsymbol{\beta}$ as follows. Let $C_n^{(k)} = [\mathbf{c}_n, \ldots, \mathbf{c}_{n+k-1}] \in \mathbb{R}^{p \times k}$. Instead of (11), we solve the system

$$Y^T \Delta C_n^{(k)} \boldsymbol{\beta} = Y^T \mathbf{c}_{n+k},\tag{15}$$

where $Y \in \mathbb{R}^{p \times k}$.

Similarly, by defining the matrix $\overline{C}_i^{(j)}$ as made for $\overline{S}_i^{(j)}$, we can, instead of (14), solve

$$Y^T \Delta \overline{C}_n^{(k)} \boldsymbol{\beta} = Y^T \overline{C}_{n+k}^{(1)}, \tag{16}$$

where now $Y \in \mathbb{R}^{kp \times k}$,

Particular choices of Y and of the coupled sequence (\mathbf{c}_n) give expressions similar to those of well known methods (see [18] for more details).

3 Shanks-based transformations for general sequences

The approaches described in the previous Section are all equivalent for a sequence belonging to the Shanks kernel and they yield the exact limit or antilimit. It is clear however, that this is an idealistic situation. For extrapolating sequences that do not belong to the Shanks kernel (1), we still write down the systems of linear equations or the optimization problems giving the coefficients α_i or β_i (which now depend of k and n), and define a sequence transformation as the same linear combination of terms as above.

In the sequel, for the extrapolated vector, we use the double indexing $\mathbf{t}_i^{(j)}$ that highlights the fact that the transformations, require the j + 1 elements $\mathbf{s}_n, \ldots, \mathbf{s}_{n+j}$ of the sequence, in order to compute $\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$.

- Minimal residual: In the case of the Minimal residual approaches there are k + 1 vectors involved in the linear combination. Thus, since to compute $\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$, we need the k + 2 vectors $\mathbf{s}_n, \ldots, \mathbf{s}_{n+k+1}$, we have only the following two different transformations, with the same $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ (we denote the second transformation with a tilde symbol over the \mathbf{t})
 - $\mathbf{t}_{n}^{(k+1)} = [\mathbf{s}_{n+1}, \dots, \mathbf{s}_{n+k+1}] \boldsymbol{\alpha} = S_{n+1}^{(k+1)} \boldsymbol{\alpha}$, or equivalently $\mathbf{t}_{n}^{(k+1)} = \mathbf{s}_{n+k+1} - [\Delta \mathbf{s}_{n+1}, \dots, \Delta \mathbf{s}_{n+k}] \boldsymbol{\beta} = \mathbf{s}_{n+k+1} - \Delta S_{n+1}^{(k)} \boldsymbol{\beta}$ • $\widetilde{\mathbf{t}}_{n}^{(k+1)} = [\mathbf{s}_{n}, \dots, \mathbf{s}_{n+k}] \boldsymbol{\alpha} = S_{n}^{(k+1)} \boldsymbol{\alpha}$, or equivalently $\widetilde{\mathbf{t}}_{n}^{(k+1)} = \mathbf{s}_{n+k} - [\Delta \mathbf{s}_{n}, \dots, \Delta \mathbf{s}_{n+k-1}] \boldsymbol{\beta} = \mathbf{s}_{n+k} - \Delta S_{n}^{(k)} \boldsymbol{\beta}$

where $\boldsymbol{\alpha} \in \mathbb{R}^{k+1}$ solves (6) or (7) (Approach 1) and $\boldsymbol{\beta} \in \mathbb{R}^k$ solves (9) or (11) (Approaches 2 or 3), or (15) (coupled approach).

Topological: In the Topological case, there are again k + 1 vectors involved in the linear combination, but since we need the 2k + 1 vectors $\mathbf{s}_n, \ldots, \mathbf{s}_{n+2k}$ to compute $\boldsymbol{\alpha}$ or $\boldsymbol{\beta}$, we have k + 1 different transformations (depending on the choice of the vectors used in the linear combination), but with the same $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, and we have

•
$$\mathbf{t}_{n,i}^{(2k)} = [\mathbf{s}_{n+i}, \dots, \mathbf{s}_{n+i+k}] \boldsymbol{\alpha} = S_{n+i}^{(k+1)} \boldsymbol{\alpha}, \quad \text{for } i = 0, \dots, k$$

or equivalently
 $\mathbf{t}_{n,i}^{(2k)} = \mathbf{s}_{n+i+k} - [\Delta \mathbf{s}_{n+i}, \dots, \Delta \mathbf{s}_{n+i+k-1}] \boldsymbol{\beta} = \mathbf{s}_{n+i+k} - \Delta S_{n+i}^{(k)} \boldsymbol{\beta}, \quad \text{for } i = 0, \dots, k$

where $\boldsymbol{\alpha} \in \mathbb{R}^{k+1}$ solves (12) (Approach 4) and $\boldsymbol{\beta} \in \mathbb{R}^k$ given by (13) or (14) (Approaches 5 or 6), or (16) (coupled approach).

Among all the possible linear combinations, it seems more appropriate to use those involving the last available vector of the sequence, that is the transformation with i = k that uses \mathbf{s}_{n+2k} . In the sequel, for simplifying the notation we will set $\mathbf{t}_n^{(2k)} = \mathbf{t}_{n,k}^{(2k)}$.

Of course, if the sequence belongs to the Shanks kernel, all the preceding transformations are equivalent and give the same result, that is s.

Now, let us show how to adapt and extend to our approaches the idea proposed in [54]. All the transformations summarized at the beginning of this Section can be used, and the only change deals with the computation of the coefficients α_i or the β_i . In [54], in order to overcome the problems due to the ill-conditioning of problem (6) (our Approach 1) the authors consider the following regularized problem for the computation of the α_i in the minimal residual approach

$$\boldsymbol{\alpha}_{\lambda} = \operatorname*{arg\,min}_{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^{T}\boldsymbol{\gamma} = 1} \left(\|\Delta S_{n}^{(k+1)}\boldsymbol{\gamma}\|^{2} + \lambda \|\boldsymbol{\gamma}\|^{2} \right),$$

with $\lambda \in \mathbb{R}$, and whose solution is (assuming that $\Delta S_n^{(k+1)}$ is of full rank)

$$\boldsymbol{\alpha}_{\lambda} = \frac{((\Delta S_n^{(k+1)})^T \Delta S_n^{(k+1)} + \lambda I)^{-1} \mathbf{e}}{\mathbf{e}^T ((\Delta S_n^{(k+1)})^T \Delta S_n^{(k+1)} + \lambda I)^{-1} \mathbf{e}}.$$

Observe that an alternative approach would be to change the metric in the evaluation of the norm, i.e., instead of using the Euclidean norm, solve the problem

$$\boldsymbol{\alpha}_{M,\lambda} = \operatorname*{arg\,min}_{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^T \boldsymbol{\gamma} = 1} \left(\|\Delta S_n^{(k+1)} \boldsymbol{\gamma}\|_M^2 + \lambda \|\boldsymbol{\gamma}\|^2 \right), \tag{17}$$

where $\|\mathbf{x}\|_M^2 = (\mathbf{x}, M\mathbf{x})$ and $M \in \mathbb{R}^{p \times p}$ is a positive definite matrix. In what follows we will need M to be positive semi-definite only instead of positive definite. In this case $\|\cdot\|_M$ is a semi-norm but we abuse the terminology by calling it a 'norm'.

With this, we have the following lemma.

Lemma 1 The solution of problem (17) is

$$\boldsymbol{\alpha}_{M,\lambda} = \frac{((\Delta S_n^{(k+1)})^T M \Delta S_n^{(k+1)} + \lambda I)^{-1} \mathbf{e}}{\mathbf{e}^T ((\Delta S_n^{(k+1)})^T M \Delta S_n^{(k+1)} + \lambda I)^{-1} \mathbf{e}},$$
(18)

and the corresponding extrapolated vector is

$$\mathbf{t}_{n}^{(k+1)} = S_{n+1}^{(k+1)} \boldsymbol{\alpha}_{M,\lambda} \quad or \quad \widetilde{\mathbf{t}}_{n}^{(k+1)} = S_{n}^{(k+1)} \boldsymbol{\alpha}_{M,\lambda}.$$
(19)

Proof: The result follows by writing the problem (17) as

$$\boldsymbol{\alpha}_{M,\lambda} = \operatorname*{arg\,min}_{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^T \boldsymbol{\gamma} = 1} \left(\boldsymbol{\gamma}^T (\Delta S_n^{(k+1)})^T M \Delta S_n^{(k+1)} \boldsymbol{\gamma} + \lambda \boldsymbol{\gamma}^T \boldsymbol{\gamma} \right),$$

and by applying a technique analogous to that used in [54]. From (4) we obtain (19).

Motivated by the equivalence of all the approaches described in Section 2.1 for sequences in the Shanks kernel, we can thus introduce the following problem

$$\boldsymbol{\beta}_{M,\lambda} = \underset{\boldsymbol{\eta} \in \mathbb{R}^k}{\operatorname{arg\,min}} \left(\|\Delta \mathbf{s}_{n+k} - \Delta^2 S_n^{(k)} \boldsymbol{\eta}\|_M^2 + \lambda \|\boldsymbol{\eta}\|^2 \right),$$
(20)

where M is a semi-positive definite matrix. Referring to the gradient of the function $g(\eta) =$ $\|\Delta \mathbf{s}_{n+k} - \Delta^2 S_n^{(k)} \boldsymbol{\eta}\|_M^2 + \lambda \|\boldsymbol{\eta}\|^2$, the solution of (20) is given by

$$\boldsymbol{\beta}_{M,\lambda} = ((\Delta^2 S_n^{(k)})^T M \Delta^2 S_n^{(k)} + \lambda I)^{-1} (\Delta^2 S_n^{(k)})^T M \Delta \mathbf{s}_{n+k},$$
(21)

and hence, the corresponding extrapolated vector is

$$\mathbf{t}_{n}^{(k+1)} = \mathbf{s}_{n+k+1} - [\Delta \mathbf{s}_{n+1}, \dots, \Delta \mathbf{s}_{n+k}]\boldsymbol{\beta}_{M,\lambda},$$
(22)

or

$$\widetilde{\mathbf{t}}_{n}^{(k+1)} = \mathbf{s}_{n+k} - [\Delta \mathbf{s}_{n}, \dots, \Delta \mathbf{s}_{n+k-1}]\boldsymbol{\beta}_{M,\lambda}$$

In particular, if $M = YY^T$ where $Y \in \mathbb{R}^{p \times k}$ is a given matrix and $\lambda = 0$, we have,

$$(\Delta^2 S_n^{(k)})^T Y \left(Y^T \Delta^2 S_n^{(k)} \boldsymbol{\beta}_{YY^T,0} - Y^T \Delta \mathbf{s}_{n+k} \right) = \mathbf{0}.$$

When rank $(Y^T \Delta^2 S_n^{(k)}) = k$, we see that Approach 3 (11) is a particular case of problem (20). As we already observed, different choices of $Y \in \mathbb{R}^{p \times k}$ give rise to different *acceleration* performances for different type of sequences.

Similarly, following the idea of the topological approaches of Section 2.2, we consider the problems

$$\boldsymbol{\alpha}_{M,\lambda} = \operatorname*{arg\,min}_{\boldsymbol{\gamma} \in \mathbb{R}^{k+1}, \mathbf{e}^T \boldsymbol{\gamma} = 1} \left(\|\Delta \overline{S}_n^{(k+1)} \boldsymbol{\gamma}\|_M^2 + \lambda \|\boldsymbol{\gamma}\|^2 \right), \tag{23}$$

or

$$\boldsymbol{\beta}_{M,\lambda} = \operatorname*{arg\,min}_{\boldsymbol{\eta} \in \mathbb{R}^k} \left(\|\Delta \overline{S}_{n+k}^{(1)} - \Delta^2 \overline{S}_n^{(k)} \boldsymbol{\eta}\|_M^2 + \lambda \|\boldsymbol{\eta}\|^2 \right), \tag{24}$$

where, in both cases, $M \in \mathbb{R}^{kp \times kp}$ is a semi-positive definite matrix. The solution of (23) is

$$\boldsymbol{\alpha}_{M,\lambda} = \frac{((\Delta \overline{S}_n^{(k+1)})^T M \Delta \overline{S}_n^{(k+1)} + \lambda I)^{-1} \mathbf{e}}{\mathbf{e}^T ((\Delta \overline{S}_n^{(k+1)})^T M \Delta \overline{S}_n^{(k+1)}) + \lambda I)^{-1} \mathbf{e}},$$
(25)

and the corresponding extrapolated vector is

$$\mathbf{t}_{n}^{(2k)} = S_{n+k}^{(k+1)} \boldsymbol{\alpha}_{M,\lambda}.$$
(26)

The solution of problem (24) is

$$\boldsymbol{\beta}_{M,\lambda} = ((\Delta^2 \overline{S}_n^{(k)})^T M \Delta^2 \overline{S}_n^{(k)} + \lambda I)^{-1} (\Delta^2 \overline{S}_n^{(k)})^T M \Delta \overline{S}_{n+k}^{(1)}$$

and the corresponding extrapolated vector is

$$\mathbf{t}_{n}^{(2k)} = \mathbf{s}_{n+2k} - [\Delta \mathbf{s}_{n+k}, \dots, \Delta \mathbf{s}_{n+2k-1}]\boldsymbol{\beta}_{M,\lambda}.$$
(27)

We set $M = YY^T$ with $Y \in \mathbb{R}^{kp \times k}$ and $\operatorname{rank}(Y^T \Delta^2 \overline{S}_n^{(k)}) = k$. If $\lambda = 0$, we see that the Approach 6 is a particular case of the problem (24). If $Y = I_k \otimes \mathbf{y}$, for some $\mathbf{y} \in \mathbb{R}^p$, we obtain a method similar to the Topological Shanks transformation [8].

We refer the reader to Section 6 for a discussion of different possible strategies for the selection of the regularization parameter λ .

4 Possible uses of acceleration strategies

In this Section and in the following one, we consider the solution of the fixed point problem $G(\mathbf{s}) = \mathbf{s}$. There are three ways to proceed.

The simplest way is to use an extrapolation method. The vectors \mathbf{s}_n are generated one by one by Picard's iteration as $\mathbf{s}_{n+1} = G(\mathbf{s}_n), n = 0, 1, \ldots$, from a given \mathbf{s}_0 . The extrapolation method is applied after each computation of a new vector \mathbf{s}_n by using a certain number of the preceding Picard's iterates to produce a completely new extrapolated sequence. This procedure is called the *Acceleration Method* but it is not used in this paper (see [14] for details).

The second way consists in computing a certain number of Picard's iterates, then to use these in one of the extrapolation techniques introduced in Section 3, and finally to restart the Picard's iterates from the extrapolated vector that has been obtained. This is the *Restarted* method treated below.

In the third way, the process builds its own sequence step by step. Each term of the sequence is obtained by combining, in a certain manner, Picard's iterates, preceding terms of the sequence and extrapolated ones. We will focus on three possible algorithms of this type that are termed *Continuous-Updating*, presented in this Section, the *Anderson-type* and the *Periodic Anderson-type* methods, both discussed in Section 5. The difference between these procedures lies in the way in which previous iterates are combined together in the process to obtain a new vector.

4.1 Restarted method

In this methodology, already described, for example, in [5, 14, 35], a certain number of Picard's iterates are produced, an extrapolation strategy is then applied to them, and the Picard's iterates are *restarted* from the extrapolated vector; see Algorithm 1. The sequence of the successive extrapolated terms will be denoted by (\mathbf{x}_i) .

Algorithm 1: The Restarted Method (RM).

Input: Choose M, λ , k, and $\mathbf{x}_0 \in \mathbb{R}^p$. 1 for j = 0, 1, ... do 2 Set $\mathbf{s}_0 = \mathbf{x}_j$ 3 for $i = 1, ..., \ell_k - 1$ (basic or inner iterations) do 4 Compute $\mathbf{s}_i = G(\mathbf{s}_{i-1})$ 5 end 6 Compute $\mathbf{t}_0^{(\ell_k - 1)}$ using (19) or (22) or (26) or (27) 7 Set $\mathbf{x}_{j+1} = \mathbf{t}_0^{(\ell_k - 1)}$ 8 end

Observe that $\ell_k = k + 2$ if we use (19) or (22), and $\ell_k = 2k + 1$ if we use (26) or (27). In the particular case of (22), we have

$$\mathbf{t}_0^{(k+1)} = \mathbf{s}_{k+1} - G_{M,\lambda} \Delta \mathbf{s}_k$$

where

$$G_{M,\lambda} = [\Delta \mathbf{s}_1, \dots, \Delta \mathbf{s}_k] ((\Delta^2 S_0^{(k)})^T M \Delta^2 S_0^{(k)} + \lambda I)^{-1} (\Delta^2 S_0^{(k)})^T M,$$

Setting $\mathbf{f}_k = G(\mathbf{s}_k) - \mathbf{s}_k = \Delta \mathbf{s}_k$, we have

$$\mathbf{t}_0^{(k+1)} = \mathbf{s}_{k+1} - G_{M,\lambda} \mathbf{f}_k.$$

Therefore, we can interpret the Restarted Method as a cyclic projection method (see [33] and [11] for the linear case) for the solution of the problem $F(\mathbf{s}) = 0$ where $F(\mathbf{s}) = G(\mathbf{s}) - \mathbf{s}$.

The idea of the RM, that is to interleave a certain number of Picard's iterates with one extrapolation step, can also be used in the *Continuous-Updating* and in the *Anderson-type* methods (see Section 5 where a general 'periodic' algorithm of this type is presented).

A particular case of the RM is the Generalized Steffensen Method (GSM) which corresponds to the case where the dimension of the projection space coincides with the dimension of the system, that is for k = p. Under some assumptions, when $\lambda = 0$ and M = I, the sequence (\mathbf{x}_j) obtained by the GSM asymptotically converges quadratically to the fixed point \mathbf{s}^* of G even if G is not a contraction. The GSM is a generalization of the well-known Steffensen method [62] when p = 1. It was first proposed by Brezinski [5] and Gekeler [35] for the case of the vector ε -algorithm, but there was a gap in their proofs as in that of Skelboe for the MPE [61] as noticed in [60] The first complete proof of the quadratic convergence of the GSM was given by Ortega and Rheinbolt [46, p. 373] for Henrici's method [39, pp. 115 ff.] (a particular case of the MMPE), Le Ferrand [43] for the first Topological Shanks transformation of Brezinski [8], and Jbilou and Sadok for the MPE and the RRE [41].

4.2 Continuous-Updating method

In this approach, the sequence is *continuously accelerated* by computing a new basic iterate at each step, using it in the extrapolation process, and, after the computation of the extrapolated vector, replacing the new basic iterate computed before by it. Thus, when compared with the original fixed point sequence, the continuous updating scheme builds a completely new sequence whose iterates replace those of the original sequence.

We start with the Minimal residual approach for computing the α_i . We have the following Continuous-Updating Method (Algorithm 2)

Algorithm 2: Continuous-Updating Method (CU) with $\alpha_{M,\lambda}$.

Input: Choose M, λ , $m \in \mathbb{N}$, $m \ge 1$, $\mathbf{s}_0 \in \mathbb{R}^p$. 1 for j = 0, 1, ... do 2 Set $m_j = \min(m, j)$ 3 Compute $\mathbf{s}_{j+1} = G(\mathbf{s}_j)$ (Picard iteration) 4 Set $S_{j-m_j}^{(m_j+1)} = [\mathbf{s}_{j-m_j}, ..., \mathbf{s}_j]$ 5 Compute $\boldsymbol{\alpha}_{M,\lambda}$ using (18) and $\Delta S_{j-m_j}^{(m_j+1)}$ 6 Compute $\tilde{\mathbf{t}}_{j-m_j}^{(m_j+1)} = S_{j-m_j}^{(m_j+1)} \boldsymbol{\alpha}_{M,\lambda}$ 7 Set $\mathbf{s}_{j+1} = \tilde{\mathbf{t}}_{j-m_j}^{(m_j+1)}$ 8 end

Algorithm 3 listed next, uses formulas (21–22), (i.e. the β_i 's, are computed by (21), that solve the problem (20))

Algorithm 3: Continuous-Updating Method (CU) with $\beta_{M,\lambda}$.

Input: Choose M, λ , $m \in \mathbb{N}$, $m \ge 1$, $\mathbf{s}_0 \in \mathbb{R}^p$. 1 Compute $\mathbf{s}_1 = G(\mathbf{s}_0)$ 2 for j = 1, 2, ... do 3 Set $m_j = \min(m, j)$ 4 Compute $\mathbf{s}_{j+1} = G(\mathbf{s}_j)$ (Picard iteration) 5 Set $\Delta S_{j-m_j}^{(m_j)} = [\Delta \mathbf{s}_{j-m_j}, ..., \Delta \mathbf{s}_{j-1}]$ 6 Compute $\boldsymbol{\beta}_{M,\lambda}$ using (21) and $\Delta^2 S_{j-m_j}^{(m_j)}$ 7 Compute $\tilde{\mathbf{t}}_{j-m_j}^{(m_j+1)} = \mathbf{s}_j - \Delta S_{j-m_j}^{(m_j)} \boldsymbol{\beta}_{M,\lambda}$ 8 Set $\mathbf{s}_{j+1} = \tilde{\mathbf{t}}_{j-m_j}^{(m_j+1)}$ 9 end

As in the preceding algorithm, the new fixed point iterate \mathbf{s}_{j+1} is used only for computing $\boldsymbol{\beta}_{M,\lambda}$. Thereafter, this iterate is not used in the linear combination for computing the extrapolated vector as it is replaced by the extrapolated one that is computed.

It is possible to highlight the connection between acceleration techniques and the projection framework. We define

$$G_{M,\lambda}^{(j)} = [\Delta \mathbf{s}_{j-m_j}, \dots, \Delta \mathbf{s}_{j-1}] ((\Delta^2 S_{j-m_j}^{(m_j)})^T M \Delta^2 S_{j-m_j}^{(m_j)} + \lambda I)^{-1} (\Delta^2 S_{j-m_j}^{(m_j)})^T M.$$

If we set $\mathbf{f}_j = G(\mathbf{s}_j) - \mathbf{s}_j = \mathbf{s}_{j+1} - \mathbf{s}_j$ (where here \mathbf{s}_{j+1} denotes the Picard iteration) we can compute a new vector \mathbf{s}_{j+1} as

$$\mathbf{s}_{j+1} = \mathbf{s}_j - G_{M,\lambda}^{(j)} \mathbf{f}_j.$$

Observe that $G_{M,\lambda}^{(j)}$ satisfies the following *multisecant* condition, see, e.g., [31], (when $\lambda = 0$)

$$G_{M,\lambda}^{(j)}\Delta^2 S_{j-m_j}^{(m_j)} = [\Delta \mathbf{s}_{j-m_j}, \dots, \Delta \mathbf{s}_{j-1}].$$

It is interesting to notice that, when $\lambda \neq 0$, we obtain a class of *regularized projection methods*, that do not yet seem to have been fully investigated in the literature.

For the sake of simplicity, we did not present here the topological approaches of Section 2.2, but the preceding algorithms can be easily modified for these transformations.

5 Anderson-type Mixing (ATM) methods

Anderson Acceleration (AA) (also known as Anderson Mixing) is a technique originally presented in [2] for solving systems of nonlinear equations written as $F(\mathbf{s}) = G(\mathbf{s}) - \mathbf{s} = 0$. In this section, we generalize the basic version of AA as given by Walker and Ni [64] or by Higham and Strabić [40]. The main idea of this generalization is that a procedure similar to Anderson Acceleration can be built up with any of the Shanks transformations. We will name such methods Anderson-type Mixing (ATM) to emphasize the fact that, as it will be explained, these methods use a Continuous-Updating scheme which mixes information coming out from two different sequences. Indeed, in the framework of the Continuous-Updating scheme presented in Section 4.2, two different sequences are generated, i.e., the continuously updated sequence (\mathbf{s}_j) on the one hand, and the sequence $(G(\mathbf{s}_j))$ on the other. The main feature of the Anderson-Mixing strategy is that it combines the information coming from these two sequences in order to obtain a better acceleration procedure. We will prove that it coincides with a quasi-Newton strategy. Since, in this case, the sequence (\mathbf{s}_j) is not generated by a *fixed point iteration*, we also consider the sequence (\mathbf{f}_j) , where $\mathbf{f}_j = G(\mathbf{s}_j) - \mathbf{s}_j = \mathbf{g}_j - \mathbf{s}_j$, that do not coincide with the sequence $(\Delta \mathbf{s}_j)$.

Algorithm 4 shown below is a prototype version of *Anderson-type Mixing* method where we define:

$$F_{j-m_j}^{(m_j)} \equiv [\mathbf{f}_{j-m_j}, \dots, \mathbf{f}_{j-1}]$$

and use the previous notation $S_{j-m_j}^{(m_j)} \equiv [\mathbf{s}_{j-m_j}, \dots, \mathbf{s}_{j-1}].$

Algorithm 4:	The Anderson	-Type Mixing	(ATM) method.	
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Input: Choose $m \in \mathbb{N}, m \ge 1, \beta \in \mathbb{R}, \mathbf{s}_0 \in \mathbb{R}^p$. 1 Compute $\mathbf{f}_0 = G(\mathbf{s}_0) - \mathbf{s}_0$ and $\mathbf{s}_1 = \mathbf{s}_0 + \beta \mathbf{f}_0$ 2 for $j = 1, 2, \dots$ do 3 Compute $\mathbf{f}_j = G(\mathbf{s}_j) - \mathbf{s}_j$ 4 Set $m_j = \min(m, j)$ 5 Set $\Delta S_{j-m_j}^{(m_j)} = [\Delta \mathbf{s}_{j-m_j}, \dots, \Delta \mathbf{s}_{j-1}]$ and $\Delta F_{j-m_j}^{(m_j)} = [\Delta \mathbf{f}_{j-m_j}, \dots, \Delta \mathbf{f}_{j-1}]$ 6 Compute $\boldsymbol{\theta}^{(j)} \in \mathbb{R}^{m_j}$ 7 Compute $\overline{\mathbf{s}}_j = \mathbf{s}_j - \Delta S_{j-m_j}^{(m_j)} \boldsymbol{\theta}^{(j)}$ and $\overline{\mathbf{f}}_j = \mathbf{f}_j - \Delta F_{j-m_j}^{(m_j)} \boldsymbol{\theta}^{(j)}$ 8 Set $\mathbf{s}_{j+1} = \overline{\mathbf{s}}_j + \beta \overline{\mathbf{f}}_j$ 9 end

The scalar β , usually a fixed positive value with $0 < \beta \leq 1$, is called *mixing* or *damping* parameter. It is also possible to change it at each cycle, and it can be used to improve convergence. A common choice is to take $\beta = 1$. In this case, since $\mathbf{g}_j = G(\mathbf{s}_j) = \mathbf{s}_j + \mathbf{f}_j$ we can define

$$G_{j-m_j}^{(m_j)} = [\mathbf{g}_{j-m_j}, \dots, \mathbf{g}_{j-1}] = S_{j-m_j}^{(m_j)} + F_{j-m_j}^{(m_j)}.$$

By denoting $\overline{\mathbf{g}}_j = \overline{\mathbf{s}}_j + \overline{\mathbf{f}}_j = \mathbf{g}_j - \Delta G_{j-m_j}^{(m_j)} \boldsymbol{\theta}^{(j)}$, the new iterate can be simply computed as $\mathbf{s}_{j+1} = \overline{\mathbf{g}}_j$. This is the so-called *undamped iterate*.

Let us point out that Line 8 in Algorithm 4 can be alternatively written as

$$\mathbf{s}_{j+1} = \mathbf{s}_j - \left(-\beta \mathbf{f}_j + \left(\Delta S_{j-m_j}^{(m_j)} + \beta \Delta F_{j-m_j}^{(m_j)}\right) \boldsymbol{\theta}^{(j)}\right),\tag{28}$$

and that different choices of $\boldsymbol{\theta}^{(j)}$ give rise to different ATMs. Some particular cases are described in the sequel.

The original AA is obtained when

$$\boldsymbol{\theta}^{(j)} = \underset{\boldsymbol{\eta} \in \mathbb{R}^{m_j}}{\arg\min} \|\mathbf{f}_j - \Delta F_{j-m_j}^{(m_j)} \boldsymbol{\eta}\|^2,$$
(29)

that is, assuming that the columns of $\Delta F_{j-m_j}^{(m_j)}$ are linearly independent,

 $\boldsymbol{\theta}^{(j)} = ((\Delta F_{j-m_j}^{(m_j)})^T \Delta F_{j-m_j}^{(m_j)})^{-1} (\Delta F_{j-m_j}^{(m_j)})^T \mathbf{f}_j.$

Remark 2 It is interesting to observe that defining $\theta^{(j)}$'s as

$$\boldsymbol{\theta}^{(j)} = \underset{\boldsymbol{\eta} \in \mathbb{R}^{m_j}}{\arg\min} \|\Delta \mathbf{s}_j - \Delta^2 S_{j-m_j}^{(m_j)} \boldsymbol{\eta}\|^2$$

i.e., using (8), would be a good choice if the sequence (\mathbf{s}_j) is close to the Shanks kernel. Instead, in the original AA the derivation of the $\boldsymbol{\theta}^{(j)}$ using (29) could be interpreted as an implicit assumption that the sequence (\mathbf{f}_j) is closer to the Shanks kernel than the sequence (\mathbf{s}_j) .

From (28), we have

$$\mathbf{s}_{j+1} = \mathbf{s}_j - (-\beta I + (\Delta S_{j-m_j}^{(m_j)} + \beta \Delta F_{j-m_j}^{(m_j)})((\Delta F_{j-m_j}^{(m_j)})^T \Delta F_{j-m_j}^{(m_j)})^{-1} (\Delta F_{j-m_j}^{(m_j)})^T) \mathbf{f}_j,$$
(30)

as also observed in [18, 31].

Formula (28) highlights the connections between Anderson Mixing and quasi-Newton methods. Indeed, in this case, defining

$$H_{j}^{(\beta)} = -\beta I + (\Delta S_{j-m_{j}}^{(m_{j})} + \beta \Delta F_{j-m_{j}}^{(m_{j})})((\Delta F_{j-m_{j}}^{(m_{j})})^{T} \Delta F_{j-m_{j}}^{(m_{j})})^{-1} (\Delta F_{j-m_{j}}^{(m_{j})})^{T},$$

we can write

$$\mathbf{s}_{j+1} = \mathbf{s}_j - H_j^{(\beta)} \mathbf{f}_j,$$

with $H_j^{(\beta)}$ satisfying the multisecant condition $H_j^{(\beta)}\Delta F_{j-m_j}^{(m_j)} = \Delta S_{j-m_j}^{(m_j)}$. In the next section we will fully make use of this idea: by introducing a *stabilization procedure* to overcome problems connected to the ill-conditioning of the matrix $(\Delta F_{j-m_j}^{(m_j)})^T \Delta F_{j-m_j}^{(m_j)}$, it is possible to prove the local linear convergence of the AA method.

As indicated in the previous Section, it is also possible to define a *Periodic Anderson-Type* Mixing method whereby acceleration steps are interspersed into linear updates at regular intervals. Fixing the period $\mu \in \mathbb{N}$, with $\mu \geq 1$, an Anderson-type update is made each μ iterations. In between these updates, when $\mu > 1$, the iterates are computed simply as a linear mixing $\mathbf{s}_{j+1} = \mathbf{s}_j + \beta \mathbf{f}_j$, where β is the mixing parameter ($\beta = 1$ corresponds to Picard's iteration). Clearly, when $\mu = 1$ Algorithm 5 coincides with Algorithm 4.

Algorithm 5: The Periodic Anderson-Type Mixing method.

Input: Choose $m, \mu \in \mathbb{N}, m, \mu \geq 1, \beta \in \mathbb{R}, \mathbf{s}_0 \in \mathbb{R}^p$. 1 Compute $\mathbf{f}_0 = G(\mathbf{s}_0) - \mathbf{s}_0$ and $\mathbf{s}_1 = \mathbf{s}_0 + \beta \mathbf{f}_0$ **2** for j = 1, 2, ... do Compute $\mathbf{f}_i = G(\mathbf{s}_i) - \mathbf{s}_i$ 3 if $(j+1) \mod \mu = 0$ then 4 Compute \mathbf{s}_{j+1} using steps 4 to 8 of Algorithm 4 (Anderson-type update) $\mathbf{5}$ else 6 Compute $\mathbf{s}_{j+1} = \mathbf{s}_j + \beta \mathbf{f}_j$ (linear mixing update) 7 end 8 9 end

It is important to underline that the values of μ and m can be chosen independently. However, when $\mu \geq 3$ and we choose $m = \mu - 2$, then the terms used for computing the Anderson-type

update are only those terms obtained by the linear mixing update, and therefore in this situation Algorithm 5 proceeds as a RM method of Algorithm 1, with a different restarting formula. It must also be noticed that Algorithm 5 with $\theta^{(j)}$ computed as in (29), is exactly the Periodic Pulay method [4] (compare also with (30)). Interleaving Anderson Acceleration with fixed point iterations for improving the global convergence properties, but not necessarily the speed, has been recognized before in the physics literature as can be seen from the related discussion and the references in [4]. This idea is somewhat similar also to the A2DR (Anderson accelerated Douglas– Rachford) algorithm proposed in [32].

To start the derivation of the new ATMs, we observe that a possible generalization for the derivation of the $\theta^{(j)}$ can be obtained by using the coupled sequences defined in Section 2.3, that is by taking

$$\boldsymbol{\theta}^{(j)} = (Y^T \Delta C_{j-m_j}^{(m_j)})^{-1} Y^T \mathbf{c}_j.$$
(31)

If we take $\mathbf{c}_j = \mathbf{f}_j$, for all j, and $Y = \Delta C_{j-m_j}^{(m_j)} = \Delta F_{j-m_j}^{(m_j)}$ we recover the AA choice for $\boldsymbol{\theta}^{(j)}$. It is easy to see that taking into account the transformations defined at the beginning of Section 3, if we consider the extrapolated vector $\tilde{\boldsymbol{t}}_{j-m_j}^{(m_j+1)} = \mathbf{s}_j - \Delta S_{j-m_j}^{(m_j)} \boldsymbol{\theta}^{(j)}$ we recover exactly the $\overline{\mathbf{s}}_j$'s computed in Algorithms 4 and 5. If we consider the same $\boldsymbol{\theta}^{(j)}$, in the same relation, and by using, as sequence to be extrapolated the coupled one (\mathbf{f}_j) , we obtain $\overline{\mathbf{f}}_j$.

Another additional generalization can be made by considering, as in problem (20) of Section 3, a different metric in the evaluation of the norm, and also a regularization parameter λ . We consider the problem

$$\boldsymbol{\theta}_{M,\lambda}^{(j)} = \underset{\boldsymbol{\eta} \in \mathbb{R}^{m_j}}{\arg\min} \left(\| \mathbf{c}_j - \Delta C_{j-m_j}^{(m_j)} \boldsymbol{\eta} \|_M^2 + \lambda \| \boldsymbol{\eta} \|^2 \right).$$
(32)

The solution is

$$\boldsymbol{\theta}_{M,\lambda}^{(j)} = ((\Delta C_{j-m_j}^{(m_j)})^T M \Delta C_{j-m_j}^{(m_j)} + \lambda I)^{-1} (\Delta C_{j-m_j}^{(m_j)})^T M \mathbf{c}_j.$$
(33)

By taking in (33) $\mathbf{c}_j = \mathbf{f}_j$ and M = I, that is by introducing only a ℓ_2 -regularization term to the original AA problem, we obtain a method that we call *Regularized Anderson Acceleration* (in short RAA).

If we take $M = YY^T$ and $\lambda = 0$, it is possible to see that $\boldsymbol{\theta}_{M,\lambda}^{(j)}$ in (33) can be obtained, alternatively, as the solution of the linear system

$$(\Delta C_{j-m_j}^{(m_j)})^T Y (Y^T \Delta C_{j-m_j}^{(m_j)} \boldsymbol{\theta}_{YY^T,0}^{(j)} - Y^T \mathbf{c}_j) = 0,$$

which correspond exactly to (31), assuming that $\operatorname{rank}((\Delta C_{j-m_i}^{(m_j)})^T Y) = m_j$.

The ATMs methods can thus be obtained by considering the coupled sequence $(\mathbf{c}_j) = (\mathbf{f}_j)$ fixed, and changing the matrix Y. The following particular cases are of interest:

1. ATM-RRE: $Y = [\Delta^2 \mathbf{s}_{j-m_j}, \dots, \Delta^2 \mathbf{s}_{j-1}] = \Delta^2 S_{j-m_j}^{(m_j)} \in \mathbb{R}^{p \times m_j}$ corresponds to a method in the style of the RRE. For this choice, since we also need the knowledge of the vector \mathbf{s}_{j+1} we have to edit slightly Algorithm 4 by beginning the loop (line 2) with j = 2 and by adding before it the computation of $\mathbf{s}_2 = \mathbf{s}_1 + \beta \mathbf{f}_1$. Modifications that take this into account must also be made in Algorithm 5. The choice $Y = [\Delta^2 \mathbf{f}_{j-m_j}, \dots, \Delta^2 \mathbf{f}_{j-1}] = \Delta^2 F_{j-m_j}^{(m_j)} \in \mathbb{R}^{p \times m_j}$ is also possible.

- 2. ATM-MPE: $Y = [\Delta \mathbf{s}_{j-m_j}, \dots, \Delta \mathbf{s}_{j-1}] = \Delta S_{j-m_j}^{(m_j)} \in \mathbb{R}^{p \times m_j}$ or $Y = [\mathbf{f}_{j-m_j}, \dots, \mathbf{f}_{j-1}] = F_{j-m_j}^{(m_j)} \in \mathbb{R}^{p \times m_j}$ leads to two methods in the style of the MPE;
- 3. ATM-MMPE: $Y = [\mathbf{y}_1, \dots, \mathbf{y}_{m_j}] \in \mathbb{R}^{p \times m_j}$ which leads to an ATM in the style of the MMPE.
- 4. ATM-TEA: suitably modifying the structure of Algorithms 4 and 5, it is possible to use a topological approach (see Section 2.2) to obtain the coefficients $\boldsymbol{\theta}_{M,\lambda}^{(j)}$. As in Section 4.2 we omit all the details for the sake of brevity.

Before concluding this section, we point out that the introduction of an ℓ_2 -regularization term for AA has already been studied in the recent papers [3,32,47], and that (32) represents a generalization to the ATM methods of the ℓ_2 -regularization approach for AA. In Section 6, for the particular AA case, we will propose and experimentally analyze the choice of the regularization parameter λ using the *Generalized Cross Validation* [36]. This choice represents a major difference with the above mentioned works, where the choice of the regularization parameter is made adaptively based on quantities related to the most recent iterates (see, for example, [32, eq. (3.4)] and [47, eq. (3)]). Sections 5.1 and 5.2 below further justify/clarify the introduction of an ℓ_2 -regularization strategy.

5.1 Stabilized AA

The aim of this Section is to present an algorithm which can be viewed as a *stabilized* version of the AA method. In particular, in this new version of AA, a check on the linear independence of the vectors $\Delta \mathbf{f}_d$ is performed (Lines 7 -16): the residual difference $\Delta \mathbf{f}_d$ is discarded if its projection $\mathbf{\hat{f}}_d$ onto the orthogonal of the previously computed residual differences is *close* to the null vector, i.e., if it results in a vector of sufficiently small norm when compared to the original one (see Section 5.2 for further details). It is interesting to note that when, in Algorithm 6, we choose m = 1 (and likely for small values of m) the introduced stabilization procedure is not required and Algorithm 6 coincides with the classic AA scheme (compare, in this case, (30) and the update at Line 20 in Algorithm 6).

Algorithm 6: Stabilized Anderson Acceleration.

Input: Choose $m \in \mathbb{N}, m \geq 1, \beta \in \mathbb{R}, \mathbf{s}_0 \in \mathbb{R}^p$ and $\tau > 1$. 1 Compute $\mathbf{f}_0 = G(\mathbf{s}_0) - \mathbf{s}_0$ and $\mathbf{s}_1 = \mathbf{s}_0 + \beta \mathbf{f}_0$ 2 for j = 1, ... do Set $m_i = \min(m, j)$. 3 Compute $\mathbf{f}_i = G(\mathbf{s}_i) - \mathbf{s}_i$ 4 Compute $\widehat{\mathbf{f}}_{j-m_j} = \Delta \mathbf{f}_{j-m_j}$ Set $P_{j-m_j} = (\widehat{\mathbf{f}}_{j-m_j} \widehat{\mathbf{f}}_{j-m_j}^T) / (\widehat{\mathbf{f}}_{j-m_j}^T \widehat{\mathbf{f}}_{j-m_j})$ $\mathbf{5}$ 6 for $d = j - m_i + 1, ..., j - 1$ do 7 $\begin{aligned} u &= j \quad m_j + 1, \dots, j \quad 1 \quad \mathrm{d}\mathbf{b} \\ \mathrm{Set} \ Q_{j-m_j}^{d-1} &= \sum_{i=j-m_j}^{d-1} P_i \\ \mathrm{Compute} \ \widehat{\mathbf{f}}_d &= (I - Q_{j-m_j}^{d-1}) \Delta \mathbf{f}_d \end{aligned}$ 8 9 if $\|\widehat{\mathbf{f}}_d\|_{\tau} \geq \|\Delta \mathbf{f}_d\|$ then 10 Set $P_d = (\widehat{\mathbf{f}}_d \, \widehat{\mathbf{f}}_d^T) / (\widehat{\mathbf{f}}_d^T \, \widehat{\mathbf{f}}_d)$ 11 else 12 Set $\widehat{\mathbf{f}}_d = \mathbf{0}$ Set $P_d = \mathbf{0}$ $\mathbf{13}$ $\mathbf{14}$ end 15end 16Set $\mathcal{I}_j = \{k_1, \ldots, k_{\widehat{m}_j}\} \subseteq \{j - m_j, \ldots, j - 1\}$ the set of indices such that $\widehat{\mathbf{f}}_{k_1}, \cdots, \widehat{\mathbf{f}}_{k_{\widehat{m}_j}}$ $\mathbf{17}$ are non null vectors Set $\Delta F_{\mathcal{I}_j} = [\Delta \mathbf{f}_{k_1}, \dots, \Delta \mathbf{f}_{k_{\widehat{m}_j}}], \ \Delta S_{\mathcal{I}_j} = [\Delta \mathbf{s}_{k_1}, \dots, \Delta \mathbf{s}_{k_{\widehat{m}_j}}]$ 18 Set $H_j^{(\beta)} = \left[-\beta I + (\Delta S_{\mathcal{I}_j} + \beta \Delta F_{\mathcal{I}_j})((\Delta F_{\mathcal{I}_j})^T \Delta F_{\mathcal{I}_j})^{-1} (\Delta F_{\mathcal{I}_j})^T \right]$ 19 Compute $\mathbf{s}_{i+1} = \mathbf{s}_i - H_i^{(\beta)} \mathbf{f}_i$ $\mathbf{20}$ 21 end

5.1.1 Local convergence

There already exist in the literature different proofs of the local convergence for the stabilized versions of AA, see for example [32, 34, 47, 52, 53]. In principle, our convergence analysis can be obtained using ideas and techniques from [52, Sec. 4.2], but we prefer to present here a full detailed proof. The reasons to present such a detailed proof can be mainly summarized as follows: a) our derivation is not completely analogous to that in [52]: simplifying some arguments, we are able to obtain slightly more general results than those presented in [52, Sec. 4.2] (the interested reader can compare our Theorem 1 with [52, Th. 4.10]); b) our analysis does not require the contractivity or non-expansivity of the fixed point map G, a major difference if compared to what has been proved in [32, 47]; c) our proof of convergence holds for every mixing parameter $\beta \in \mathbb{R}$ shedding further light on the significance and the relevance of the parameter β in the AA procedure: it can be interpreted as a scaling factor of the initial Jacobian approximation (see Theorem 1); d) when m = 1, since Algorithm 6 coincides with the classic AA scheme (see the beginning of Section 5.1), we obtain, as a by-product of our analysis, an alternative proof of that given in [63, Sec. 2.3] for the convergence of the classic AA with m = 1 without assuming, once more, any contractivity of

the fixed point map G. We consider the function $F(\mathbf{s}) = G(\mathbf{s}) - \mathbf{s}$, and we made the following assumption:

Assumption 1 $F : \mathbf{R}^n \to \mathbf{R}^n$ is differentiable in a open convex set $E \subseteq \mathbb{R}^n$ and there exists $\mathbf{s}^* \in E$ such that $\mathbf{f}^* = F(\mathbf{s}^*) = \mathbf{0}$. Moreover, $J = F'(\mathbf{s}^*)$ is invertible and for all $\mathbf{s} \in E$ we have

$$|F'(\mathbf{s}) - F'(\mathbf{s}^*)|| \le L ||\mathbf{s} - \mathbf{s}^*||.$$

The above assumption implies that,

$$||F(\mathbf{u}) - F(\mathbf{v}) - J(\mathbf{u} - \mathbf{v})|| \le L ||\mathbf{u} - \mathbf{v}|| \max\{||\mathbf{u} - \mathbf{s}^*||, ||\mathbf{v} - \mathbf{s}^*||\},\$$

for all $\mathbf{u}, \mathbf{v} \in E$ and that there exists $U_{\kappa}(\mathbf{s}^*) := \{\mathbf{u} \in \mathbb{R}^n : \|\mathbf{u} - \mathbf{s}^*\| \le \kappa\}$ s.t., for some $\rho > 0$,

$$\frac{1}{\rho} \|\mathbf{u} - \mathbf{v}\| \le \|F(\mathbf{u}) - F(\mathbf{v})\| \le \rho \|\mathbf{u} - \mathbf{v}\|.$$

In the remainder of this section we use the notations introduced in Algorithm 6.

Lemma 2 The matrices $H_i^{(\beta)}$ (defined at Line 19 of Algorithm 6) satisfy the multisecant condition

$$H_j^{(\beta)} \Delta F_{\mathcal{I}_j} = \Delta S_{\mathcal{I}_j}$$

Proof: The proof is by direct verification.

Lemma 3 $H_i^{(\beta)}$ can be computed recursively from $H_i^0 = -\beta I$ using

$$H_j^d = H_j^{d-1} + \frac{(\Delta \mathbf{s}_{k_d} - H_j^{d-1} \Delta \mathbf{f}_{k_d}) \widehat{\mathbf{f}}_{k_d}^T}{\widehat{\mathbf{f}}_{k_d}^T \Delta \mathbf{f}_{k_d}} \text{ for } d = 1, \dots, \widehat{m}_j$$

with $H_j^{\widehat{m}_j} = H_j^{(\beta)}$ (see Line 17 in Algorithm 6 for the definitions of $\widehat{\mathbf{f}}_{k_d}$). In particular, for all $d = 1, \ldots, \widehat{m}_j$, we have: $H_j^d \Delta \mathbf{f}_{k_p} = \Delta \mathbf{s}_{k_p}$ for $p = 1, \ldots, d$.

Proof: Define $Z \in \mathbb{R}^{n \times n - \widehat{m}_j}$ as a basis for $\operatorname{span}(\Delta F_{\mathcal{I}_j})^{\perp}$. From the definition of $H_j^{(\beta)}$ we have $H_j^{(\beta)}Z = -\beta Z$ and $H_j^{(\beta)}\Delta F_{\mathcal{I}_j} = \Delta S_{\mathcal{I}_j}$. To prove the theorem, we will prove (by induction) that $H_j^{\widehat{m}_j}$ satisfies the same relations. For d = 1 we have $H_j^1 = H_j^0 + \frac{(\Delta \mathbf{s}_{k_1} - H_j^0 \Delta \mathbf{f}_{k_1}) \widehat{\mathbf{f}}_{k_1}^T}{\widehat{\mathbf{f}}_{k_1}^T \Delta \mathbf{f}_{k_1}}$ and hence $H_j^1 \Delta \mathbf{f}_{k_1} = \Delta \mathbf{s}_{k_1}$. Suppose now the assumption true for $d = \ell$. By definition we have that $H_j^{\ell+1} \Delta \mathbf{f}_{k_{\ell+1}} = \Delta \mathbf{s}_{k_{\ell+1}}$ and $H_j^{\ell+1} \Delta \mathbf{f}_{k_p} = \Delta \mathbf{s}_{k_p}$ for all $p = 1, \ldots, \ell$ since $\widehat{\mathbf{f}}_{k_{\ell+1}} \perp \Delta \mathbf{f}_{k_p}$. Finally, since

$$\operatorname{span}(\widehat{\mathbf{f}}_{k_1},\ldots,\widehat{\mathbf{f}}_{k_{\widehat{m}_j}}) = \operatorname{span}(\Delta \mathbf{f}_{k_1},\ldots,\Delta \mathbf{f}_{k_{\widehat{m}_j}}),$$

implies that Z is also a basis for span $(\widehat{\mathbf{f}}_{k_1}, \ldots, \widehat{\mathbf{f}}_{k_{\widehat{m}_j}})^{\perp}$, we have $H_j^{\widehat{m}_j}Z = -\beta Z$. The result follows observing that, since $[\Delta F_{\mathcal{I}_j}, Z]$ is invertible, the equation $B[\Delta F_{\mathcal{I}_j}, Z] = [\Delta S_{\mathcal{I}_j}, -\beta Z]$ has a unique solution.

Observe that, as already pointed out in [67], Lemma 3 highlights the connections between the Jacobian approximations produced by the *Bad (or type-II) Broyden* update [19] and the matrices produced by AA.

Lemma 4 Let us define $\widehat{\mathbf{s}}_{k_1} = \Delta \mathbf{s}_{k_1}$ and for $d = 2, \ldots, \widehat{m}_j$ define $\widehat{\mathbf{s}}_{k_d} = \Delta \mathbf{s}_{k_d} - H_j^{d-1} Q_{k_1}^{k_{d-1}} \Delta \mathbf{f}_{k_d}$ being $Q_{k_1}^{k_{d-1}} = \sum_{p=1}^{d-1} (\widehat{\mathbf{f}}_{k_p} \widehat{\mathbf{f}}_{k_p}^T / \widehat{\mathbf{f}}_{k_p}^T \widehat{\mathbf{f}}_{k_p})$. Then $H_j^{(\beta)}$ can be computed recursively from $H_j^0 = -\beta I$ using

$$H_j^d = H_j^{d-1} + \frac{(\widehat{\mathbf{s}}_{k_d} - H_j^{d-1} \widehat{\mathbf{f}}_{k_d}) \widehat{\mathbf{f}}_{k_d}^T}{\widehat{\mathbf{f}}_{k_d}^T \widehat{\mathbf{f}}_{k_d}} \text{ for } d = 1, \dots, \widehat{m}_j$$

with $H_j^{\widehat{m}_j} = H_j^{(\beta)}$. In particular, for all $d = 1, \ldots, \widehat{m}_j$, we have: $H_j^d \widehat{\mathbf{f}}_{k_p} = \widehat{\mathbf{s}}_{k_p}$ for $p = 1, \ldots, d$.

Proof: The proof follows from the definition of H_i^d , and observing that

$$\widehat{\mathbf{f}}_{k_d} = (I - Q_{k_1}^{k_{d-1}}) \Delta \mathbf{f}_{k_d} \Rightarrow \widehat{\mathbf{f}}_{k_d}^T \widehat{\mathbf{f}}_{k_d} = \widehat{\mathbf{f}}_{k_d}^T \Delta \mathbf{f}_{k_d}$$

(since $(I - Q_{k_1}^{k_{d-1}})$ is a projector) and that $\widehat{\mathbf{s}}_{k_d} - H_j^{d-1} \widehat{\mathbf{f}}_{k_d} = \Delta \mathbf{s}_{k_d} - H_j^{d-1} \Delta \mathbf{f}_{k_d}$.

Lemma 5 Suppose that $\mathbf{s}_{k_d}, \mathbf{s}_{k_d+1} \in U_{\kappa}(\mathbf{s}^*)$ for all $d = 1, \ldots, \widehat{m}_j$. Then, the following inequality is satisfied

$$\|\widehat{\mathbf{s}}_{k_d} - J^{-1}\widehat{\mathbf{f}}_{k_d}\| \le C \|\Delta \mathbf{f}_{k_d}\| \sum_{p=1}^d n_{k_p}^{k_p+1} (2\tau)^{p-d},$$

where $C = \|J^{-1}\|L\rho$ and $n_{k_p}^{k_p+1} = \max\{\|\mathbf{s}_{k_p+1} - \mathbf{s}^*\|, \|\mathbf{s}_{k_p} - \mathbf{s}^*\|\}.$

Proof: For d = 1 we have

$$\|\widehat{\mathbf{s}}_{k_1} - J^{-1}\widehat{\mathbf{f}}_{k_1}\| = \|\Delta \mathbf{s}_{k_1} - J^{-1}\Delta \mathbf{f}_{k_1}\| \le C \|\Delta \mathbf{f}_{k_1}\| n_{k_1}^{k_1+1},$$

where the last inequality follows from Assumption 1. Suppose now the assumption true for $d = \ell$. To prove the statement for $d = \ell + 1$ we have

$$\begin{split} \|\widehat{\mathbf{s}}_{k_{\ell+1}} - J^{-1}\widehat{\mathbf{f}}_{k_{\ell+1}}\| &\leq \|\Delta \mathbf{s}_{k_{\ell+1}} - J^{-1}\Delta \mathbf{f}_{k_{\ell+1}}\| + \|H_{j}^{\ell}Q_{k_{1}}^{k_{\ell}}\Delta \mathbf{f}_{k_{\ell+1}} - J^{-1}Q_{k_{1}}^{k_{\ell}}\Delta \mathbf{f}_{k_{\ell+1}}\| \\ &\leq C\|\Delta \mathbf{f}_{k_{\ell+1}}\|n_{k_{\ell+1}}^{k_{\ell+1}+1} + \sum_{p=1}^{\ell} \frac{\|H_{j}^{\ell}\widehat{\mathbf{f}}_{k_{p}} - J^{-1}\widehat{\mathbf{f}}_{k_{p}}\|}{\|\widehat{\mathbf{f}}_{k_{p}}\|} \|\Delta \mathbf{f}_{k_{\ell+1}}\| \\ &= C\|\Delta \mathbf{f}_{k_{\ell+1}}\|n_{k_{\ell+1}}^{k_{\ell+1}+1} + \sum_{p=1}^{\ell} \frac{\|\widehat{\mathbf{s}}_{k_{p}} - J^{-1}\widehat{\mathbf{f}}_{k_{p}}\|}{\|\widehat{\mathbf{f}}_{k_{p}}\|} \|\Delta \mathbf{f}_{k_{\ell+1}}\| \\ &\leq C\|\Delta \mathbf{f}_{k_{\ell+1}}\|(n_{k_{\ell+1}}^{k_{\ell+1}+1} + \tau \sum_{p=1}^{\ell} \sum_{h=1}^{p} n_{k_{h}}^{k_{h}+1}(2\tau)^{p-h}) = C\|\Delta \mathbf{f}_{k_{\ell+1}}\|(n_{k_{\ell+1}}^{k_{\ell+1}+1} + \tau \sum_{p=1}^{\ell} n_{k_{p}}^{k_{p}+1}h = 0^{\ell-p}(2\tau)^{h}) \end{split}$$

where, in the first inequality, we use the definition of $\widehat{\mathbf{s}}_{k_{\ell+1}}$, in the second inequality, we use the definition of $Q_{k_1}^{k_{\ell}}$, in the first equality, we use the fact that $H_j^{\ell} \widehat{\mathbf{f}}_{k_p} = \widehat{\mathbf{s}}_{k_p}$ for $p = 1, \ldots, \ell$ (see Lemma 4), and, in the last inequality, our induction hypothesis. Finally, since

$$\sum_{h=0}^{\ell-p} (2\tau)^h \le \tau^{\ell-p} \sum_{h=0}^{\ell-p} 2^h = \tau^{\ell-p} (2^{\ell-p+1} - 1) \le \tau^{\ell-p} 2^{\ell-p+1},$$

we have that

$$C\|\Delta \mathbf{f}_{k_{\ell+1}}\|(n_{k_{\ell+1}}^{k_{\ell+1}+1} + \tau \sum_{p=1}^{\ell} n_{k_p}^{k_p+1} \sum_{h=0}^{\ell-p} (2\tau)^h) \le C\|\Delta \mathbf{f}_{k_{\ell+1}}\| \sum_{p=1}^{\ell+1} n_{k_p}^{k_p+1} (2\tau)^{\ell+1-p}$$

which concludes the proof.

Lemma 6 The following equality is satisfied

$$H_{j}^{(\beta)} - J^{-1} = (-\beta I - J^{-1})(I - Q_{k_{1}}^{k_{\widehat{m}_{j}}}) + \sum_{d=1}^{\widehat{m}_{j}} \frac{(\widehat{\mathbf{s}}_{k_{d}} - J^{-1}\widehat{\mathbf{f}}_{k_{d}})\widehat{\mathbf{f}}_{k_{d}}^{T}}{\widehat{\mathbf{f}}_{k_{d}}^{T}\widehat{\mathbf{f}}_{k_{d}}}.$$

Moreover, if $\mathbf{s}_{k_d}, \mathbf{s}_{k_d+1} \in U_{\kappa}(\mathbf{s}^*)$ and $n_{k_d}^{k_d+1} \leq \varepsilon$ for all $d = 1, \ldots, \overline{m}_j$, there exists a constant $\alpha = \alpha(\tau, m, C)$ such that

$$\sum_{d=1}^{\widehat{m}_j} \frac{\|(\widehat{\mathbf{s}}_{k_d} - J^{-1}\widehat{\mathbf{f}}_{k_d})\widehat{\mathbf{f}}_{k_d}^T\|}{\widehat{\mathbf{f}}_{k_d}^T\widehat{\mathbf{f}}_{k_d}} \le \alpha\varepsilon.$$

Proof: The first part of the statement follows from direct computation using the fact that the vectors $\hat{\mathbf{f}}_{k_d}$ are orthogonal (see also [52, Lemma 4.17]). For the second part, observe that

$$\begin{split} & \sum_{d=1}^{\widehat{m}_j} \frac{\|(\widehat{\mathbf{s}}_{k_d} - J^{-1}\widehat{\mathbf{f}}_{k_d})\widehat{\mathbf{f}}_{k_d}^T\|}{\widehat{\mathbf{f}}_{k_d}^T \widehat{\mathbf{f}}_{k_d}} \leq \sum_{d=1}^{\widehat{m}_j} \frac{\|(\widehat{\mathbf{s}}_{k_d} - J^{-1}\widehat{\mathbf{f}}_{k_d})\|}{\|\widehat{\mathbf{f}}_{k_d}\|} \\ & \leq C \sum_{d=1}^{\widehat{m}_j} \frac{\|\Delta \mathbf{f}_{k_d}\|}{\|\widehat{\mathbf{f}}_{k_d}\|} \sum_{p=1}^d n_{k_d}^{n_d+1} (2\tau)^{d-p} \leq \varepsilon C\tau \sum_{d=1}^{\widehat{m}_j} \sum_{p=1}^d (2\tau)^{d-p} \\ & \leq \varepsilon C\tau \sum_{d=1}^m \sum_{h=0}^{d-1} (2\tau)^h \leq \varepsilon Cm (2\tau)^m, \end{split}$$

where, in the second inequality, we use Lemma 5, and, in the fourth one, the fact that $\widehat{m}_j \leq m_j \leq m$ for all j.

Theorem 1 Let $\mathbf{s}_0, \mathbf{s}_1, \ldots$, be the iterates produced by Algorithm 6 (Stabilized Anderson Acceleration). Then, for all $q \in (0, 1)$, there exists $\delta = \delta(q, \alpha)$, $\varepsilon(q, \alpha)$ such that if

 $\|-\beta I - J^{-1}\| \leq \delta \text{ and } \|\mathbf{s}_0 - \mathbf{s}^*\| \leq \varepsilon,$

we have

$$\mathbf{s}_{j+1} \in E \text{ and } \|\mathbf{s}_{j+1} - \mathbf{s}^*\| \le q \|\mathbf{s}_j - \mathbf{s}^*\|$$

for all $j \in \mathbf{N}$.

Proof: For a fixed q, choose δ and ε such that

$$\|J^{-1}\|L\varepsilon + \rho(\delta + \alpha\varepsilon) < q$$

in a way that $U_{\varepsilon}(\mathbf{s}^*) \subseteq U_{\kappa}(\mathbf{s}^*) \subseteq E$ (where κ and α are the same as in Lemma 6, and ρ is the same as in Assumption 1). For j = 0 we have

$$\begin{aligned} \|\mathbf{s}_{1} - \mathbf{s}^{*}\| &\leq \|\mathbf{s}_{0} + \beta \mathbf{f}_{0} - \mathbf{s}^{*}\| \leq \|\mathbf{s}_{0} - \mathbf{s}^{*} - J^{-1}(\mathbf{f}_{0} - \mathbf{f}^{*})\| + \|(-\beta I - J^{-1})(\mathbf{f}_{0} - \mathbf{f}^{*})\| \\ &\leq \|J^{-1}\|\|J(\mathbf{s}_{0} - \mathbf{s}^{*}) - (\mathbf{f}_{0} - \mathbf{f}^{*})\| + \delta\|\mathbf{f}_{0} - \mathbf{f}^{*}\| \leq (\|J^{-1}\|L\varepsilon + \delta\rho)\|\mathbf{s}_{0} - \mathbf{s}^{*}\| \leq q\|\mathbf{s}_{0} - \mathbf{s}^{*}\| \leq \varepsilon, \end{aligned}$$

which proves that $\mathbf{s}_1 \in U_{\varepsilon}(\mathbf{s}^*)$. Assume now that, for all $j \ge 0$, $\|\mathbf{s}_j - \mathbf{s}^*\| \le q^j \|\mathbf{s}_0 - \mathbf{s}^*\|$ and hence that $\mathbf{s}_j \in U_{\varepsilon}(\mathbf{s}^*)$. We have

$$\begin{aligned} \|\mathbf{s}_{j+1} - \mathbf{s}^*\| &= \|\mathbf{s}_j - H_j^{(\beta)} \mathbf{f}_j - \mathbf{s}^*\| \\ &\leq \|J^{-1}\| \|J(\mathbf{s}_j - \mathbf{s}^*) - (\mathbf{f}_j - \mathbf{f}^*)\| + \|H_j^{(\beta)} - J^{-1}\| \|\mathbf{f}_j - \mathbf{f}^*\| \\ &\leq \|J\|^{-1}L \|\mathbf{s}_j - \mathbf{s}^*\|^2 + \rho \|H_j^{(\beta)} - J^{-1}\| \|\mathbf{s}_j - \mathbf{s}^*\| \\ &\leq (\|J\|^{-1}Lq^j\varepsilon + \rho(\delta + \alpha\varepsilon)) \|\mathbf{s}_j - \mathbf{s}^*\| \leq q \|\mathbf{s}_j - \mathbf{s}^*\|, \end{aligned}$$

where, in the last inequality, we use our induction hypothesis and Lemma 6. \blacksquare

It is interesting to note that, in the particular case that G is contractive, Theorem 1 proves that, at least locally, the stabilized version of AA (Algorithm 6) could improve the rate of convergence of the fixed point map $\mathbf{s}_{j+1} = G(\mathbf{s}_j)$ since the linear convergence parameter q in Theorem 1 can be chosen smaller than the contraction factor of G (see also [29, 47]). Observe, moreover, that if the inequality $\| -\beta I - J^{-1} \| \leq \delta$ could not be fulfilled, we can consider the *preconditioned* non linear function $\tilde{F} = P^{-1}F$ where P is some approximation of $J = F(\mathbf{s}^*)$, and we obtain in this way $\| -\beta I - J^{-1}P \| \leq \delta$.

Finally, let us observe that, as customary in the quasi-Newton literature, we can improve the global convergence properties of the AA procedure by introducing a step-length parameter α_j and transforming the sequence generated by Algorithm 6 into the sequence

$$\mathbf{s}_{j+1} = \mathbf{s}_j - \alpha_j H_j^{(\beta)} \mathbf{f}_j.$$

5.2 Connections between stabilized AA and regularized ATM

As already pointed out in the previous section, from a theoretical point of view, the stabilization procedure introduced in Algorithm 6, in order to ensure the convergence, aims to detect a subset of the vectors in $\Delta F_{j-m_j}^{(m_j)}$ that are sufficiently linearly independent: the proposed stabilization procedure in Algorithm 6 (Lines 7 -16) can be interpreted simply as a Gram-Schmidt procedure with threshold, i.e., the residual difference $\Delta \mathbf{f}_d$ is discarded if it is close to a vector linearly dependent from the previously computed residual differences. The above observation naturally links the stabilization procedure with Rank-Revealing QR factorizations [21,37]. We find this issue particularly interesting and deserving further investigation. Here, we prefer to adopt a regularization point of view, as in [3,32,47,54], to motivate the introduction of the regularization parameter λ in the Anderson-Type Mixing methods as we did at the beginning of Section 5. To this end, let us consider the ATM obtained by (33) with $\mathbf{c}_j = \mathbf{f}_j$ and M = I. As already pointed out, when $\lambda = 0$ it coincides with the classical AA but, when $\lambda \neq 0$, the method obtained can be viewed as a Regularized Anderson Acceleration (RAA).

In this setting, we interpret the magnitude of the singular values of the matrix $\Delta F_{j-m_j}^{(m_j)}$ as a measure of the linear independence of its columns: the presence of linearly dependent vectors in

 $\Delta F_{j-m_j}^{(m_j)}$ is highlighted by the presence of very small singular values. Let us consider now the SVD decomposition $\Delta F_{j-m_j}^{(m_j)} = U\Sigma V^T$. We add a regularization parameter λ to the matrix Σ and, we set $\Delta \widetilde{F}_{j-m_j}^{(m_j)} = U\sqrt{\Sigma^2 + \lambda I}V^T$. By direct computation, it is possible to show that (33) can be written as

$$\boldsymbol{\theta}_{I,\lambda}^{(j)} = ((\Delta \widetilde{F}_{j-m_j}^{(m_j)})^T \Delta \widetilde{F}_{j-m_j}^{(m_j)})^{-1} (\Delta F_{j-m_j}^{(m_j)})^T \mathbf{f}_j.$$

The statement regarding the linear independence of the columns of the matrix $\Delta \tilde{F}_{j-m_j}^{(m_j)}$ can be obtained by observing that all its singular values are bounded from below by $\sqrt{\lambda}$. We consider the above argument as an explanation of the fact that the introduction of a regularization parameter in the AA method (and, in general, in all the ATMs) could achieve numerically the same task of the stabilization procedure of Algorithm 6. Adopting a quasi-Newton point of view, it is important to observe that using Formula (28) with $\boldsymbol{\theta}^{(j)} = \boldsymbol{\theta}_{I,\lambda}^{(j)}$, the ATM update (see Line 8 in Algorithm 4) can be written as

$$\mathbf{s}_{j+1} = \mathbf{s}_j - \widetilde{H}_j^{(\beta)} \mathbf{f}_j,$$

with

$$\widetilde{H}_{j}^{(\beta)} = -\beta I + (\Delta S_{j-m_{j}}^{(m_{j})} + \beta \Delta F_{j-m_{j}}^{(m_{j})}) ((\Delta \widetilde{F}_{j-m_{j}}^{(m_{j})})^{T} \Delta \widetilde{F}_{j-m_{j}}^{(m_{j})})^{-1} (\Delta F_{j-m_{j}}^{(m_{j})})^{T}.$$
(34)

The quasi-Newton matrices defined in (34) satisfy only an *approximated multisecant condition*, namely

$$\widetilde{H}_{j}^{(\beta)}\Delta F_{j-m_{j}}^{(m_{j})} = \Delta S_{j-m_{j}}^{(m_{j})} + \beta (\Delta F_{j-m_{j}}^{(m_{j})} ((\Delta \widetilde{F}_{j-m_{j}}^{(m_{j})})^{T} \Delta \widetilde{F}_{j-m_{j}}^{(m_{j})})^{-1} \Delta F_{j-m_{j}}^{(m_{j})} \Delta F_{j-m_{j}}^{(m_{j})} - \Delta F_{j-m_{j}}^{(m_{j})})^{-1} \Delta F_{j-m_{j}}^{(m_{j})} \Delta F_{j-m_{j}}^{(m_{j})} - \Delta F_{j-m_{j}}^{(m_{j})})^{-1} \Delta F_{j-m_{j}}^{(m_{j})} \Delta F_{j-m_{j}}^{(m_{j})} - \Delta F_{j-m_{$$

which represents a noteworthy difference with the multisecant conditions satisfied by the quasi-Newton matrices used in the classical AA and in its stabilized version (see Lemma 2).

6 Numerical results

In this Section, we investigate the numerical behavior of some of the methods studied in the previous sections for different test problems.

6.1 Details on the methods and their implementations

We select a subset of the methods presented in the previous sections with the main aim to compare their numerical performance (with a focus on the rate of convergence), and to prove that the acceleration performance they deliver behave consistently. Our choices are, among other things, driven by the fact that all the acceleration methods considered share the same order of complexity (linear in the dimension of the problem) per acceleration step. A comprehensive detailed numerical study and the relative implementations of all the methods described in the previous sections is out of the scope of this work and is postponed to future works. Table 1 summarizes the methods we consider in our numerical experiments. In the first column we report the name and the relative abbreviation for the particular acceleration scheme we consider. In the second column we report the reference equations of the acceleration scheme and, for the sake of completeness, in the third column we report the strategy type of the considered acceleration: *Restarted Method* (RM) or *Continuous-Updating* (CU). Finally, in the last column, we report the details concerning the choice of the regularization parameter: in the *Grid Search* (GS) approach the regularization parameter $\overline{\lambda}$ is chosen, as proposed in [54], as the parameter which achieves the smallest fixed point residual; the interval $[10^{-12}, 1]$ is discretized logarithmically into 7 values of λ , (for more details see Algorithm 7 which is a modification of Algorithm 1) among which, one of them, $\overline{\lambda}$, is selected. For the sake of completeness, let us recall that, also in this new algorithm, $\ell_k = k + 2$ if we use (19) or (22), and $\ell_k = 2k + 1$ if we use (26) or (27) For the *Generalized Cross Validation* (GCV) approach, which is a natural approach for regularizing ill-posed regression-like problems, we refer the interested reader to [36].

Name	Ref. Eq.	Type	Choice of λ
Singular Value Decomposition Acceleration (SVDA)	(7)	RM	$\lambda = 0$
Regularized Nonlinear Acceleration (RNA)	(18)	RM	GS (Alg. 7)
Regularized Reduced Rank Extrapolation (RRRE)	(21)	RM	GCV [36]
Regularized Topological Shanks Acceleration (RTSA)	(25)	RM	GS (Alg. 7)
Anderson Acceleration (AA) with $0 < \beta \leq 1$	(30)	CU	$\lambda = 0$
Regularized Anderson Acceleration (RAA)	(34)	CU	GCV [36]

Table 1: Methods tested.

Let us point out that, to the best of our knowledge, among the methods presented in Table 1, RTSA and RRRE/RAA with the regularization parameter chosen using the GCV are new approaches introduced in this work. Instead, for the other methods, we refer in particular to [57] for the SVDA (which is called SVD-MPE in the original paper) and to [54] for the RNA.

Finally, we mention that in all the numerical experiments we used M = I and that, in the SVDA approach, we use as extrapolated term $\mathbf{t}_n^{(k+1)} = S_{n+1}^{(k+1)} \boldsymbol{\alpha}$ where $\boldsymbol{\alpha}$ is the normalized singular vector corresponding to the smallest singular value of $\Delta S_n^{(k+1)}$ (see equation (7)).

Algorithm 7: The Restarted Method (RM) with grid-search (GS).

Input: Choose $M, k, \lambda_{\min}, \lambda_{\max}, n$, and $\mathbf{x}_0 \in \mathbb{R}^p$. 1 for $j = 0, 1, \dots$ do Set $\mathbf{s}_0 = \mathbf{x}_i$ $\mathbf{2}$ for $i = 1, ..., \ell_k - 1$ (basic or inner iterations) do 3 Compute $\mathbf{s}_i = G(\mathbf{s}_{i-1})$ $\mathbf{4}$ end 5 Choose $\lambda_0, \ldots, \lambda_{n-1} \in [\lambda_{\min}, \lambda_{\max}]$ 6 for i = 0, ..., n - 1 do 7 Compute $\mathbf{t}_{0,\lambda_i}^{(\ell_k-1)}$ using (19) or (22) or (26) or (27) 8 end 9
$$\begin{split} \overline{\lambda} &= \underset{\lambda_i \in \{\lambda_0, \dots, \lambda_{n-1}\}}{\arg\min} \| G(\mathbf{t}_{0, \lambda_i}^{(\ell_k - 1)}) - \mathbf{t}_{0, \lambda_i}^{(\ell_k - 1)} \| \\ \text{Set } \mathbf{x}_{j+1} &= \mathbf{t}_{0, \overline{\lambda}}^{(\ell_k - 1)} \end{split}$$
10 11 12 end

All the numerical experiments are performed on a laptop running Linux with 16Gb memory

and CPU Intel[®] CoreTM i7-4510U with a clock speed of 2.00GHz. The code is written and executed in Python. For the discretization of the PDE's we used Fenics [1] and, for the GCV choice of the regularization parameter, we used the Scikit-learn package [48]. Throughout the experiments, to show and test the robustness of the different extrapolation approaches, we base all our extrapolation schemes on 7 previous iterates, i.e., $\ell_k = 7$ in Algorithm 7 or m = 7 in Algorithm 4

6.2 PageRank

The aim of this first numerical example is to highlight the benefits of introducing regularization strategies in Shanks-based extrapolation methods. In particular, in this section, we consider the PageRank problem (see [28]), i.e., the problem of computing the Perron eigenvector of the matrix

$$G = \alpha S + \frac{(1-\alpha)}{n} \mathbf{e} \mathbf{e}^T, \ \alpha \in (0,1).$$

where S is a nonnegative column stochastic matrix. For the solution of this problem, we consider the Power Method, i.e., $\mathbf{u}_{k+1} = G(\mathbf{u}_k)$ where \mathbf{u}_0 is a nonnegative stochastic vector, which is known to be a linear fixed point iteration globally convergent with a rate of convergence of $O(\alpha^k)$ [28]. As the previous convergence bound confirms, the rate of convergence of the Power Method for the PageRank computation becomes slower as α approaches 1, but this is usually the case of interest in applications [28]. In this experiment we use as stopping criterion $||G(\mathbf{u}_k) - \mathbf{u}_k|| < 10^{-7}$.



Figure 1: PageRank Problem

In the left panel of Figure 1, we report the acceleration performance of the regularized versions of the methods considered when compared to the non regularized ones (in the right panel), for the computation of the PageRank vector of the matrix amazon-0202 from [24] (which has been suitably modified in order to be stochastic and Dangling-Nodes free [28]). Recall that the sequence generated by the Power Method belongs to the Shanks kernel and hence, at least theoretically, all the extrapolation strategies should be equivalent and should work consistently without any requirement of regularization. Nevertheless, as Figure 1 clearly shows, the introduction of a regularization strategy improves the robustness of the extrapolation procedures permitting, for the restarted extrapolation methods (namely RNA, RTSA, RRRE), to obtain a more effective acceleration performance across different choices of the parameter α . Observe also that, in this case, the introduction of a regularization procedure in the AA scheme (RAA) does not sensibly improves the acceleration performance.

6.3 Nonlinear Poisson problems

In this Section, we consider the solution of the nonlinear PDE (see equation (35))

$$-\nabla(q(u)\nabla u) + g(u) + u_x = f \text{ in } \mathcal{D} = [0,1] \times [0,1],$$

$$u = v \text{ on } \partial \mathcal{D}.$$
(35)

We use a 1/64 uniform triangular mesh of $\Omega = [0, 1]^2$ with a (P_2) discretization [1] that provides a total of 16,641 degrees of freedom. In particular, we consider the following choices of the functions

- $q(u) = 1 + u^2$ or $q(u) = 1 + u^4$, g(u) = 0 and f such that the exact solution of (35) is given by $\overline{u} = \exp(-2x)\sin(3\pi y)$ and $v = \overline{u}$ on $\partial\Omega$. We refer to these choices as the Nonlinear Poisson Problem;
- q(u) = 1, $g(u) = \lambda e^u$ with $\lambda = 1$ or $\lambda = -1$, f = 0 and v = 0 on $\partial \Omega$. We refer to these choices as the *Bratu Problem* [38].

After the discretization of (35), the corresponding problems can be written as the solution of $F(\mathbf{s}) = 0$, i.e., as the solution of a linear system of equations. We assume that the derivative of F are not readily available or that a sufficiently accurate initial guess is not at our disposal in order to apply Newton's method. In this experiment we use as stopping criterion $||F(\mathbf{u}_k)|| < 10^{-7}$. Figures 2 and 3, show the acceleration performance of AA when compared to its regularized version RAA (these problems are not well scaled and a good choice for the mixing parameter was $\beta = 0.1$) for the problems previously discussed. The Figures clearly show that the introduction of the regularization strategy, in these cases characterized by a higher nonlinearity than for the PageRank example, leads to a better robustness of the schemes with respect to the choice of the memory parameter m. In particular, the introduction of the regularization procedure permits to have a satisfactory rate of convergence independently from the value m. We point out that, interestingly enough, the need for a stabilization procedure needed from the theoretical point of view to prove the convergence of the AA scheme (see Algorithm 6), is echoed by the experimental observation that increasing m could result in a lost of efficiency for the AA scheme (see Figure 3). The introduction of a regularization procedure mitigates such a drawback.



Figure 2: Nonlinear Poisson Problem.



Figure 3: Bratu Problem.

6.3.1 Navier-Stokes equation

In this Section, we compare the numerical performance of the different restarted extrapolation approaches on the incompressible Navier-Stokes Equation (NSE)

$$\begin{split} u \cdot \nabla u + \nabla p - \nu \Delta u &= f, \\ \nabla \cdot u &= 0, \\ u|_{\partial \Omega} &= g, \end{split}$$

where ν is the kinematic viscosity, f is the forcing, u and p represent velocity and pressure and Ω is a given domain in \mathbb{R}^2 . Following [49], we consider a Picard iteration (equations (36)) to solve the problem. The iteration, which is commonly used for its stability and global convergence properties, takes the form

$$u_k \cdot \nabla u_{k+1} + \nabla p_{k+1} - \nu \Delta u_{k+1} = f,$$

$$\nabla \cdot u_{k+1} = 0,$$

$$u_{k+1}|_{\partial\Omega} = g.$$
(36)



Figure 4: Lid driven Problem: Acceleration Performance.

The above scheme is written in the fixed point form $u_{k+1} = G(u_k)$, where G denotes the solution operator for the linearization (36). To be specific, we consider the 2D lid driven cavity ($\Omega = (0, 1)^2$) and a "deep" lid driven cavity with $(\Omega = (0, 1) \times (0, 3))$. No slip (u = 0) boundary conditions are imposed on the sides and the bottom, and the Dirichlet boundary condition $u(x,1) = (1,0)^T$ is imposed on the top to enforce the "moving lid" condition. There is no forcing (f = 0) and the kinematic viscosity ($\nu = Re^{-1}$) is considered at benchmark values Re = 5000, 7500. We discretize with (P_2, P_1) Taylor Hood elements. In the case $\Omega = (0, 1)^2$ we use a $\frac{1}{64}$ uniform triangular mesh that provides a 37,507 total degrees of freedom and in the case $\Omega = (0, 1) \times (0, 3)$ we use a $\frac{1}{40} \times \frac{1}{120}$ mesh that provides 87, 203 total degrees of freedom. Similarly to the results presented in [49], our experiments confirm that Newton's method starting with a zero initial guess, never converges. In this experiment we use as stopping criterion $||G(\mathbf{u}_k) - \mathbf{u}_k|| < 10^{-5}$. Figures 4 and 5 show the acceleration performance of the methods described in Table 1 for the solution of the steady NSE. The best performer in terms of achieved acceleration is AA and the introduction of a regularization procedure in this scheme (RAA) seems not to have a relevant impact on the rate of convergence. This is probably due to the fact that the fixed point iteration we are considering generates a sequence that is *close* to being a linear sequence and, as in the PageRank case, regularization of the AA scheme does not seem to have a great influence. Concerning the restarted regularized methods, we should notice that the RTSA is not able to achieve an acceleration performance in the Deep case for Re = 7500. Finally, let us highlight the particularly interesting performance of the SVDA approach: this approach does not require the computation of any regularization parameter



Figure 5: Lid driven Problem: Acceleration Performance.

and only one SVD decomposition every $\ell_k - 1$ fixed point iterations is needed, whereas AA requires the solution of a least square solution per step, and all the regularized methods which use the RM approach require the selection of a regularization parameter. The non-regularized versions of the methods using the RM strategy, as in the PageRank case, exhibited a worst performance and are not reported for this reason.

7 Conclusions

In this work, we presented a unified framework for Shanks-based transformations. If, on one hand, the introduction of this framework allowed us to link apparently different extrapolation/acceleration techniques with Shanks-based transformations, on the other hand, it allowed us to introduce suitable generalizations able to numerically outperform the existing ones, as highlighted in the preliminary numerical results presented, especially on problems characterized by a high degree of nonlinearity. To conclude, we note that the highlighted connection between the Shanks-based transformations and the quasi-Newton methods and Anderson Acceleration, shed light into some of its theoretical and numerical behaviors, furthering our knowledge of the powerful, but poorly understood, Anderson acceleration [42].

Acknowledgments:

We would like to thank the reviewers for their very careful reading of our paper, and for their constructive comments.

C.B. acknowledges support from the Labex CEMPI (ANR-11-LABX-0007-01). S.C. and M.R.-Z. are a members of the INdAM Research group GNCS. The work of S.C. was partially supported by the GNCS – INdAM project "Efficient Methods for large scale problems with applications to data analysis and preconditioning" and from Dept. of Computer Science & Engineering, University of Minnesota, Project No. UMF0002384. The work of M.R.-Z. was partially supported by the University of Padua, Project No. DOR 1903575/19 Numerical Linear Algebra and Extrapolation methods with applications. The work of Y.S. was supported in part by NSF grant DMS-1912048.

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