DESCENT PROPERTIES OF AN ANDERSON ACCELERATED GRADIENT METHOD WITH RESTARTING*

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Abstract. Anderson Acceleration (AA) is a popular acceleration technique to enhance the convergence of fixed-point schemes. The analysis of AA approaches often focuses on the convergence behavior of a corresponding fixed-point residual, while the behavior of the underlying objective function values along the accelerated iterates is currently not well understood. In this paper, we investigate local properties of AA with restarting applied to a basic gradient scheme (AA-R) in terms of function values. Specifically, we show that AA-R is a local descent method and that it can decrease the objective function at a rate no slower than the gradient method up to higher-order error terms. These new results theoretically support the good numerical performance of AA(-R) when heuristic descent conditions are used for globalization and they provide a novel perspective on the convergence analysis of AA-R that is more amenable to nonconvex optimization problems. Numerical experiments are conducted to illustrate our theoretical findings.

Key words. Anderson Acceleration, Descent Properties, Restarting

AMS subject classifications. 90C30, 65K05, 90C06, 90C53

1. Introduction. In this work, we consider the smooth optimization problem

(1.1)
$$\min_{x \in \mathbb{P}^n} f(x)$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function. If the gradient mapping ∇f is additionally Lipschitz continuous with modulus L, then the basic gradient descent method with fixed step size,

(1.2)
$$x^{k+1} = x^k - \frac{1}{L} \nabla f(x^k) =: g(x^k),$$

can be utilized to solve problem (1.1). Here, $g : \mathbb{R}^n \to \mathbb{R}^n$ represents the associated gradient step mapping with step size $\frac{1}{L}$. The gradient descent step (1.2) can be viewed as a fixed-point iteration and the fixed-points of g are exactly the stationary points of the objective function f.

Anderson Acceleration (AA) applies to fixed-point iterations of the form (1.2) and is a popular technique to accelerate the convergence of such iterative fixedpoint schemes. For instance, AA-based algorithms have been applied successfully in computer graphics [31, 52, 27], reinforcement learning [15, 43], machine learning [49], and numerical methods for PDEs [34]. In iteration k and based on the past m iterations $\{x^{k-m}, \ldots, x^k\}$, AA first computes the mixing coefficients $\alpha^k = (\alpha_1^k, \ldots, \alpha_m^k)^\top \in \mathbb{R}^m$ as solution of the following optimization problem:

(1.3)
$$\min_{\alpha \in \mathbb{R}^m} \left\| h(x^{k-m}) + \sum_{i=1}^m \alpha_i (h(x^{k-m+i}) - h(x^{k-m})) \right\|^2,$$

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where h(x) := g(x) - x denotes the residual map and m is a corresponding memory parameter. AA then performs the accelerated iteration:

(1.4)
$$x^{k+1} = g(x^{k-m}) + \sum_{i=1}^{m} \alpha_i^k (g(x^{k-m+i}) - g(x^{k-m}))$$

The parameter m is usually chosen to be fixed or it is allowed to increase each iteration until a given threshold is reached after which m is reinitialized. We will refer to such a restarted version of the Anderson accelerated gradient scheme (1.4) as AA-R (cf. Algorithm 2.1 in section 2). The goal of this paper is to analyze and establish novel descent properties of AA-R. In particular, we show that AA-R not only decreases the norm of the residual ||h(x)||, but it can also decrease the underlying objective function f. Therefore, we answer the following question affirmatively:

Can Anderson accelerated schemes achieve descent on the underlying objective function values?

1.1. Related Work and Literature. Originally proposed by Anderson [1] for solving partial differential equations, AA has gained steadily growing attention during the last decade [31, 30, 19, 23, 27]. Though widely used in various fields and applications, the theoretical analysis and properties of AA are still somewhat limited. AA is known to belong to the class of multi-secant quasi-Newton methods [11, 12, 38]. When applied to linear problems, AA is equivalent to the generalized minimal residual method (GMRES) [47, 35]. For nonlinear problems, AA is also closely related to the nonlinear generalized minimal residual method (NGMRES) [48]. The convergence analysis in [46] shows that AA converges locally r-linearly under a smoothness condition on the map g and uniform boundedness of the coefficients $\{\alpha^k\}_k$, but the obtained linear rate is slower than the rate of the original scheme. Later, in [10], the authors prove that AA can achieve an improved linear rate with additional quadratic error terms which overall yields r-linear convergence. This result is further improved in [33] by assuming sufficient linear independence on the set of difference vectors of the residuals $h(x^k)$ and q-linear convergence of AA is established with a rate faster than the Picard iteration (1.2). Moreover, if the coefficients $\{\alpha^k\}_k$ are assumed to be constant in each iteration, an asymptotic rate is given in [48]. The convergence behavior of AA applied to nonsmooth algorithmic schemes is also considered in [23, 6].

Since AA is known to only converge locally [46, 23], globalization mechanisms are required to use it in practice. A simple and heuristic choice is to check whether AA decreases the objective function value f and to perform a fixed-point iteration if the decrease of the AA step is not sufficient. Such a strategy is utilized in [31, 27, 41, 17] However, to the best of our knowledge, no consistent global-local convergence proofs are known in this case. Alternatively, one can check whether AA decreases the residual ||h(x)|| and to reject the step if no sufficient decrease is observed. This strategy is more common and has been used in [51, 28, 14, 9]. Transition to local fast convergence of such a globalized AA approach is provided in [28]. Unfortunately, the convergence analyses in [51, 28, 14, 9] require global nonexpansiveness of g^1 , which often necessitates convexity of f. Notably, it is also possible to combine function value- and residual-based globalization techniques, see, e.g., [17, 45].

Restarting strategies are part of many numerical algorithms. For instance, restarting is used in the conjugate gradient method (CG) [36], the generalized minimal residual method (GMRES) [40], and in quasi-Newton methods [24]. Restarting strategies have

¹Though residual-based globalizations of AA without nonexpansiveness are possible, it is not fully clear which type of convergence guarantees can be achieved.

also been widely applied in the context of AA. In [4, 12], AA is restarted whenever the ratio of the square of the current residual to the sum of the squares of the previous residuals exceeds a predetermined constant. Similar ideas are discussed in [51, Section 3.2] and [32]. Restarting strategies are sometimes also used in tandem with regularization techniques to enhance the numerical stability of AA, see, e.g., [19, 43, 41]. A comprehensive comparison between AA with restarting and the original AA scheme on linear problems with parallel implementation can be found in [22]. The results in [22] suggest that the performance of AA with restarting is generally comparable to the performance of the original AA method. Further supporting observations for the effectiveness of restarted AA are provided in [37].

1.2. Contributions. The convergence analyses of AA [46, 10, 33, 28] focus on the decrease of the residual ||h(x)||, which is natural since AA aims to minimize this norm in the AA subproblem (1.3). However, as mentioned, such globalization strategies usually require global nonexpansiveness of g in order to obtain global convergence results, see, e.g., [51, 28, 14, 9]. Hence, the heuristic idea to base the acceptance of an AA step on the decrease of the objective function value seems attractive, since the Picard iteration (1.2) can decrease the function value even if f is nonconvex. So far, there seems to be no theoretical backing ensuring that AA(-R) can achieve descent on the underlying objective function — even if strong convexity is assumed and an appropriate initial point is selected. Our aim is to investigate this gap and to show that AA-R can decrease the objective function value locally. This result provides theoretical guarantees for algorithms that utilize descent conditions for f as globalization mechanism without hindering the local fast convergence of AA-R. We now summarize our main contributions:

- To the best of our knowledge, we establish the first descent properties of AA-R iterations for the gradient descent scheme (1.2). On the one hand, this illuminates the success of algorithms that have used heuristic descent-type conditions to globalize AA(-R) [31, 27, 41]. On the other hand, our findings can be utilized in the design of novel globalization techniques for AA-R methods.
- We verify that the iterates generated by AA-R in one restarting cycle are equivalent to the iterates generated by GMRES when being run on a perturbed linear system model (for the same amount of iterations). This model, without perturbation, is exactly the quadratic expansion of f and the Hessian of this model is symmetric and positive definite if we assume local strong convexity. Hence, AA-R is close to running the conjugate residual method (CR) [44] on such a quadratic model of f. Motivated by these observations, we analyze and specify the error between GMRES and CR under small perturbations of the system matrix which will allow us to link AA-R, CR, and CG. Based on classical results for CG [20], we then show that AA-R not only decreases the objective function value, but the overall achieved descent is actually no smaller than the one obtained by performing a gradient descent step with step size $\frac{1}{L}$ up to higher-order error terms. Some byproducts of our results indicate that CR itself decreases the objective function value no slower than the gradient descent method.
- We design a practical function value-based globalization mechanism for AA-R. Unlike residual-based globalizations, this allows to apply AA-R directly to nonconvex problems without requiring any adjustments of the underlying AA-R scheme. We illustrate the numerical performance of our simple globalization and numerically confirm the derived theoretical descent guarantees of AA-R

on several nonconvex large-scale problems.

1.3. Organization. This work is organized as follows. In section 2, we introduce the algorithmic details of AA-R and list the standing assumptions. In section 3, we derive the core descent properties of AA-R. This is done step by step. In subsection 3.1, we first establish q-linear convergence. The mentioned equivalence between AA-R and GMRES is shown in subsection 3.3. Next, in subsection 3.4, we analyze the error between the sequences generated by CR and GMRES which allows to connect GMRES and CR. The detailed connection between CR and CG is investigated in subsection 3.5. An objective function value-based globalization of AA-R is presented in section 4. Finally, in section 5, we verify our theoretical results and test the proposed globalized AA-R algorithm on several examples.

1.4. Notation. Throughout this work, we consider the fixed-point mapping $g(x) = x - \nabla f(x)/L$ and the corresponding residual $h(x) := g(x) - x = -\nabla f(x)/L$. For a given sequence of iterates $\{x^k\}_k$, we define the terms:

$$M_h^k := \max_{k - \hat{m} \le i \le k} \|h(x^i) - h(x^{k - \hat{m}})\|, \quad M_x^k := \max_{k - \hat{m} \le i \le k} \|x^i - x^{k - \hat{m}}\|,$$

where $\hat{m} = \text{mod}(k, m+1)$. We further introduce the following matrices and notations:

$$\begin{aligned} X_k &:= [x^{k-\hat{m}+1} - x^{k-\hat{m}}, \dots, x^k - x^{k-\hat{m}}] \in \mathbb{R}^{n \times \hat{m}}, \\ H_k &:= [h(x^{k-\hat{m}+1}) - h(x^{k-\hat{m}}), \dots, h(x^k) - h(x^{k-\hat{m}})] \in \mathbb{R}^{n \times \hat{m}}, \\ G_k &:= [g(x^{k-\hat{m}+1}) - g(x^{k-\hat{m}}), \dots, g(x^k) - g(x^{k-\hat{m}})] \in \mathbb{R}^{n \times \hat{m}}, \end{aligned}$$

 $\hat{x}^0 := x^0, \, \hat{x}^k := x^{k-\hat{m}} + X_k \alpha^k, \, g^k := g(x^k), \, \hat{g}^k := g^{k-\hat{m}} + G_k \alpha^k, \, h^k := h(x^k), \text{ and } \hat{h}^k := \hat{g}^k - \hat{x}^k.$ The definition of \hat{x}^k follows [10, Equation (2.4)]. We further note that the AA subproblem (1.3) can be viewed as finding the minimal value of the linearized residual of \hat{x}^k which is \hat{h}^k . Based on these notations, we can express the solution to (1.3) explicitly by $\alpha^k = -(H_k^\top H_k)^{-1} H_k^\top h^{k-\hat{m}}$ provided that $H_k^\top H_k$ is invertible.

For given $n \in \mathbb{N}$, we set $[n] := \{1, \ldots, n\}$. For a matrix A, $\sigma_{\max}(A)$ $(\lambda_{\max}(A))$ denotes the largest singular value (eigenvalue) of A and $\sigma_{\min}(A)$ $(\lambda_{\min}(A))$ is the smallest singular value (eigenvalue) of A. The condition number of A is given by $\kappa(A) := \sigma_{\max}(A)/\sigma_{\min}(A)$. Unless specified otherwise, the norm $\|\cdot\|$ refers to the standard Euclidean norm for vectors and the spectral norm for matrices. We will use $\|\cdot\|_F$ to denote the Frobenius norm of a matrix. The space $\mathcal{K}^t(A, b) := \operatorname{span}\{b, Ab, \ldots, A^{t-1}b\}$ is used to denote the *t*-th Krylov space generated by A and b.

2. Anderson Acceleration with Restarting. Throughout this paper, we assume that:

ASSUMPTION 2.1. There is some r > 0 and a stationary point $x^* \in \mathbb{R}^n$ of f (i.e., $\nabla f(x^*) = 0$) such that:

- (A.1) The function f is L-smooth on \mathbb{R}^n .
- (A.2) The function f is μ -strongly convex on $\mathbb{B}_r(x^*) := \{x : ||x x^*|| < r\}.$
- (A.3) The Hessian $\nabla^2 f$ is Lipschitz continuous with modulus L_H on $\mathbb{B}_r(x^*)$.

We note that the conditions formulated in Assumption 2.1 are common in the convergence analysis of Anderson accelerated gradient methods, see, e.g., [46, 10] for comparison. Let $\kappa_r := \frac{L}{\mu}$ denote the condition number of the Hessian $\nabla^2 f$ on $\mathbb{B}_r(x^*)$. Then, under Assumption 2.1, it follows:

(2.1)
$$||g(x) - g(y)|| \le \left\|I - \frac{1}{L}\bar{F}\right\| ||x - y|| \le \left(1 - \frac{1}{\kappa_r}\right) ||x - y||, \quad \forall x, y \in \mathbb{B}_r(x^*),$$

where $\bar{F} := \int_0^1 \nabla^2 f(y + t(x - y)) \, dt$. Hence, g is contractive on $\mathbb{B}_r(x^*)$ with Lipschitz constant $1 - \frac{1}{\kappa_n}$.

We study local properties of AA with restarting applied to the gradient mapping $g(x) = x - \frac{1}{L} \nabla f(x)$. In particular, given some initial point x^0 which is sufficiently close to x^* , we apply AA on $\{x^0, \ldots, x^{k-1}\}$ to obtain the new iterate x^k . After m iterations (m is the fixed memory parameter), this procedure is stopped and AA is restarted with x^{m+1} as new initial point of the next cycle. The full algorithm of the restarted AA scheme for problem (1.1) – AA-R – is shown below in Algorithm 2.1.

Algorithm 2.1 AA with Restarting (AA-R)

Require: Choose the initial point x⁰ and the memory parameter m ∈ N. Set the current memory parameter as m̂ = 0.
1: for k = 0, 1, ... do
2: m̂ = mod(k, m + 1).
3: if m̂ = 0 then
4: Set x^{k+1} = g(x^k).
5: else
6: Calculate the coefficient α^k based on the sequence {h(x^k),...,h(x^{k-m̂})} via solving (1.3) and set x^{k+1} = g^{k-m̂} + G_kα^k.

- 7: **end if**
- 8: end for

3. Convergence and Descent Properties of AA-R. Most classical convergence analyses of AA are based on the same idea — linearization [46, 10, 23, 28]. It is wellknown that AA(-R) is equivalent to GMRES if the mapping g is affine [35] and therefore, AA(-R) can be viewed as GMRES being applied to a linear approximation of g along with some linearization error. When specialized to the gradient mapping, these analyses ignore the structural information that g has a symmetric Hessian. Taking this information into account, we can deduce that the system matrix of the GMRES procedure is essentially close to a symmetric positive definite matrix, which means that GMRES is close to CR in this case. This observation motivates us to utilize classical tools for CR to show that AA-R locally performs descent steps for f. The main technical difficulty lies in the fact that the iterates generated by AA-R only coincide with the iterates generated by GMRES after one additional gradient step. We resolve this complication by connecting GMRES and CG (via CR) and by analyzing the relevant properties via a CG-based perspective.

3.1. Q-Linear Convergence of AA-R. We first present an additional assumption and several basic properties of AA-R (and AA) that allow to establish q-linear convergence. This will serve as a foundation for our later results.

ASSUMPTION 3.1. (A.4) The condition number of $X_k^{\top} X_k$ is bounded by M^2 for every $k \in \mathbb{N}$.

Let us note that the analogous assumption on H_k is more common, since H_k appears directly in the computation of the coefficient α_k in (1.3). We address this issue in the following proposition and show that condition (A.4) is actually equivalent to assuming that the condition number of $H_k^{\top}H_k$ is bounded locally. Hence, in practice, (A.4) can be ensured by monitoring the condition number of $H_k^{\top}H_k$. For instance, we can restart the current cycle whenever the condition number of $H_k^{\top}H_k$ exceeds a given tolerance. Alternative strategies are further discussed in [33, Section 5.1.3]. It is also possible to mitigate condition (A.4) and related boundedness assumptions on the mixing coefficients $\{\alpha^k\}_k$, [46, 10, 23, 6] via algorithmic independence checks or adaptive depth mechanisms, see, e.g., [7]. However, such adjustments naturally affect the achievable convergence and acceleration results.

PROPOSITION 3.2. Suppose that the conditions (A.1)-(A.3) are satisfied. Then, the following statements hold:

- (i) For every $M_X > 0$ there is a neighborhood U_1 of x^* such that if $x^{k-\hat{m}} \dots, x^k \in U_1 \cup U_2 \cup U_2$
- $\begin{array}{l} U_1 \ and \ \kappa(X_k^\top X_k) \leq M_X^2, \ then \ it \ holds \ that \ \kappa(H_k^\top H_k) \leq 4\kappa_r^2\kappa(X_k^\top X_k). \\ (\text{ii)} \ For \ every \ M_H > 0 \ there \ is \ a \ neighborhood \ U_2 \ of \ x^* \ such \ that \ if \ x^{k-\hat{m}}, \ldots, x^k \in \\ U_2 \ and \ \kappa(H_k^\top H_k) \leq M_H^2, \ then \ we \ have \ \kappa(X_k^\top X_k) \leq 4\kappa_r^2\kappa(H_k^\top H_k). \end{array}$

Proof. Without loss of generality and in order to simplify the notation, we assume $\hat{m} = m$ and k = m. Let us first define $U_1 := \mathbb{B}_{\delta_1}(x^*)$ where $\delta_1 := \min\{r, (1 - \frac{1}{\sqrt{2}})\frac{\mu}{\sqrt{m}M_XL_H}\}$. We further set $b_i := \nabla f(x^i) - \nabla f(x^0) - \nabla^2 f(x^0)(x^i - x^0)$ and $B_k := [b_1, \ldots, b_k]$. Utilizing [25, Lemma 4.1.1], it follows $||b_i|| \leq \frac{L_H}{2} ||x^i - x^0||^2$ for all $i \in [k]$ and we obtain

$$||B_k|| \le ||B_k||_F \le \sqrt{m} \max_{1 \le i \le k} ||b_i|| \le \frac{\sqrt{m}L_H}{2} \max_{1 \le i \le k} ||x^i - x^0||^2 = \frac{\sqrt{m}L_H(M_x^k)^2}{2}.$$

Defining $E_k := B_k (X_k^{\top} X_k)^{-1} X_k^{\top}$ (E_k is well-defined since $X_k^{\top} X_k$ is invertible) and $A_k = \nabla^2 f(x^0) + E_k$, a direct calculation yields

(3.1)
$$A_k(x^i - x^0) = \nabla f(x^i) - \nabla f(x^0) \quad \forall \ i \in [k].$$

In other words, we have $A_k X_k = -LH_k$. Moreover, the norm of E_k can be estimated as follows

(3.2)
$$\|E_k\| \le \|B_k\| \| (X_k^\top X_k)^{-1} X_k^\top \|$$
$$= \|B_k\| \sqrt{\| (X_k^\top X_k)^{-1} \|} \le \frac{\|B_k\|_F M_X}{\|X_k\|} \le \frac{\sqrt{m} L_H M_X M_x^k}{2},$$

where we used $||X_k|| \ge \max_{1\le i\le k} ||X_k e_i|| = M_x^k$ with $e_i \in \mathbb{R}^k$ being the *i*-th unit vector. Due to $M_x^k \le 2\delta_1$, we can further infer $||E_k|| \le \sqrt{m}L_H M_X \delta_1 \le (1 - \frac{1}{\sqrt{2}})\mu$. Therefore, it holds that $\sigma_{\max}(A_k) \le \lambda_{\max}(\nabla^2 f(x^0)) + \sigma_{\max}(E_k) \le \sqrt{2}L$ and $\sigma_{\min}(A_k) \ge \lambda_{\min}(\nabla^2 f(x^0)) - \sigma_{\max}(E_k) \ge \frac{1}{\sqrt{2}}\mu$. Consequently, we have $\kappa(A_k) \le 2\kappa_r$. This allows to bound the condition number of H_k :

$$\kappa(H_k^\top H_k) = \kappa(X_k^\top A_k^\top A_k X_k) \le \kappa(X_k^\top X_k) \kappa(A_k^\top A_k) \le 4\kappa_r^2 M_X^2$$

and proves part (i). We now turn to the proof of the second statement. We define $U_2 := \mathbb{B}_{\delta_2}(x^*), \ \delta_2 := \min\{r, (1 - \frac{1}{\sqrt{2}})\frac{\mu^2}{\sqrt{m}LL_HM_H}\}, \ \tilde{b}_i = \frac{1}{L}[(\nabla^2 f(x^0))^{-1}(\nabla f(x^i) - \nabla f(x^0)) - (x^i - x^0)], \ \text{and} \ \tilde{B}_k = [\tilde{b}_1, \dots, \tilde{b}_k].$ As before, we obtain

$$\|\tilde{B}_k\| = \frac{1}{L} \|\nabla f(x^0)^{-1} B_k\| \le \frac{1}{L\mu} \|B_k\| \le \frac{\sqrt{mL_H(M_x^k)^2}}{2L\mu}$$

Let $j \in [k]$ be given with $M_x^k = \max_{1 \le i \le k} \|x^i - x^0\| = \|x^j - x^0\|$. Using (A.2), it then holds that

(3.3)
$$||H_k|| \ge M_h^k \ge ||h^j - h^0|| = \frac{1}{L} ||\nabla f(x^j) - \nabla f(x^0)|| \ge \frac{1}{\kappa_r} ||x^j - x^0|| = \frac{M_x^k}{\kappa_r}.$$

Therefore, setting $\tilde{E}_k := \tilde{B}_k (H_k^\top H_k)^{-1} H_k^\top$, it follows

$$\|\tilde{E}_k\| \le \|\tilde{B}_k\| \sqrt{\|(H_k^\top H_k)^{-1}\|} \le \frac{\sqrt{m}L_H (M_x^k)^2 M_H}{2L\mu \|H_k\|} \le \frac{\sqrt{m}L_H M_H M_x^k}{2\mu^2}$$

and by the definition of δ_2 , we have $M_x^k \leq 2\delta_2$ and $\|\tilde{E}_k\| \leq \frac{\sqrt{m}L_H M_H \delta_2}{\mu^2} \leq (1 - \frac{1}{\sqrt{2}})\frac{1}{L}$. Next, defining $\tilde{A}_k := (\nabla^2 f(x^0))^{-1} + \tilde{E}_k$, we can again infer

$$\tilde{A}_k(\nabla f(x^i) - \nabla f(x^0)) = x^i - x^0, \quad i \in [k] \implies L\tilde{A}_k H_k = -X_k$$

$$\begin{split} \sigma_{\max}(\tilde{A}_k) &\leq \lambda_{\max}(\nabla^2 f(x^0)^{-1}) + \sigma_{\max}(\tilde{E}_k) \leq \frac{\sqrt{2}}{\mu}, \text{ and } \sigma_{\min}(\tilde{A}_k) \geq \lambda_{\min}(\nabla^2 f(x^0)^{-1}) - \\ \sigma_{\max}(\tilde{E}_k) &\geq 1/(\sqrt{2}L). \text{ This yields } \kappa(\tilde{A}_k) \leq 2\kappa_r \text{ and } \kappa(X_k^\top X_k) \leq \kappa(H_k^\top H_k)\kappa(\tilde{A}_k^\top \tilde{A}_k) \leq 4\kappa_r^2 M_H^2. \end{split}$$

We note that the matrix $A_k = \nabla^2 f(x^0) + E_k$ defined in the proof of Proposition 3.2 is a key technical ingredient in this paper and will be used in the subsequent sections. The matrix A_k consists of the symmetric Hessian $\nabla^2 f(x^0)$ and the perturbation matrix E_k . Our goal in the next subsections is to suitably control the norm of E_k promoting a link between AA-R and CR.

Based on condition (A.4), we now verify q-linear convergence of the sequence $\{\|h^k\|\}_k$. Let us remark that assumption (A.4) (or its equivalent formulation for the matrices $H_k^{\top}H_k$) is generally stronger than the condition appearing in [33]. Namely, in [33, Theorem 5.1], q-linear convergence of AA(-R) is shown under a sufficient linear independence condition on each of the columns of (a permutation of) H_k . Here, we will work with the slightly stronger assumption (A.4) as it allows us to study the behavior of $(H_k^{\top}H_k)^{-1}H_k^{\top}$ under perturbations which is required to link AA-R and CR. More details can be found in the proof of Theorem 3.12. In addition, in [33], contraction and Lipschitz differentiability of ∇f is assumed on the whole space \mathbb{R}^n , while we consider the local case in a neighborhood of x^* . Following the derivation in [33], we first analyze the behavior of the residuals $\{\|h^k\|\}_k$ in one cycle of AA-R.

PROPOSITION 3.3. Let the conditions (A.1)–(A.4) be satisfied and let us further assume $g(x^i), x^i \in U_1$ with $i = k - \hat{m}, \ldots, k$ and $\hat{x}^k, \hat{g}^k \in U_1$ (where U_1 is introduced in Proposition 3.2 for $M_X = M$). Then, it holds that:

(3.4)
$$||h^{k+1}|| \le \left(1 - \frac{1}{\kappa_r}\right) ||h^k|| + \mathcal{O}\left(||h^k|| \left(\sum_{i=k-\hat{m}}^k ||h^i||\right)\right).$$

Proof. This result basically follows from [33, Theorem 5.1]. A comprehensive proof is presented in Appendix A. $\hfill \Box$

In order to transfer the statement in Proposition 3.3 to the full sequence $\{||h^k||\}_k$, we need to show that AA-R stays indeed local.

LEMMA 3.4. Let the conditions (A.1)-(A.3) hold and assume $x^{k-\hat{m}}, \ldots, x^k \in \mathbb{B}_r(x^*)$. If $\kappa(H_k^{\top}H_k) \leq M_H^2$, then we have:

$$\|\hat{x}^k - x^{k-\hat{m}}\| \le \sqrt{m}M_H\kappa_r \|h^{k-\hat{m}}\|$$
 and $\|\hat{g}^k - x^{k-\hat{m}}\| \le (1 + \sqrt{m}M_H\kappa_r)\|h^{k-\hat{m}}\|.$

Proof. We start with bounding the coefficient α^k . As mentioned, the closed-form expression for α^k is given by $\alpha^k = -(H_k^{\top}H_k)^{-1}H_k^{\top}h^{k-\hat{m}}$. Therefore, it holds that

$$\|\alpha^{k}\| \leq \sqrt{\|(H_{k}^{\top}H_{k})^{-1}\|} \|h^{k-\hat{m}}\| \leq \frac{M_{H}}{\|H_{k}\|} \|h^{k-\hat{m}}\| \leq \frac{M_{H}\kappa_{r}}{M_{x}^{k}} \|h^{k-\hat{m}}\|,$$

where we used (3.3) in the last inequality. Due to $||X_k||_F \leq \sqrt{\hat{m}} M_x^k$, the definition of \hat{h}^k , and (1.3), this implies

$$\|\hat{x}^{k} - x^{k-\hat{m}}\| = \|X_{k}\alpha^{k}\| \le \|X_{k}\| \|\alpha^{k}\| \le \|X_{k}\|_{F} \|\alpha^{k}\| \le \sqrt{m}M_{H}\kappa_{r}\|h^{k-\hat{m}}\|$$

and $\|\hat{g}^k - x^{k-\hat{m}}\| \le \|\hat{h}^k\| + \|\hat{x}^k - x^{k-\hat{m}}\| \le (1 + \sqrt{m}M_H\kappa_r)\|h^{k-\hat{m}}\|.$

PROPOSITION 3.5. Let (A.1)-(A.4) be satisfied and let $\{x^k\}_k$ be generated by Algorithm 2.1. Then there exists a neighborhood U of x^* such that if $x^0 \in U$, it follows $\{x^k\}_k \subset U$ and $\|h(x^{k+1})\| \leq (1 - \frac{1}{2\kappa_r})\|h(x^k)\|$ for all $k \in \mathbb{N}$.

Proof. We define $S_{\epsilon} = \{x \in \mathbb{R}^n : ||h(x)|| \le \epsilon\} \cap \mathbb{B}_r(x^{\star})$. Due to (A.2), we obtain

$$\|h(x)\| = \frac{1}{L} \|\nabla f(x)\| \ge \frac{\mu}{L} \|x - x^{\star}\| = \frac{1}{\kappa_r} \|x - x^{\star}\| \quad \forall \ x \in \mathbb{B}_r(x^{\star}).$$

Let U_1 be defined as in Proposition 3.2 for $M_X = M$. The previous inequality implies that there is some $\epsilon_1 > 0$ such that $S_{\epsilon_1} \subset U_1$. Moreover, by Proposition 3.3, there exists another neighborhood S_{ϵ_2} such that if $x^k, \ldots, x^{k-\hat{m}}, \hat{x}^k, \hat{g}^k \in S_{\epsilon_2}$, then we have

(3.5)
$$||h(\hat{g}^k)|| \le (1 - (2\kappa_r)^{-1})||h(x^k)||.$$

We now take $\bar{\epsilon} = \min\{\epsilon_1, \frac{\epsilon_2}{2+2\sqrt{m}\kappa_r^2 M}, \frac{r}{1+(2\sqrt{m}\kappa_r M+1)\kappa_r}\}$ and set $U = S_{\bar{\epsilon}}$. Let us further suppose $x^0 \in U$. We use an induction to show $\|h^k\| \leq (1-(2\kappa_r)^{-1})\|h^{k-1}\|$ and $x^k \in U$ for all k. It is clear that we only need to prove this conclusion for $k = 1, \ldots, m+1$, since the analysis is identical for the next cycle of the restarted AA method. We start with k = 1. By definition, we have $x^1 = g(x^0)$ and according to (2.1), it follows:

$$||x^{1} - x^{\star}|| = ||g(x^{0}) - g(x^{\star})|| \le (1 - \kappa_{r}^{-1})||x^{0} - x^{\star}|| \le r.$$

This proves $x^1 \in \mathbb{B}_r(x^*)$. Moreover, it holds that:

$$\|h(x^1)\| = \|g(x^1) - x^1\| = \|g(x^1) - g(x^0)\| \le (1 - \kappa_r^{-1})\|h(x^0)\| \le \bar{\epsilon},$$

which shows $||h(x^1)|| \leq (1 - (2\kappa_r)^{-1})||h(x^0)||$ and $x^1 \in S_{\bar{\epsilon}}$. Next, let us assume that the induction hypothesis is true for $i = 1, \ldots, k$ and let us prove the conclusion for i = k + 1. Applying Proposition 3.2 and (A.4), we obtain $\kappa(H_k^{\top}H_k) \leq 4\kappa_r^2 M^2$ and using Lemma 3.4, we can further infer:

$$\|x^{k+1} - x^{\star}\| \le \|\hat{g}^k - x^0\| + \|x^0 - x^{\star}\| \le (1 + 2\sqrt{m}M\kappa_r^2)\|h^0\| + \kappa_r\|h^0\| \le r.$$

This establishes $x^{k+1} \in \mathbb{B}_r(x^*)$. Similarly, we also have $\hat{x}^k \in \mathbb{B}_r(x^*)$ and it holds that

$$\|h(\hat{x}^k)\| \le \|h(\hat{x}^k) - h(x^0)\| + \|h^0\| \le \|\hat{x}^k - x^0\| + \bar{\epsilon} \le (1 + 2\sqrt{m\kappa_r^2}M)\bar{\epsilon} \le \epsilon_2$$

and $||h(\hat{g}^k)|| \le \epsilon_2$. Hence, by (3.5), we can conclude $||h^{k+1}|| = ||h(\hat{g}^k)|| \le (1 - \frac{1}{2\kappa_r})||h^k||$ and $x^{k+1} \in S_{\bar{\epsilon}}$.

3.2. Local Descent Properties of AA-R. We now formulate and present one of the main theoretical results of this paper.

THEOREM 3.6. Let the conditions (A.1)–(A.4) hold and let $\{x^k\}_k$ be generated by Algorithm 2.1. There is a neighborhood U of x^* such that if $x^0 \in U$, then we have:

(3.6)
$$f(x^{k+1}) \le f(g(x^k)) + \mathcal{O}(\|\nabla f(x^{k-\hat{m}})\|^3)$$

for all $k \in \mathbb{N}$, where $\hat{m} = \text{mod}(k, m+1)$.

As already outlined, the proof of Theorem 3.6 relies on subtle connections between AA-R, GMRES, CR, and CG. We will establish and discuss these connections step-by-step in the subsequent subsections.

Before proceeding with further details, let us briefly discuss GMRES, CR, and CG, cf. [39]. All of these algorithms are designed to solve linear systems of form Ax = bvia Krylov subspace techniques. For GMRES and CR, the k-th iterate is the point in the k-th Krylov subspace $\mathcal{K}^k(A, b)$ with minimal residual norm ||Ax - b||. Here, CR typically requires the matrix A to be symmetric positive semidefinite, which can be exploited in (faster) implementations. No additional assumptions (on A) need to be made when applying GMRES. CG is connected to CR and requires A to be symmetric, positive (semi)definite. Instead of finding elements with minimal residual norm, CG aims at minimizing the quadratic form $\frac{1}{2}x^{T}Ax - b^{T}x$ within the subspace $\mathcal{K}^{k}(A, b)$.

We now summarize the core components of our proof. In subsection 3.3, we show that the AA-R iterate x^{k+1} coincides with an iterate \bar{x}_G^k that can be generated via performing an additional gradient step on the GMRES iterate x_G^k . Here, GMRES is applied to a non-symmetric perturbed linear system $A(x - x^0) = b$ that is connected to AA-R. In addition, the gradient step $g(x^k)$ can be viewed as applying two gradient steps on the previous GMRES iterate x_G^{k-1} resulting in \tilde{x}_G^{k-1} . Since the system matrix Acan be interpreted as a perturbed version of the symmetric Hessian $\nabla^2 f(x^0)$, our idea is to run CR on the linear system $B(x - x^0) = b$ with $B = \nabla^2 f(x^0)$ and $b = -\nabla f(x^0)$ and to bound the differences between the CR and GMRES iterates. In subsection 3.4, we verify that this error has order $\mathcal{O}(||b||^2)$. Finally, in subsection 3.5, we connect CR and CG and use the rich computational properties of CG, [20], to show that the CR iterates achieve the desired descent on a local quadratic model of f. In the last subsection, we combine these different components to prove that the AA-R iterate x^{k+1} itself decreases the objective function value up to certain higher-order error terms.

3.3. Connecting AA-R and GMRES. We now establish equivalence of GMRES and AA-R when running one restarting cycle. Let us introduce the matrix $A := A_m = \nabla^2 f(x^0) + E_m$, where A_m and E_m have been defined in the proof of Proposition 3.2, i.e., it holds that

(3.7)
$$A = \nabla^2 f(x^0) + E_m, \quad E_m = B_m (X_m^\top X_m)^{-1} X_m^\top, \quad B_m = [b_1, \dots, b_m],$$

where $b_i = \nabla f(x^i) - \nabla f(x^0) - \nabla^2 f(x^0)(x^i - x^0), i \in [m].$

The matrix A can be utilized to construct a new perturbed gradient mapping $\bar{g}(x) := x - \frac{1}{L}(A(x - x^0) + \nabla f(x^0))$. Recalling (3.1), it can be shown that the function \bar{g} is exact at x^k for all $k = 0, \ldots, m$, i.e., we have $\bar{g}(x^k) = g(x^k)$. We now study GMRES applied to the linear system $A(x - x^0) = -\nabla f(x^0)$. While there are various implementations of GMRES [40, 5], each of these variants will yield the same iteration sequence $\{x_G^k\}_k$. The following proposition (which holds for general input data $A \in \mathbb{R}^{n \times n}$ and $b, x^0 \in \mathbb{R}^n$) is taken from [35, Equation (4)] and characterizes the iterates x_G^k more explicitly.

PROPOSITION 3.7. Let $A \in \mathbb{R}^{n \times n}$ be nonsingular and let $b, x^0 \in \mathbb{R}^n$ be given. Suppose further that $\{x_G^k\}_k$ is generated by GMRES to solve the system $A(x - x^0) = b$ with $x_G^0 = x^0$. Then, we have:

$$x_G^k = \operatorname{argmin}_{x \in x^0 + \mathcal{K}^k(A,b)} \|A(x - x^0) - b\|^2$$

Next, we verify the equivalence of AA-R and GMRES (in one restarting cycle) in the general nonlinear setting. As we will see, the matrix A in (3.7) and the perturbed

gradient mapping \bar{g} will play an important role when connecting AA-R and GMRES. We further note that the linear case has been already covered in [35, Proposition 2].

PROPOSITION 3.8. Let $\{x^k\}_{k=0,...,m+1}$ be generated by Algorithm 2.1 and suppose that (A.4) is satisfied. Let the sequence $\{x_G^k\}_{k=0,...,m}$ be generated by GMRES applied to $A(x-x^0) = -\nabla f(x^0)$ with initial point $x_G^0 = x^0$, where A is defined as in (3.7). Suppose that the matrix A is nonsingular. Setting $\hat{x}^0 := x^0$, it then holds that

$$\bar{x}_G^k := \bar{g}(x_G^k) = x^{k+1}$$
 and $x_G^k = \hat{x}^k \quad \forall \ k = 0, \dots, m$

In particular, we have $\kappa((\bar{X}_G^k)^{\top}\bar{X}_G^k) \leq M^2$ for each $k = 1, \ldots, m$, where $\bar{X}_G^k := [\bar{x}_G^0 - x^0, \ldots, \bar{x}_G^{k-1} - x^0]$.

Proof. We prove Proposition 3.8 by induction. The base case k = 0 is obviously satisfied. Next, let us suppose that the induction hypothesis is true for any $i \leq k - 1$. By definition, we have $\hat{x}^k = x^0 + \sum_{i=1}^k \alpha_i^k (x^i - x^0)$ where α^k is the solution to

$$\min_{\alpha} \|h(x^0) + \sum_{i=1}^k \alpha_i (h(x^i) - h(x^0))\|^2.$$

Based on the definition of the matrix A (see (3.7)) and by (3.1), we further obtain:

(3.8)
$$A(x^{i} - x^{0}) = \nabla f(x^{i}) - \nabla f(x^{0}) = -L(h(x^{i}) - h(x^{0})) \quad \forall i = 0, \dots, m.$$

Hence, α^k is also the solution to the problem $\min_{\alpha} \|A[\sum_{i=1}^k \alpha_i(x^i - x^0)] + \nabla f(x^0)\|^2$ and it holds that $\hat{x}^k = \operatorname{argmin}_{x \in x^0 + \operatorname{span}\{x^1 - x^0, \dots, x^k - x^0\}} \|A(x - x^0) + \nabla f(x^0)\|^2$. In addition, using assumption (A.4), we can infer that the vectors $\{x^1 - x^0, \dots, x^k - x^0\}$ are linearly independent. Applying Proposition 3.7, we have $x_G^k - x^0 \in \mathcal{K}^k(A, -\nabla f(x^0))$ and thus, it follows $\bar{x}_G^k - x^0 = x_G^k - x^0 - \frac{1}{L}(A(x_G^k - x^0) + \nabla f(x^0)) \in \mathcal{K}^{k+1}(A, -\nabla f(x^0))$ (for all k). Combining these observations and using the induction hypothesis, this yields $\operatorname{span}\{x^1 - x^0, \dots, x^k - x^0\} = \operatorname{span}\{\bar{x}_G^1 - x^0, \dots, \bar{x}_G^{k-1} - x^0\} = \mathcal{K}^k(A, -\nabla f(x^0))$, where the last equality follows from dim($\operatorname{span}\{x^1 - x^0, \dots, x^k - x^0\}) = k$. Thus, by Proposition 3.7, we can deduce:

$$\begin{aligned} x_G^k &= \operatorname{argmin}_{x \in x^0 + \mathcal{K}^k(A, -\nabla f(x^0))} \|A(x - x^0) + \nabla f(x^0)\|^2 \\ &= \operatorname{argmin}_{x \in x^0 + \operatorname{span}\{x^1 - x^0, \dots, x^k - x^0\}} \|A(x - x^0) + \nabla f(x^0)\|^2 = \hat{x}^k \end{aligned}$$

and thanks to (3.8), we obtain

$$\bar{x}_G^k = \bar{g}(x_G^k) = \bar{g}(\hat{x}^k) = \hat{x}^k - L^{-1} \cdot \sum_{i=1}^k \alpha_i^k A(x^i - x^0) + h(x^0) = \hat{g}^k = x^{k+1}.$$

The last assertion in Proposition 3.8 now follows from $\bar{x}_G^k = x^{k+1}$ and (A.4).

3.4. Connecting GMRES and CR. In this section, we study GMRES and CR applied to the general linear systems

$$A(x-x^0) = b$$
 and $B(x-x^0) = b$, $A, B \in \mathbb{R}^{n \times n}$, $b, x^0 \in \mathbb{R}^n$.

Let x_G^k denote the k-th iteration of GMRES applied to $A(x-x^0) = b$ and let x_R^k denote the k-th iteration of CR applied to the linear system $B(x-x^0) = b$ (in our case, we will have $B = \nabla^2 f(x^0)$ and $b = -\nabla f(x^0)$). Here, we want to investigate and bound the distance between the iterates x_G^k and x_R^k . In our analysis, we further assume $x_G^0 = x_R^0 = x^0$ and $b \neq 0$. We will largely utilize the following simple fact:

PROPOSITION 3.9. Let a_1, b_1, a_2, b_2 be given scalars, vectors, or matrices with appropriate dimensions such that a_1b_1 , a_2b_2 , $a_1 - a_2$, $b_1 - b_2$, and $a_1b_1 - a_2b_2$ are well-defined. Then, we have $||a_1b_1 - a_2b_2|| \le ||a_1 - a_2|| ||b_1|| + ||b_1 - b_2|| ||a_2||$.

As usual, the concrete implementation of CR is not of our concern and we only require the following property of CR:

PROPOSITION 3.10. [13, Section 2.2] Suppose $B \in \mathbb{R}^{n \times n}$ is symmetric and positive definite and let $b, x^0 \in \mathbb{R}^n$ be given. Let $\{x_R^k\}_k$ be generated by CR applied to the linear system $B(x - x^0) = b$ with $x_B^0 = x^0$. Then, we have:

 $x_{R}^{k} = \operatorname{argmin}_{x \in x^{0} + \mathcal{K}^{k}(B,b)} \|B(x - x^{0}) - b\|^{2}.$

Based on our earlier discussion, we now introduce several additional terms:

$$\bar{x}_{G}^{k} = x_{G}^{k} - \frac{1}{L} (A(x_{G}^{k} - x^{0}) - b), \qquad \bar{x}_{R}^{k} = x_{R}^{k} - \frac{1}{L} (B(x_{R}^{k} - x^{0}) - b),$$

$$\tilde{x}_{G}^{k} = \bar{x}_{G}^{k} - \frac{1}{L} (A(\bar{x}_{G}^{k} - x^{0}) - b), \qquad \tilde{x}_{R}^{k} = \bar{x}_{R}^{k} - \frac{1}{L} (B(\bar{x}_{R}^{k} - x^{0}) - b),$$

$$\bar{x}_{G}^{k} = [\bar{x}_{G}^{0} - x^{0}, \dots, \bar{x}_{G}^{k} - x^{0}], \qquad \bar{x}_{R}^{k} = [\bar{x}_{R}^{0} - x^{0}, \dots, \bar{x}_{R}^{k} - x^{0}].$$

Our first lemma in this section allows to connect the residuals of \bar{x}_G^k and x_G^k .

LEMMA 3.11. Let $B \in \mathbb{R}^{n \times n}$ be a symmetric, positive definite matrix with $L \geq C$ $\lambda_{\max}(B), \ \lambda_{\min}(B) \geq \mu > 0$ and suppose that $A \in \mathbb{R}^{n \times n}$ satisfies $||A - B|| < \mu$. Let $x, b \in \mathbb{R}^n$ be given and set $\bar{x} = x - L^{-1}(Ax - b)$. It holds that:

$$||A\bar{x} - b|| \le ||Ax - b||.$$

Proof. First notice that $\sigma_{\min}(A) \geq \sigma_{\min}(B) - ||A - B|| > 0$, which shows that A is nonsingular. We can then define $x^* := A^{-1}b$ and rewrite $Ax - b = A(x - x^*)$. Furthermore, it holds that

$$||A\bar{x} - b|| = ||A(\bar{x} - x^*)|| = ||(I - L^{-1}A)A(x - x^*)|| \le ||I - L^{-1}A|| ||A(x - x^*)||.$$

Hence, it suffices to verify $||I - L^{-1}A|| \le 1$. Indeed, we have $||I - L^{-1}A|| \le ||I - L^{-1}A|$ $L^{-1}B \| + \|L^{-1}(A - B)\| \le 1 - \frac{\mu}{L} + \frac{\mu}{L} \le 1$ which finishes the proof. Π

Next, we present our main result of this subsection.

THEOREM 3.12. Let $B \in \mathbb{R}^{n \times n}$ be a symmetric, positive definite matrix with $\begin{array}{l} \lambda_{\max}(B) \leq L \ and \ \lambda_{\min}(B) \geq \mu > 0 \ and \ let \ A \in \mathbb{R}^{n \times n}, \ b, x^0 \in \mathbb{R}^n, \ and \ \mathbb{N} \ni m \leq n \ be \\ given. \ Let \ the \ sequences \ \{x_G^k\}_k \ and \ \{x_R^k\}_k \ be \ generated \ by \ \mathsf{GMRES} \ and \ \mathsf{CR} \ applied \ to \\ the \ linear \ systems \ A(x-x^0) = b \ and \ B(x-x^0) = b \ with \ x_G^0 = x_R^0 = x^0, \ respectively. \end{array}$ Suppose further that there are constants $C_1, C_2, C_3 > 0$ such that:

- (i) $||A B|| \le C_1 ||b||$.
- (ii) For each $\bar{k} = 0, ..., m$, we have $\|\bar{x}_G^k x_G^0\| \le C_2 \|b\|$. (iii) We have $\kappa((\bar{X}_G^k)^\top \bar{X}_G^k) \le C_3$ for all k = 1, ..., m.

There exists a constant $\epsilon_{\sharp} > 0$ such that if $||b|| \leq \epsilon_{\sharp}$, then there is C > 0 such that:

$$\|x_G^k - x_R^k\| \le C \|b\|^2, \quad \|\bar{x}_G^k - \bar{x}_R^k\| \le C \|b\|^2, \quad \|\tilde{x}_G^k - \tilde{x}_R^k\| \le C \|b\|^2, \quad \forall \ 0 \le k \le m.$$

Proof. Without loss of generality, we can assume $b \neq 0$. We define the following quantities recursively: $\zeta_0 = 0, c_{k,1} = L^{-1}C_1C_2 + L^{-2}C_1 + \zeta_k, c_{k,2} = (k+1)C_1C_2 + C_1C_2 + C_2C_1 + \zeta_k$ $L(\sum_{i=0}^{k} c_{i,1}^{2})^{\frac{1}{2}}, c_{k,3} = 3c_{k,2}L(k+1)C_{2}, c_{4} = \frac{16}{9\mu^{2}}C_{3}L^{2}, c_{k,5} = c_{4}c_{k,2} + \frac{7}{2}c_{4}^{2}c_{k,3}(k+1)C_{2}, c_{4} = \frac{16}{9\mu^{2}}C_{3}L^{2}, c_{5} = \frac{16}{9\mu^{2}}C_{5}L^{2}, c$ $\begin{aligned} \zeta_{k+1} &= \frac{7}{4}L(k+1)C_2c_{k,5} + \sqrt{c_4}c_{k,2}, \ c_j = \max_{k=0,\dots,m} c_{k,j}, \ \text{for all } j = 1,2,3,5 \ \text{and} \\ \epsilon_{\sharp} &:= \frac{1}{2}\min\{(L^2C_3\sum_{i=0}^m c_{i,1}^2)^{-\frac{1}{2}}, \frac{\mu}{2C_1}, \frac{L}{c_2}, \frac{1}{c_3c_4}\}. \ \text{Next, let us assume } \|b\| \leq \epsilon_{\sharp}. \ \text{Due to} \\ C_1\epsilon_{\sharp} \leq \frac{1}{4}\mu \leq \frac{1}{4}L, \ \text{we then immediately obtain:} \end{aligned}$

(3.10)
$$||A|| \le ||B|| + ||A - B|| \le \frac{5}{4}L$$
 and $\sigma_{\min}(A) \ge \lambda_{\min}(B) - ||A - B|| \ge \frac{3}{4}\mu$.

This shows that A is nonsingular. Our goal is now to establish $||x_G^k - x_R^k|| \le \zeta_k ||b||^2$ by induction. The base case k = 0 is trivial. Let us suppose that the induction hypothesis is true for all $0 \le i \le k$. By Proposition 3.7 and Proposition 3.10, we have:

$$x_G^{k+1} = \underset{x \in x^0 + \mathcal{K}^{k+1}(A,b)}{\operatorname{argmin}} \|A(x - x^0) - b\|^2, \quad x_R^{k+1} = \underset{x \in x^0 + \mathcal{K}^{k+1}(B,b)}{\operatorname{argmin}} \|B(x - x^0) - b\|^2.$$

Furthermore, mimicking the proof of Proposition 3.8 and using (iii), we can deduce

(3.11)
$$\bar{x}_G^k - x^0 \in \mathcal{K}^{k+1}(A, b) \text{ and } \bar{x}_R^k - x^0 \in \mathcal{K}^{k+1}(B, b)$$

for all k and span{ $\bar{x}_G^0 - x^0, \ldots, \bar{x}_G^k - x^0$ } = $\mathcal{K}^{k+1}(A, b)$. In addition, applying (i) and (ii), it holds that

$$\begin{aligned} \|\bar{x}_{G}^{i} - \bar{x}_{R}^{i}\| &= \|x_{G}^{i} - L^{-1}A(x_{G}^{i} - x^{0}) - x_{R}^{i} + L^{-1}B(x_{R}^{i} - x^{0})\| \\ &= \|L^{-1}(A - B)(x^{0} - x_{G}^{i}) + (I - L^{-1}B)(x_{G}^{i} - x_{R}^{i})\| \\ &\leq L^{-1}\|A - B\|(\|\bar{x}_{G}^{i} - x^{0}\| + \|\bar{x}_{G}^{i} - x_{G}^{i}\|) + \|I - L^{-1}B\|\|x_{G}^{i} - x_{R}^{i}\| \\ &\leq C_{1}L^{-1}\|b\|(\|\bar{x}_{G}^{i} - x^{0}\| + \|\bar{x}_{G}^{i} - x_{G}^{i}\|) + \|x_{G}^{i} - x_{R}^{i}\| \\ &\leq C_{1}L^{-1}\|b\|(C_{2}\|b\| + L^{-1}\|b\|) + \zeta_{i}\|b\|^{2} = c_{i,1}\|b\|^{2}, \end{aligned}$$

$$(3.12)$$

where we used $||I - L^{-1}B|| \le 1 - \frac{\mu}{L} \le 1$ and Proposition 3.7 to show that:

$$\|\bar{x}_G^i - x_G^i\| = L^{-1} \min_{x \in x^0 + \mathcal{K}^i(A, b)} \|A(x - x^0) - b\| \le L^{-1} \|A(x^0 - x^0) - b\| = L^{-1} \|b\|.$$

Therefore, we are able to bound the error between \bar{X}_G^k and \bar{X}_R^k :

$$\|\bar{X}_{G}^{k} - \bar{X}_{R}^{k}\| \le \left(\sum_{i=0}^{k} \|\bar{x}_{G}^{i} - \bar{x}_{R}^{i}\|^{2}\right)^{1/2} \le \left(\sum_{i=0}^{k} c_{i,1}^{2}\right)^{1/2} \|b\|^{2} \le \frac{1}{2L\sqrt{C_{3}}} \|b\|,$$

where we applied the definition of ϵ_{\sharp} . Furthermore, due to (iii), we can infer:

(3.13)
$$\|\bar{X}_G^k\| \ge \|\bar{x}_G^0 - x^0\| = \frac{\|b\|}{L} \implies \sigma_{\min}(\bar{X}_G^k) \ge \frac{\sigma_{\max}(\bar{X}_G^k)}{\sqrt{C_3}} \ge \frac{\|b\|}{(L\sqrt{C_3})}$$

Consequently, it holds that $\sigma_{\min}(\bar{X}_R^k) \geq \sigma_{\min}(\bar{X}_G^k) - \|\bar{X}_G^k - \bar{X}_R^k\| \geq \frac{1}{2L\sqrt{C_3}}\|b\| > 0$. Thus, the column vectors of \bar{X}_R^k are also linearly independent and by (3.11), it follows $\operatorname{span}\{\bar{x}_R^0 - x^0, \dots, \bar{x}_R^k - x^0\} = \mathcal{K}^{k+1}(B, b)$. Combining the previous arguments, we can now rewrite x_G^{k+1} and x_R^{k+1} as:

$$\begin{split} x_G^{k+1} &= \operatorname{argmin}_{x \in x^0 + \operatorname{span}\{\bar{x}_G^0 - x^0, \dots, \bar{x}_G^k - x^0\}} \ \|A(x - x^0) - b\|^2, \\ x_R^{k+1} &= \operatorname{argmin}_{x \in x^0 + \operatorname{span}\{\bar{x}_R^0 - x^0, \dots, \bar{x}_R^k - x^0\}} \ \|B(x - x^0) - b\|^2. \end{split}$$

The closed-form expressions of x_G^{k+1} and x_R^{k+1} are therefore given by:

$$x_G^{k+1} = x^0 + Y_G^k((Y_G^k)^\top Y_G^k)^{-1}(Y_G^k)^\top b, \quad x_R^{k+1} = x^0 + Y_R^k((Y_R^k)^\top Y_R^k)^{-1}(Y_R^k)^\top b$$

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where $Y_G^k = A\bar{X}_G^k$ and $Y_R^k = B\bar{X}_R^k$. Our first task is to estimate the error between Y_G^k and Y_R^k . Using (i) and (ii), we have:

$$\begin{aligned} \|Y_G^k - Y_R^k\| &\leq \|(A - B)\bar{X}_G^k\| + \|B(\bar{X}_G^k - \bar{X}_R^k)\| \\ &\leq (k+1)C_1\|b\|\|\bar{X}_G^k\|_{\infty} + L\left(\sum_{i=0}^k c_{i,1}^2\right)^{1/2}\|b\|^2 \leq c_{k,2}\|b\|^2 \leq c_2\|b\|^2 \end{aligned}$$

Moreover, applying (3.10), we can infer $||Y_G^k|| \leq ||A|| ||\bar{X}_G^k|| \leq \frac{5L}{4} ||\bar{X}_G^k|| \leq \frac{5L(k+1)C_2}{4} ||b||$ and due to $c_2 \epsilon_{\sharp} \leq \frac{L}{2} \leq \frac{L(k+1)}{2}$, we have $c_2 ||b||^2 \leq \frac{L(k+1)C_2}{2} ||b||$. This allows to establish a bound for the norm of Y_R^k :

$$||Y_R^k|| \le ||Y_G^k|| + ||Y_G^k - Y_R^k|| \le \frac{7}{4}L(k+1)C_2||b||.$$

Therefore, by Proposition 3.9, we can bound the norm of the term $(Y_G^k)^\top Y_G^k - (Y_R^k)^\top Y_R^k$ as follows:

$$\begin{aligned} \|(Y_G^k)^\top Y_G^k - (Y_R^k)^\top Y_R^k\| &\leq \|Y_G^k - Y_R^k\| (\|Y_G^k\| + \|Y_R^k\|) \\ &\leq c_{k,2} \|b\|^2 \left(\frac{7}{4}L(k+1)C_2 + \frac{5}{4}L(k+1)C_2\right) \|b\| = 3c_{k,2}L(k+1)C_2 \|b\|^3 = c_{k,3} \|b\|^3. \end{aligned}$$

Our next task is to bound $\|((Y_G^k)^\top Y_G^k)^{-1}\|$. Using $A^\top A \succeq \frac{9}{16}\mu^2 I$ and (3.13), we have:

$$\begin{aligned} \| ((Y_G^k)^\top Y_G^k)^{-1} \| &= \| ((\bar{X}_G^k)^\top A^\top A \bar{X}_G^k)^{-1} \| \\ &\leq \frac{16}{9\mu^2} \| ((\bar{X}_G^k)^\top \bar{X}_G^k)^{-1} \| \leq \frac{16C_3}{9\mu^2 \| \bar{X}_G^k \|^2} \leq \frac{16C_3 L^2}{9\mu^2 \| b \|^2} = \frac{c_4}{\| b \|^2} \end{aligned}$$

Since ϵ_{\sharp} is chosen such that $1 - c_{k,3}c_4 \|b\| \ge \frac{1}{2} > 0$, we can now apply Banach's perturbation lemma, see, e.g., [16, Theorem 2.3.4], which implies:

$$\begin{split} \|((Y_G^k)^\top Y_G^k)^{-1} - ((Y_R^k)^\top Y_R^k)^{-1}\| &\leq \frac{\|((Y_G^k)^\top Y_G^k)^{-1}\|^2 \|(Y_G^k)^\top Y_G^k - (Y_R^k)^\top Y_R^k\|}{1 - \|((Y_G^k)^\top Y_G^k)^{-1}\| \|(Y_G^k)^\top Y_G^k - (Y_R^k)^\top Y_R^k\|} \\ &\leq \frac{c_4^2 c_{k,3}}{\|b\| - c_4 c_{k,3}\|b\|^2} \leq \frac{2c_4^2 c_{k,3}}{\|b\|}. \end{split}$$

Consequently, applying Proposition 3.9, it follows:

$$\begin{aligned} \|Y_G^k((Y_G^k)^\top Y_G^k)^{-1} - Y_R^k((Y_R^k)^\top Y_R^k)^{-1}\| \\ & \leq \|((Y_G^k)^\top Y_G^k)^{-1}\| \|Y_G^k - Y_R^k\| + \|((Y_G^k)^\top Y_G^k)^{-1} - ((Y_R^k)^\top Y_R^k)^{-1}\| \|Y_R^k\| \\ & \leq c_4 c_{k,2} + \frac{7}{2} c_4^2 c_{k,3}(k+1) C_2 = c_{k,5} \end{aligned}$$

and $||Y_G^k((Y_G^k)^\top Y_G^k)^{-1}|| = \sqrt{||((Y_G^k)^\top Y_G^k)^{-1}||} \le \frac{\sqrt{c_4}}{||b||}$. Altogether, this yields: $||x_G^{k+1} - x_R^{k+1}|| = ||Y_G^k((Y_G^k)^\top Y_G^k)^{-1}(Y_G^k)^\top b - Y_R^k((Y_R^k)^\top Y_R^k)^{-1}(Y_R^k)^\top b||$

 $\leq \|Y_G^k((Y_G^k)^\top Y_G^k)^{-1} - Y_R^k((Y_R^k)^\top Y_R^k)^{-1}\|\|Y_R^k\|\|b\| + \|Y_G^k((Y_G^k)^\top Y_G^k)^{-1}\|\|Y_R^k - Y_G^k\|\|b\| \\ \leq \frac{7}{4}L(k+1)C_2c_{k,5}\|b\|^2 + \sqrt{c_4}c_{k,2}\|b\|^2 = \zeta_{k+1}\|b\|^2.$

This shows $||x_G^k - x_R^k|| \le \zeta_k ||b||^2$ by induction. Mimicking (3.12), we now obtain:

$$\begin{aligned} \|\tilde{x}_{G}^{k} - \tilde{x}_{R}^{k}\| &\leq \|L^{-1}(A - B)(\bar{x}_{G}^{k} - x^{0})\| + \|(I - L^{-1}B)(\bar{x}_{G}^{k} - \bar{x}_{R}^{k})\| \\ &\leq L^{-1}C_{1}C_{2}\|b\|^{2} + \|\bar{x}_{G}^{k} - \bar{x}_{R}^{k}\| \leq (L^{-1}C_{1}C_{2} + c_{1})\|b\|^{2}. \end{aligned}$$

Therefore, it suffices to choose $C := \max\{\max_{k=0,\dots,m} \zeta_k, L^{-1}C_1C_2 + c_1\}.$

3.5. Connecting CR and CG. In this subsection, we assume that the matrix B is symmetric and positive definite. Suppose we apply CR to the linear system $B(x - x^0) = b$ starting at x^0 . Then, by Proposition 3.10, we have:

$$x_{R}^{k} = \operatorname{argmin}_{x \in x^{0} + \mathcal{K}^{k}(B,b)} \|B(x - x^{0}) - b\|^{2} = \operatorname{argmin}_{x \in x^{0} + \mathcal{K}^{k}(B,b)} \|B(x - x^{*})\|,$$

where $x^* := B^{-1}b + x^0$ is the optimal solution of the linear system $B(x - x^0) = b$. Next, for k = 0, ..., m, we set $y^* := B^{\frac{1}{2}}x^*$, $\overline{b} := B^{\frac{1}{2}}b$ and $y^k := B^{\frac{1}{2}}x_R^k$. Then, by definition, we obtain:

$$y^{k} = \operatorname{argmin}_{y \in y^{0} + \mathcal{K}^{k}(B,\bar{b})} (y - y^{*})^{\top} B(y - y^{*})$$

According to [18, Theorem 2], this means that y^k coincides with the k-th iteration of CG applied to the linear system $B(y-y^*) = 0$ with initial value $y^0 = B^{\frac{1}{2}}x^0$. Moreover, in this case, it follows $(x_R^k - x^*)^\top B(x_R^k - x^*) = ||y^k - y^*||^2$. Based on this observation and connection between the CR- and CG-iterates, we now want to apply classical techniques for CG, [20], to study the behavior of the distance $||y^k - y^*||$ as the iteration k increases. Our goal is to then transfer the obtained results back to CR and AA-R. As usual, we define the following terms: $\bar{y}^k = y^k - L^{-1}B(y^k - y^*)$,

$$\tilde{y}^k = \bar{y}^k - L^{-1}B(\bar{y}^k - y^*), \text{ and } \psi(y) = \frac{1}{2}(y - y^*)^\top B(y - y^*).$$

Notice that the introduced linear transformations also preserve the latter gradient descent steps, i.e., it holds that $\bar{y}^k = B^{\frac{1}{2}} \bar{x}_R^k$ and $\tilde{y}^k = B^{\frac{1}{2}} \tilde{x}_R^k$. Here, the point \bar{y}^k is obtained by applying one gradient step (for the objective function ψ) with stepsize L^{-1} on the CG-iteration y^k and \tilde{y}^k results from applying two gradient steps with stepsize L^{-1} on y^k . Next, we collect several results from [20] for convenience and to fix the notations. The full CG algorithm is shown in Algorithm 3.1.

Algorithm 3.1 CG for the linear system $B(y - y^*) = 0$.

1: Choose an initial point $y^0 \in \mathbb{R}^n$ and set $p^0 = r^0 = -B(y^0 - y^*)$. 2: for i = 0, 1, ..., n do 3: if $||r^i|| = 0$ then Break; end if 4: $a_i = \frac{||r^i||^2}{\langle p^i, Bp^i \rangle}$. 5: $y^{i+1} = y^i + a_i p^i$. 6: $r^{i+1} = r^i - a_i Bp^i$. 7: $b_i = \frac{||r^{i+1}||^2}{||r^i||^2}$. 8: $p^{i+1} = r^{i+1} + b_i p^i$. 9: end for

PROPOSITION 3.13. Let the sequence $\{y^k\}_k$ be generated by CG and let $y^{(k)}$ denote the projection of y^* onto the affine space $\mathcal{A}^k := y^0 + \operatorname{span}\{y^1 - y^0, \ldots, y^k - y^0\}$. Then, the following properties are satisfied:

- (i) ([20, Theorem 6.5]) $y^{(k+1)} = y^{k+1} + \frac{2\psi(y^{k+1})}{\|r^k\|^2} p^k$.
- (ii) ([20, Equation (5:3a)]) For all $i \neq j$: $\langle r^i, r^j \rangle = 0$.
- (iii) ([20, Equation (5:3c)]) For all i < j, we have ⟨pⁱ, r^j⟩ = 0 and for all i ≥ j, it holds that ⟨pⁱ, r^j⟩ = ||rⁱ||².
- (iv) ([20, Equation (5:6b)]) For all $0 \le i \le n$: $||p^i||^2 = ||r^i||^4 \sum_{j=0}^i \frac{1}{||r^j||^2}$.

- (v) ([20, Equation (5:11)]) For all $0 \le i \le n-1$: $\langle r^{i+1}, Br^i \rangle = \langle r^{i+1}, Bp^i \rangle = \langle r^{i+1}, Bp^i \rangle$ $-a_i^{-1} \| r^{i+1} \|^2.$
- (vi) ([20, Equation (5:6a)]) For all $0 \le i \le j \le n$: $\langle p^i, p^j \rangle = \frac{\|r^j\|^2 \|p^i\|^2}{\|r^i\|^2}$.

- (vii) ([20, Equation (5:4b)]) For all $i \neq j$: $\langle p^i, Bp^j \rangle = 0$. (viii) ([20, Equation (5:3d)]) For all $i \neq j, i \neq j + 1$: $\langle r^i, Bp^j \rangle = 0$. (ix) ([20, Equation (5:12)]) We have $a_0 = \frac{\|r^0\|^2}{\langle r^0, Br^0 \rangle}$ and $\frac{\|p^i\|^2}{\langle p^i, Br^i \rangle} > a_i > \frac{\|r^i\|^2}{\langle r^i, Br^i \rangle}$ for all i > 0.
 - (x) ([20, Equation (5:8b)]) For all $i \ge 1$: $r^{i+1} = (1 + b'_{i-1})r^i a_i Br^i b'_{i-1}r^{i-1}$, where $b'_{i-1} = \frac{a_i}{a_{i-1}} b_{i-1} = \frac{a_i}{a_{i-1}} \frac{\|r^i\|^2}{\|r^{i-1}\|^2}$.

The properties stated in Proposition 3.13 will be referred to as Property (i)–(x) in the following. Before studying the convergence behavior of CG in terms of $\|\bar{y}^k - y^*\|$ and $\|\tilde{y}^{k-1} - y^*\|$, let us briefly discuss our underlying motivation.

Our final aim is to prove $f(x^{k+1}) \leq f(g(x^k))$ (including some potential higherorder error terms), where $\{x^k\}_k$ is generated by AA-R. Applying Proposition 3.8, the AA step x^{k+1} is equal to \bar{x}_G^k , which is close to \bar{x}_R^k . On the other hand, we have $g(x^k) = \bar{g}(x^k) = \bar{g}(\bar{x}_G^{k-1}) = \tilde{x}_G^{k-1}$, which is close to \bar{x}_R^{k-1} . Hence, up to certain error terms, the descent condition " $f(x^{k+1}) \leq f(g(x^k))$ " can now be formulated as follows:

$$f(\bar{x}_R^k) \le f(\tilde{x}_R^{k-1}).$$

Expanding f at x^0 (and again ignoring higher-order error terms), this can be further rewritten as:

$$\nabla f(x^0)^\top (\bar{x}_R^k - x^0) + \frac{1}{2} (\bar{x}_R^k - x^0)^\top \nabla^2 f(x^0) (\bar{x}_R^k - x^0)$$

$$\leq \nabla f(x^0)^\top (\tilde{x}_R^{k-1} - x^0) + \frac{1}{2} (\tilde{x}_R^{k-1} - x^0)^\top \nabla f(x^0) (\tilde{x}_R^{k-1} - x^0)$$

Noticing $B = \nabla^2 f(x^0)$, $b = -\nabla f(x^0)$, and $x^* = B^{-1}b + x^0$, this is equivalent to

$$(\bar{x}_R^k - x^*)^\top B(\bar{x}_R^k - x^*) \le (\tilde{x}_R^{k-1} - x^*)^\top B(\tilde{x}_R^{k-1} - x^*),$$

which, by the previously introduced transformation, can be expressed as $\|\bar{y}^k - y^*\|^2 \leq$ $\|\tilde{y}^{k-1} - y^*\|^2$. This is exactly what we want to show in Theorem 3.14. We note that the proof of Theorem 3.14 would be significantly easier if the stepsize in the gradient mapping g is sufficiently small (potentially much smaller than L^{-1}). Here, we provide a general result covering the core case $g(x) = x - \frac{1}{L} \nabla f(x)$.

THEOREM 3.14. Suppose that $\{y^k\}_k$ is generated by CG applied to the linear system $B(y-y^*)=0$, where $B \in \mathbb{R}^{n \times n}$ is symmetric, positive definite with $\nu := \frac{L}{\|B\|} \ge 1$. Then, we have:

$$(3.14) \quad \|\bar{y}^k - y^*\|^2 + \left[2\nu + \frac{1}{\nu^2} - 3\right] \frac{\|r^k\|^2}{L^2} + \left[\nu + \frac{1}{\nu} - 2\right]^2 \frac{\|r^{k-1}\|^2}{L^2} \le \|\tilde{y}^{k-1} - y^*\|^2.$$

Proof. First, by [18, Equation (21)] and [26, Theorem 5.3], we have $\mathcal{A}^k = y^0 + \mathcal{K}^k(B, r^0)$ and $y^k \in y^0 + \mathcal{K}^k(B, r^0)$. Hence, both \bar{y}^k and \tilde{y}^{k-1} belong to the affine space $y^0 + \mathcal{K}^{k+1}(B, r^0) = \mathcal{A}^{k+1}$. Furthermore, by the definition of $y^{(k+1)}$, we can derive the following decomposition properties:

(3.15)
$$\begin{aligned} \|\bar{y}^{k} - y^{*}\|^{2} &= \|y^{(k+1)} - \bar{y}^{k}\|^{2} + \|y^{(k+1)} - y^{*}\|^{2}, \\ \|\tilde{y}^{k-1} - y^{*}\|^{2} &= \|y^{(k+1)} - \tilde{y}^{k-1}\|^{2} + \|y^{(k+1)} - y^{*}\|^{2}. \end{aligned}$$

Therefore, it holds that:

(3.16)
$$\begin{aligned} \|\tilde{y}^{k-1} - y^*\|^2 - \|\bar{y}^k - y^*\|^2 &= \|y^{(k+1)} - \tilde{y}^{k-1}\|^2 - \|y^{(k+1)} - \bar{y}^k\|^2 \\ &= \|\tilde{y}^{k-1} - \bar{y}^k\|^2 + 2\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle. \end{aligned}$$

Using Property (i) and the definition of the CG-step, we have $y^{(k+1)} = y^{k+1} + \frac{2\psi(y^{k+1})}{\|r^k\|^2}p^k$ and $y^{k+1} = y^k + a_k p^k$. Consequently, setting $\gamma_k = 2\psi(y^{k+1})/\|r^k\|^2 + a_k$ and applying $r^k = -B(y^k - y^*)$, we obtain

(3.17)
$$y^{(k+1)} - \bar{y}^k = \left[\frac{2\psi(y^{k+1})}{\|r^k\|^2} + a_k\right] p^k + [y^k - \bar{y}^k] = \gamma_k p^k - \frac{1}{L}r^k.$$

Moreover, we have $y^k - \overline{y}^{k-1} = a_{k-1}p^{k-1} - \frac{1}{L}r^{k-1}$ and

(3.18)
$$\bar{y}^k - \tilde{y}^{k-1} = (I - L^{-1}B)(y^k - \bar{y}^{k-1}) = (I - L^{-1}B)(a_{k-1}p^{k-1} - L^{-1}r^{k-1}).$$

We now consider the first term in (3.16):

$$\|\tilde{y}^{k-1} - \bar{y}^k\|^2 = \|(I - L^{-1}B)(a_{k-1}p^{k-1} - L^{-1}r^{k-1})\|^2 = T_1 - 2L^{-1}T_2 + L^{-2}T_3,$$

where $T_1 = a_{k-1}^2 ||(I - L^{-1}B)p^{k-1}||^2$, $T_2 = \langle a_{k-1}(I - L^{-1}B)p^{k-1}, (I - L^{-1}B)r^{k-1} \rangle$, and $T_3 = ||(I - L^{-1}B)r^{k-1}||^2$. The update rule for r^k yields

(3.19)
$$a_{k-1}Bp^{k-1} = r^{k-1} - r^k.$$

We first expand the term T_1 :

$$T_{1} = \|a_{k-1}p^{k-1} - L^{-1}(r^{k-1} - r^{k})\|^{2}$$

= $a_{k-1}^{2} \|p^{k-1}\|^{2} - 2a_{k-1}L^{-1}\langle p^{k-1}, r^{k-1} - r^{k}\rangle + L^{-2} \|r^{k-1} - r^{k}\|^{2}.$

Applying Property (ii) and (iii), it holds that:

$$||r^{k-1} - r^k||^2 = ||r^{k-1}||^2 + ||r^k||^2, \quad \langle p^{k-1}, r^{k-1} - r^k \rangle = ||r^{k-1}||^2,$$

and thus, it follows $T_1 = a_{k-1}^2 \|p^{k-1}\|^2 - \frac{2a_{k-1}}{L} \|r^{k-1}\|^2 + \frac{1}{L^2} (\|r^{k-1}\|^2 + \|r^k\|^2)$. Next, we estimate the term T_2 :

$$T_2 = \langle a_{k-1}p^{k-1}, r^{k-1} \rangle - 2L^{-1} \langle a_{k-1}Bp^{k-1}, r^{k-1} \rangle + L^{-2} \langle a_{k-1}Bp^{k-1}, Br^{k-1} \rangle.$$

By Property (iii), we have $\langle a_{k-1}p^{k-1}, r^{k-1} \rangle = a_{k-1} ||r^{k-1}||^2$. Furthermore, applying (3.19) and Property (ii), we obtain $\langle a_{k-1}Bp^{k-1}, r^{k-1} \rangle = \langle r^{k-1} - r^k, r^{k-1} \rangle = ||r^{k-1}||^2$ and $\langle a_{k-1}Bp^{k-1}, Br^{k-1} \rangle = \langle r^{k-1} - r^k, Br^{k-1} \rangle$. Utilizing Property (v), we can infer:

$$\langle a_{k-1}Bp^{k-1}, Br^{k-1} \rangle = \langle r^{k-1} - r^k, Br^{k-1} \rangle = ||r^{k-1}||_B^2 + a_{k-1}^{-1}||r^k||^2.$$

Substituting these expressions yields $T_2 = a_{k-1} ||r^{k-1}||^2 - \frac{2}{L} ||r^{k-1}||^2 + \frac{1}{L^2} ||r^{k-1}||_B^2 + \frac{1}{L^2 a_{k-1}} ||r^k||^2$. Finally, let us consider the term T_3 ; we have:

$$T_3 = \|r^{k-1}\|^2 - 2L^{-1}\|r^{k-1}\|_B^2 + L^{-2}\|Br^{k-1}\|^2.$$

Together, this establishes the following representation of $\|\tilde{y}^{k-1} - \bar{y}^k\|^2$:

$$(3.20) \|\tilde{y}^{k-1} - \bar{y}^k\|^2 = a_{k-1}^2 \|p^{k-1}\|^2 + \left[\frac{6}{L^2} - \frac{4a_{k-1}}{L}\right] \|r^{k-1}\|^2 \\ - \frac{4}{L^3} \|r^{k-1}\|_B^2 + \frac{1}{L^4} \|Br^{k-1}\|^2 + \left[\frac{1}{L^2} - \frac{2}{L^3a_{k-1}}\right] \|r^k\|^2$$

We continue with the inner product term $\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle$. By (3.17) and (3.18), we have:

$$\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle = \langle (I - L^{-1}B)(a_{k-1}p^{k-1} - L^{-1}r^{k-1}), \gamma^k p^k - L^{-1}r^k \rangle$$

= $Q_1 - L^{-1}Q_2,$

where $Q_1 = \langle a_{k-1}p^{k-1} - \frac{1}{L}r^{k-1}, \gamma_k p^k - \frac{1}{L}r^k \rangle$ and $Q_2 = \langle a_{k-1}Bp^{k-1} - \frac{1}{L}Br^{k-1}, \gamma_k p^k - \frac{1}{L}r^k \rangle$. Applying Property (vi), (ii) and (iii), it holds that:

$$\langle p^{k-1}, p^k \rangle = \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2}, \quad \langle r^{k-1}, p^k \rangle = \|r^k\|^2, \quad \langle p^{k-1}, r^k \rangle = \langle r^k, r^{k-1} \rangle = 0,$$

which implies $Q_1 = a_{k-1}\gamma_k \langle p^{k-1}, p^k \rangle - \frac{\gamma_k}{L} \langle r^{k-1}, p^k \rangle - \frac{a_{k-1}}{L} \langle p^{k-1}, r^k \rangle + \frac{1}{L^2} \langle r^k, r^{k-1} \rangle = a_{k-1}\gamma_k \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2} - \frac{\gamma_k}{L} \|r^k\|^2$. Similarly, we can expand Q_2 as follows:

$$Q_2 = a_{k-1}\gamma_k \langle Bp^{k-1}, p^k \rangle - \frac{\gamma_k}{L} \langle Br^{k-1}, p^k \rangle - \frac{a_{k-1}}{L} \langle Bp^{k-1}, r^k \rangle + \frac{1}{L^2} \langle Br^k, r^{k-1} \rangle.$$

Applying Property (vii), (viii), (ii), (ii), (v), and (3.19), we can infer $\langle Bp^{k-1}, p^k \rangle = 0$, $\langle Br^{k-1}, p^k \rangle = 0$, $\langle a_{k-1}Bp^{k-1}, r^k \rangle = \langle r^{k-1} - r^k, r^k \rangle = -||r^k||^2$, and $\langle Br^k, r^{k-1} \rangle = -\frac{||r^k||^2}{a_{k-1}}$, which yields $Q_2 = \frac{1}{L}(1 - \frac{1}{La_{k-1}})||r^k||^2$. Therefore, the inner product term $\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle$ is given by:

$$\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle = a_{k-1}\gamma_k \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2} - \left[\frac{\gamma_k}{L} + \frac{1}{L^2} - \frac{1}{L^3 a_{k-1}}\right] \|r^k\|^2.$$

Summing (3.20) and the previous expression, we obtain:

$$\begin{aligned} \|\tilde{y}^{k-1} - \bar{y}^k\|^2 + 2\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle \\ &= a_{k-1}^2 \|p^{k-1}\|^2 + \left[\frac{6}{L^2} - \frac{4a_{k-1}}{L}\right] \|r^{k-1}\|^2 - \frac{4}{L^3} \|r^{k-1}\|_B^2 + \frac{1}{L^4} \|Br^{k-1}\|^2 \\ (3.21) \qquad + \left[2a_{k-1}\gamma_k \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2} - \frac{2\gamma_k}{L} \|r^k\|^2 - \frac{1}{L^2} \|r^k\|^2\right]. \end{aligned}$$

We continue with two sub-cases.

Case 1: k = 1. Using the fact $r^0 = p^0$, Property (ii), and (3.19), it follows $||Br^0||^2 = ||Bp^0||^2 = a_0^{-2}||r^0 - r^1||^2 = a_0^{-2}(||r^0||^2 + ||r^1||^2)$ and $\langle r^0, Br^0 \rangle = \langle r^0, Bp^0 \rangle = a_0^{-1} \langle r^0, r^0 - r^1 \rangle = a_0^{-1} ||r^0||^2$. Using these two equalities, we can simplify (3.21) to:

$$\begin{split} \|\tilde{y}^{0} - \bar{y}^{1}\|^{2} + 2\langle \tilde{y}^{0} - \bar{y}^{1}, \bar{y}^{1} - y^{(2)} \rangle \\ &= a_{0}^{2} \|r^{0}\|^{2} + \left[\frac{6}{L^{2}} - \frac{4a_{0}}{L}\right] \|r^{0}\|^{2} - \frac{4}{L^{3}a_{0}} \|r^{0}\|^{2} + \frac{1}{L^{4}a_{0}^{2}} (\|r^{0}\|^{2} + \|r^{1}\|^{2}) \\ &+ \left[2a_{0}\gamma_{1}\|r^{1}\|^{2} - 2\gamma_{1}L^{-1}\|r^{1}\|^{2} - L^{-2}\|r^{1}\|^{2}\right] \\ &= L^{-2}(Q_{3}\|r^{0}\|^{2} + Q_{4}\|r^{1}\|^{2}), \end{split}$$

where Q_3 and Q_4 are defined as $Q_3 = a_0^2 L^2 + 6 - 4a_0 L - 4(a_0 L)^{-1} + (a_0 L)^{-2}$ and $Q_4 = 2a_0\gamma_1 L^2 - 2\gamma_1 L - 1 + (a_0 L)^{-2}$. By Property (ix), we have $a_0 = ||r^0||^2 / \langle r^0, Br^0 \rangle \ge \frac{1}{||B||} \ge \frac{1}{L}$ and $a_1 > ||r^1||^2 / \langle r^1, Br^1 \rangle \ge \frac{1}{||B||} \ge \frac{1}{L}$. Hence, by the definition of γ_1 , we can infer $\gamma_1 L \ge a_1 L > L ||B||^{-1} = \nu \ge 1$ and $a_0 L \ge \nu \ge 1$. Therefore, it holds that:

$$Q_4 = 2\gamma_1 L(a_0 L - 1) - 1 + (a_0 L)^{-2} \ge 2a_0 L + (a_0 L)^{-2} - 3 \ge 2\nu + \nu^{-2} - 3 \ge 0,$$

where – in the last equality – we used the fact that the function $x \mapsto 2x + x^{-2}$ is monotonically increasing for $x \ge 1$. Concerning Q_3 , we notice:

$$Q_3 = (a_0L + (a_0L)^{-1} - 2)^2 \ge 0.$$

Since $x \mapsto x + \frac{1}{x} - 2$ is monotonically increasing and nonnegative for $x \in [1, \infty)$, we can further infer $Q_3 = (a_0L + (a_0L)^{-1} - 2)^2 \ge (\nu + \nu^{-1} - 2)^2$, Together, we obtain $\|\bar{y}^1 - y^*\|^2 + (\nu + \nu^{-1} - 2)^2 \frac{\|r^0\|^2}{L^2} + (2\nu + \nu^{-2} - 3) \frac{\|r^1\|^2}{L^2} \le \|\tilde{y}^0 - y^*\|^2$.

Case 2: $k \ge 2$. We first utilize Property (x): $a_{k-1}Br^{k-1} = (1+b'_{k-2})r^{k-1} - r^k - b'_{k-2}r^{k-2}$. Along with Property (ii), this allows to calculate $||r^{k-1}||_B^2$ and $||Br^k||^2$:

$$\langle r^{k-1}, Br^{k-1} \rangle = \frac{1}{a_{k-1}} \langle r^{k-1}, (1+b'_{k-2})r^{k-1} - r^k - b'_{k-2}r^{k-2} \rangle = \frac{1+b'_{k-2}}{a_{k-1}} \|r^{k-1}\|^2, \\ \|Br^{k-1}\|^2 = \langle Br^{k-1}, Br^{k-1} \rangle = \frac{(1+b'_{k-2})^2}{a_{k-1}^2} \|r^{k-1}\|^2 + \frac{1}{a_{k-1}^2} \|r^k\|^2 + \frac{(b'_{k-2})^2}{a_{k-1}^2} \|r^{k-2}\|^2.$$

Therefore, the term (3.21) can be decomposed as follows: $\|\tilde{y}^{k-1} - \bar{y}^k\|^2 + 2\langle \tilde{y}^{k-1} - \bar{y}^k, \bar{y}^k - y^{(k+1)} \rangle = Q_5 + Q_6$, where

$$\begin{aligned} Q_5 &= a_{k-1}^2 \|p^{k-1}\|^2 + \left[\frac{6}{L^2} - \frac{4a_{k-1}}{L} - \frac{4(1+b_{k-2}')}{L^3 a_{k-1}} + \frac{(1+b_{k-2}')^2}{L^4 a_{k-1}^2}\right] \|r^{k-1}\|^2 + \frac{(b_{k-2}')^2}{a_{k-1}^2 L^4} \|r^{k-2}\|^2 \\ Q_6 &= 2a_{k-1}\gamma_k \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2} - \frac{2\gamma_k}{L} \|r^k\|^2 - \frac{1}{L^2} \|r^k\|^2 + \frac{1}{L^4 a_{k-1}^2} \|r^k\|^2. \end{aligned}$$

We start with bounding Q_6 . First, by Property (iv), it holds that:

$$2a_{k-1}\gamma_k \frac{\|r^k\|^2 \|p^{k-1}\|^2}{\|r^{k-1}\|^2} \ge 2a_{k-1}\gamma_k \frac{\|r^k\|^2 \|r^{k-1}\|^2}{\|r^{k-1}\|^2} = 2a_{k-1}\gamma_k \|r^k\|^2.$$

Thus, we have $Q_6 \geq \frac{1}{L^2} [2a_{k-1}\gamma_k L^2 - 2\gamma_k L - 1 + (a_{k-1}L)^{-2}] ||r^k||^2$. The coefficient in the parentheses can be shown to be larger or equal than $2\nu + \nu^{-2} - 3$ by using the same strategy as in **Case 1** for Q_4 . This yields $Q_6 \geq (2\nu + \nu^{-2} - 3)L^{-2} ||r^k||^2$. Next, recalling the definition of b'_{k-2} (see Property (x)), we obtain:

$$b_{k-2}' = \frac{a_{k-1}}{a_{k-2}} \frac{\|r^{k-1}\|^2}{\|r^{k-2}\|^2} \implies \frac{(b_{k-2}')^2}{a_{k-1}^2 L^4} \|r^{k-2}\|^2 = \frac{\|r^{k-1}\|^2}{a_{k-2}^2 L^4 \|r^{k-2}\|^2} \|r^{k-1}\|^2.$$

In addition, by Property (iv), it follows:

$$a_{k-1}^2 \|p^{k-1}\|^2 = a_{k-1}^2 \|r^{k-1}\|^4 \sum_{j=0}^{k-1} \frac{1}{\|r^j\|^2} \ge a_{k-1}^2 \|r^{k-1}\|^2 + a_{k-1}^2 \frac{\|r^{k-1}\|^2}{\|r^{k-2}\|^2} \|r^{k-1}\|^2.$$

Setting $Q_7 = a_{k-1}^2 L^2 + 6 - 4a_{k-1}L - 4(a_{k-1}L)^{-1} + (a_{k-1}L)^{-2} = (a_{k-1}L + (a_{k-1}L)^{-1} - 2)^2$ and using the previous inequalities, we can lower bound Q_5 by:

$$Q_5 \ge \left[Q_7 - \frac{4b'_{k-2}}{a_{k-1}L} + \frac{(1+b'_{k-2})^2 - 1}{a_{k-1}^2 L^2} + \left[a_{k-1}^2 L^2 + \frac{1}{a_{k-2}^2 L^2}\right] \frac{\|r^{k-1}\|^2}{\|r^{k-2}\|^2}\right] \frac{\|r^{k-1}\|^2}{L^2}.$$

Let us denote the term in parentheses by Q_8 . It suffices to show that Q_8 is nonnegative. In particular, it holds that:

$$Q_8 \ge Q_7 + \left[a_{k-1}L - \frac{1}{a_{k-2}L}\right]^2 \frac{\|r^{k-1}\|^2}{\|r^{k-2}\|^2} + \frac{2a_{k-1}}{a_{k-2}} \frac{\|r^{k-1}\|^2}{\|r^{k-2}\|^2} - \frac{4b'_{k-2}}{a_{k-1}L} + \frac{2b'_{k-2}}{a_{k-1}^2L^2} \\ \ge Q_7 + 2b'_{k-2} - \frac{4b'_{k-2}}{a_{k-1}L} + \frac{2b'_{k-2}}{a_{k-1}^2L^2} \ge \left[\nu + \nu^{-1} - 2\right]^2 + 2b'_{k-2} \left[1 - (a_{k-1}L)^{-1}\right]^2,$$

where we again used $a_{k-1}L \ge \nu$. This finally establishes (3.14), which concludes the proof of Theorem 3.14.

The previous result shows that performing two gradient steps on y^{k-1} achieves less progress in terms of the distance to the optimal solution compared to performing one gradient step on y^k . In fact, we are able to prove a similar result for CG, which is of independent interest. More precisely, CG can decrease the distance to the optimal solution no slower than the gradient method with stepsize $\frac{1}{L}$. Hence, y^k can provide more progress than \bar{y}^{k-1} . The proof is much easier and is deferred to Appendix B.

THEOREM 3.15. Let $\{y^k\}_k$ be generated by CG applied to the system $B(y-y^*) = 0$, where $B \in \mathbb{R}^{n \times n}$ is symmetric, positive definite with $||B|| \leq L$. Then, we have:

$$||y^{k+1} - y^*||^2 \le ||\bar{y}^k - y^*||^2.$$

As discussed at the beginning of this section, the sequences $\{x_R^k\}_k$ and $\{y^k\}_k$ are equivalent up to a linear transformation, i.e., it holds that $y^k = B^{\frac{1}{2}} x_R^k$. This allows to transfer our obtained results back to the CR method. We summarize our observations for CR in the following corollary.

COROLLARY 3.16. Let $B \in \mathbb{R}^{n \times n}$ be a symmetric, positive definite matrix with $||B|| \leq L$ and let $x^0 \in \mathbb{R}^n$ be given. Suppose that $\{x_R^k\}_k$ is generated by the CR method to solve the linear system $B(x - x^0) = b$. Then, we have:

$$\varphi(\bar{x}_R^k) \leq \varphi(\tilde{x}_R^{k-1}) \quad and \quad \varphi(x_R^k) \leq \varphi(\bar{x}_R^{k-1}),$$

where \bar{x}_R^k and \tilde{x}_R^k are defined in (3.9) and $\varphi(x) := \frac{1}{2}(x-x^0)^\top B(x-x^0) - b^\top (x-x^0)$.

3.6. Proof of Theorem 3.6. In this subsection, we combine our obtained results and show that AA-R locally decreases the objective function no slower than a gradient descent step with stepsize $\frac{1}{L}$ (up to a certain higher-order error term).

Throughout this section, we will work with the following choices $B = \nabla^2 f(x^0)$, $b = -\nabla f(x^0)$, and $A = B + E_m$, where E_m is defined in (3.7).

Proof of Theorem 3.6. Clearly, (3.6) holds for k = 0. Furthermore, we only need to verify (3.6) for one cycle of AA-R as all assumptions and results will also hold for subsequent cycles, since all the subsequent iterations would also belong to U by Proposition 3.5. Let $U = S_{\epsilon}$ be the neighborhood defined in Proposition 3.5. Then, for all $k \in \mathbb{N}$, we have:

$$||h(x^{k+1})|| \le (1 - (2\kappa_r)^{-1})||h(x^k)||.$$

Proposition 3.2 establishes $\kappa(H_k^{\top}H_k) \leq M_H^2$ for some $M_H > 0$ and by Lemma 3.4, we can infer $\|\hat{g}^k - x^0\| = \mathcal{O}(\|b\|)$. Due to $x^{k+1} = \hat{g}^k$, this just means $\|x^{k+1} - x^0\| = \mathcal{O}(\|b\|)$. Notice that this estimate holds for every $k = 0, 1, \ldots, m$ and therefore, it follows $M_x^m = \mathcal{O}(\|b\|)$. Furthermore, using (3.2), we obtain $\|E_m\| = \mathcal{O}(\|b\|)$. Reducing ϵ if

necessary, we may assume that $||A - B|| = ||E_m|| < \mu$, which ensures the invertibility of A as shown in the proof of Lemma 3.11. Now, let $\{x_G^k\}_k$ and $\{x_R^k\}_k$ be generated by GMRES and CR applied to the linear systems $A(x - x^0) = b$ and $B(x - x^0) = b$ with $x_G^0 = x_R^0 = x^0$, respectively. By Proposition 3.8, we have $\bar{x}_G^k = x^{k+1}$ for all $k = 0, \ldots, m$ and $\kappa((\bar{X}_G^k)^\top \bar{X}_G^k) \le M^2$ for all $k \in [m]$. Moreover, since the perturbed gradient mapping \bar{g} is exact at each x^k , $k = 0, \ldots, m$, it holds that

$$g(x^k) = \bar{g}(x^k) = \bar{g}(\bar{x}_G^{k-1}) = \tilde{x}_G^{k-1} \quad \forall \ k = 1, \dots, m.$$

In addition, we have $\|\bar{x}_G^k - x^0\| = \|x^{k+1} - x^0\| = \mathcal{O}(\|b\|)$. Reducing ϵ — if necessary — we may assume $\epsilon \leq \epsilon_{\sharp}$, where ϵ_{\sharp} was introduced in the proof of Theorem 3.12. Thus, all conditions in Theorem 3.12 are satisfied and it follows

(3.22)
$$\|\bar{x}_G^k - \bar{x}_R^k\| = \mathcal{O}(\|b\|^2)$$
 and $\|\tilde{x}_G^k - \tilde{x}_R^k\| = \mathcal{O}(\|b\|^2) \quad \forall \ k = 0, \dots, m.$

Moreover, since g is a contraction on $\mathbb{B}_r(x^*)$ and due to $||x^k - x^0|| = \mathcal{O}(||b||)$, we have $||g(x^k) - x^0|| \le ||g(x^k) - g(x^0)|| + ||g(x^0) - x^0|| = \mathcal{O}(||b||)$. Reusing the notation from Corollary 3.16, the Lipschitz continuity of the Hessian $\nabla^2 f$ then implies (3.23)

$$\begin{split} f(x^{k+1}) &= f(x^0) + \varphi(x^{k+1}) + \mathcal{O}(\|x^{k+1} - x^0\|^3) = f(x^0) + \varphi(\bar{x}_G^k) + \mathcal{O}(\|b\|^3), \\ f(g(x^k)) &= f(x^0) + \varphi(g(x^k)) + \mathcal{O}(\|g(x^k) - x^0\|^3) = f(x^0) + \varphi(\tilde{x}_G^{k-1}) + \mathcal{O}(\|b\|^3), \end{split}$$

see, e.g., [25, Lemma 4.1.1]. Since the mapping φ is quadratic, we can further write:

$$\begin{split} \varphi(\bar{x}_{G}^{k}) &= \varphi(\bar{x}_{R}^{k}) + \nabla\varphi(\bar{x}_{R}^{k})^{\top}(\bar{x}_{G}^{k} - \bar{x}_{R}^{k}) + \frac{1}{2}(\bar{x}_{G}^{k} - \bar{x}_{R}^{k})^{\top}B(\bar{x}_{G}^{k} - \bar{x}_{R}^{k}), \\ \varphi(\tilde{x}_{G}^{k-1}) &= \varphi(\tilde{x}_{R}^{k-1}) + \nabla\varphi(\tilde{x}_{R}^{k-1})^{\top}(\tilde{x}_{G}^{k-1} - \tilde{x}_{R}^{k-1}) + \frac{1}{2}(\tilde{x}_{G}^{k-1} - \tilde{x}_{R}^{k-1})^{\top}B(\tilde{x}_{G}^{k-1} - \tilde{x}_{R}^{k-1}). \end{split}$$

Next, applying Lemma 3.11 for the case A = B, it holds that:

$$\|\nabla\varphi(\bar{x}_R^k)\| = \|B(\bar{x}_R^k - x^0) - b\| \le \|B(x_R^k - x^0) - b\| \le \|B(x^0 - x^0) - b\| = \|b\|,$$

where we used Proposition 3.10 in the last step. Similarly, we can show $\|\nabla \varphi(\tilde{x}_R^{k-1})\| \leq \|b\|$. Thus, combining (3.22) and the representations of $\varphi(\bar{x}_G^k)$ and $\varphi(\tilde{x}_G^{k-1})$, we obtain

$$\begin{aligned} |\varphi(\bar{x}_{G}^{k}) - \varphi(\bar{x}_{R}^{k})| &\leq \|\nabla\varphi(\bar{x}_{R}^{k})\| \|\bar{x}_{G}^{k} - \bar{x}_{R}^{k}\| + \frac{L}{2} \|\bar{x}_{G}^{k} - \bar{x}_{R}^{k}\|^{2} = \mathcal{O}(\|b\|^{3}), \\ |\varphi(\tilde{x}_{G}^{k-1}) - \varphi(\tilde{x}_{R}^{k-1})| &\leq \|\nabla\varphi(\tilde{x}_{R}^{k-1})\| \|\tilde{x}_{G}^{k-1} - \tilde{x}_{R}^{k-1}\| + \frac{L}{2} \|\tilde{x}_{G}^{k-1} - \tilde{x}_{R}^{k-1}\|^{2} = \mathcal{O}(\|b\|^{3}), \end{aligned}$$

Using these estimates in (3.23), we can infer

$$f(x^{k+1}) = f(x^0) + \varphi(\bar{x}_R^k) + \mathcal{O}(\|b\|^3), \quad f(g(x^k)) = f(x^0) + \varphi(\bar{x}_R^{k-1}) + \mathcal{O}(\|b\|^3).$$

The conclusion then follows immediately from Corollary 3.16.

4. A Function Value-Based Globalization for AA-R. Based on the local descent properties established in the last section, we now propose a globalization mechanism for AA-R. We prove global convergence and provide simple global-to-local transition results for the globalized AA-R algorithm. To the best of our knowledge, this is the first function value-based globalization of AA-R that achieves both global and local convergence. Previously, only heuristic strategies seem to be available, see [31, 27, 42].

The full procedure is presented in Algorithm 4.1. Our core idea is to check whether the AA step x_{AA}^k satisfies a sufficient decrease condition

(4.1)
$$f(x_{\mathsf{AA}}^k) \le f(x^k) - \gamma \|\nabla f(x^k)\|^2 + \min\{c_1 \|\nabla f(x^{k-\hat{m}})\|^{\nu}, c_2 \|\nabla f(x^{k-\hat{m}})\|^2, c_3\},$$

Algorithm 4.1 A Globalized AA Scheme with Restarting

1: Choose an initial point $x^0 \in \mathbb{R}^n$, the memory parameter m, and constants $\gamma, \nu, c_1, c_2, c_3 > 0.$ Set $\hat{m} = 0.$ 2: for $k = 0, 1, \dots$ do 3: Set $\hat{m} = \text{mod}(k, m+1)$. if $\hat{m} = 0$ then 4: Set $x^{k+1} = g(x^k)$. 5: 6: else Calculate the coefficient α^k based on the sequence $\{h(x^k), \ldots, h(x^{k-\hat{m}})\}$ by 7: solving (1.3) and set $x_{\mathsf{A}\mathsf{A}}^k = g^{k-\hat{m}} + G_k \alpha^k$. if $f(x_{\mathsf{A}\mathsf{A}}^k) > f(x^k) - \gamma \|\nabla f(x^k)\|^2 + \min\{c_1 \|\nabla f(x^{k-\hat{m}})\|^\nu, c_2 \|\nabla f(x^{k-\hat{m}})\|^2, c_3\}$ 8: then Set $x^{k+1} = q(x^k)$. 9: else 10: Set $x^{k+1} = x_{AA}^k$. 11: end if 12:end if 13:14: end for

where γ , ν , and c_i , i = 1, 2, 3, are given parameters. We accept the AA step as new iterate $x^{k+1} = x_{AA}^k$ if condition (4.1) holds. Otherwise, a gradient step $x^{k+1} = g(x^k)$ is performed (which ensures decrease of the objective function values). We summarize several basic convergence properties of Algorithm 4.1 in the following theorem.

THEOREM 4.1. Suppose that (A.1) holds and let f be bounded from below. Let the sequence $\{x^k\}_k$ be generated by Algorithm 4.1 with $\gamma, c_1, c_3 > 0, c_2 < \frac{1}{2mL}$, and $\nu \in (2,3)$. Then, we have

$$\sum_{k=0}^{\infty} \|\nabla f(x^k)\|^2 < \infty \quad and \quad \lim_{k \to \infty} \|\nabla f(x^k)\| = 0.$$

In addition, if $\gamma < \frac{1}{2L}$ and if the conditions (A.2)–(A.4) are satisfied with x^* being an accumulation point of $\{x^{k(m+1)}\}_k$, then we have $x^k \to x^*$ and all AA steps will be eventually accepted, i.e., Algorithm 4.1 locally turns into Algorithm 2.1.

Proof. Notice that the k-th cycle starts at iteration (k-1)(m+1) and ends at iteration k(m+1) (with $x^{k(m+1)}$ serving as initial point for the next cycle). In order to keep the notation simple, we concentrate on the first cycle. Since the first iteration within each cycle is a gradient descent step, i.e., $x^1 = g(x^0)$, we can deduce $f(x^1) \leq f(x^0) - \frac{1}{2L} \|\nabla f(x^0)\|^2$. For all $k = 1, \ldots, m$, the iterate x^{k+1} either results from a gradient descent step or an AA step satisfying the acceptance criterion:

$$f(x^{k+1}) \le f(x^k) - \gamma \|\nabla f(x^k)\|^2 + c_2 \|\nabla f(x^0)\|^2.$$

Hence, each update k = 1, ..., m satisfies $f(x^{k+1}) \leq f(x^k) - \min\{\frac{1}{2L}, \gamma\} \|\nabla f(x^k)\|^2 + c_2 \|\nabla f(x^0)\|^2$. Summing these estimates from 1 to m, we obtain

$$f(x^{m+1}) \le f(x^0) - \min\left\{\frac{1}{2L}, \gamma\right\} \sum_{k=1}^m \|\nabla f(x^k)\|^2 - \left[\frac{1}{2L} - mc_2\right] \|\nabla f(x^0)\|^2$$

Defining $\sigma := \min\{\frac{1}{2L}, \gamma, \frac{1}{2L} - mc_2\} > 0$, this result holds for every cycle of Algorithm 4.1, i.e., we have

$$f(x^{(k+1)(m+1)}) \le f(x^{k(m+1)}) - \sigma \sum_{i=k(m+1)}^{k(m+1)+m} \|\nabla f(x^i)\|^2 \quad \forall \ k \in \mathbb{N}.$$

Summing this inequality for all $k \in \mathbb{N}$ and noticing that f is bounded from below, it follows $\sum_{i=0}^{\infty} \|\nabla f(x^i)\|^2 < \infty$ which readily implies $\|\nabla f(x^i)\| \to 0$. Next, let x^* be an accumulation point of $\{x^{k(m+1)}\}_k$ satisfying (A.2)–(A.4). By Theorem 3.6, there is a neighborhood U of x^* such that if $y^0 \in U$, then the sequence $\{y^k\}_k$ generated by Algorithm 2.1 satisfies

$$f(y^{k+1}) \le f(g(y^k)) + \mathcal{O}(\|\nabla f(y^{k-\hat{m}})\|^3) \le f(y^k) - \frac{1}{2L} \|\nabla f(y^k)\|^2 + \mathcal{O}(\|\nabla f(y^{k-\hat{m}})\|^3)$$

Thus, by shrinking U if necessary and using $\gamma < \frac{1}{2L}$, we can assume

(4.2)
$$f(y^{k+1}) \le f(y^k) - \gamma \|\nabla f(y^k)\|^2 + c_1 \|\nabla f(y^{k-\hat{m}})\|^{\nu} \quad \forall \ k$$

Since x^* is an accumulation point of $\{x^{k(m+1)}\}_k$, there exists s with $x^{s(m+1)} \in U$. We now set $y^k := x^{k+s(m+1)}$. Due to $y^0 \in U$, $\|\nabla f(x^i)\| \to 0$, and since the conditions (A.1)–(A.4) are satisfied, we can inductively infer that every AA step fulfills (4.2) and is accepted as new iterate, i.e., we have $y^{k+1} = x^{s(m+1)+k+1} = x^{s(m+1)+k}_{AA}$, $k \ge 1$. Convergence of $\{x^k\}_k$ then follows from Proposition 3.5 and (A.2).

5. Numerical Experiments. In this section, we conduct preliminary numerical experiments to illustrate the performance and convergence behavior of AA-R and to empirically verify the descent properties of Algorithm 4.1^{1} .

5.1. Nonconvex Classification. We consider two nonconvex classification problems, namely a nonlinear least-squares problem and a student's-t problem. A detailed introduction of the tested problems is deferred to the subsequent paragraphs. We will compare Algorithm 4.1 with four different methods:

- (1) The gradient descent method (GD) with fixed step size $\frac{1}{L}$. This is the original Picard iteration (1.2) and serves as a baseline.
- (2) Pure AA with and without restarting [47]. Pure AA does not use any globalization strategy, i.e., in each step, we perform an AA iteration.
- (3) AA with residual-based globalization. Our implementation is based on A2DR [14, Algorithm 3] and we consider two variants with and without restarting.
 A2DR uses a residual-based acceptance mechanism and we apply the method with the default parameters as suggested in [14].
- (4) L-BFGS. We implement L-BFGS with Wolfe conditions as in [26, Algorithm 7.5]. The line-search parameter is set to 10⁻⁴ and the parameter in Wolfe's condition is set to 0.9 as suggested in [26]. The maximum number of line-search iterations is set to 1,000.

We note that the line search procedure in L-BFGS can contain many function and gradient evaluations per iteration. Therefore, it is improper to give comparisons solely based on the number of iterations. In our plots, the x-axis is typically set as the number of oracle calls, which appears to be a more appropriate and fair measure when comparing AA algorithms and L-BFGS. Specifically, the computation of each function value is counted as one oracle call and every gradient evaluation contributes as an additional oracle call. The y-axis is set as $(f(x^k) - f^*)/\max\{f^*, 1\}$ or $\|\nabla f(x^k)\|$, respectively, where f^* denotes the best objective function value among all algorithms over the maximum oracle calls. In the figures, we will add a special mark " \star " once the current AA step is rejected and a gradient step is performed in Algorithm 4.1.

We continue with the description of the utilized training datasets and several universal implementational details. We use the CIFAR10 dataset [21], which contains

¹Code available under https://github.com/yangliu-op/AndersonAcceleration



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FIG. 1. Relative error $(f(x^k) - f^*)/\max\{f^*, 1\}$ vs. Oracle calls for the student's t(ST) and nonlinear least-squares (NLS) problem and the datasets CIFAR10 and STL10. The plots in each column are generated using the identical initial point $x^0 \sim N^d(0, 1)$. In each row, the different AA methods and L-BFGS are executed using the same memory parameter $m \in \{5, 10, 15, 20, 30\}$. The x-axes of each plot have the same scaling 0-3,000 (as shown in the bottom row).

60,000 images with 32×32 colored pixels and the STL10 dataset [8], which consists of 5,000 colored images of size 96×96 . Given that both datasets contain 10 classes, we split the data into even and odd classes to allow binary classification. We use $\{u_i, v_i\}_{i=1}^n$ to denote the training samples, where $u_i \in \mathbb{R}^d$ represents the training image and $v_i \in \{0,1\}$ is the associated label. We set $U = \{u_1, u_2, \dots, u_n\}^\top \in \mathbb{R}^{n \times d}$. We terminate the algorithms once $\|\nabla f(x^k)\| \leq 10^{-7}$ or the number of oracle calls exceeds 3,000. The memory parameter m is chosen from $m \in \{5, 10, 15, 20, 30\}$ for all AA-based methods and L-BFGS. The regularization parameter λ in (5.1) and (5.2) is set to 10^{-2} for CIFAR10 and to 10^{-1} for STL10. The initial points $x^0 \sim \mathcal{N}^d(0,1)$ are generated following a normal distribution. Finally, in Algorithm 4.1, we utilize the default parameters: $\gamma = \frac{0.01}{2L}$, $c_1 = c_3 = 1$, $c_2 = \frac{0.99}{2mL}$, and $\nu = 2.1$. Let us briefly motivate this default choice. In order to promote acceptance of AA steps (and to ensure potential acceleration), the descent condition (4.1) should not be too strict. This can be achieved when γ is small and when the min-term in (4.1) is large. Hence, we set γ fairly small, c_2 close to the theoretical threshold, and ν close to 2. Furthermore, we have found that the simple choice $c_1 = c_3 = 1$ works well enforcing sufficient progress during the first iterations. An additional ablation study for c_1 , c_2 , c_3 , and γ is



FIG. 2. $\|\nabla f(x^k)\|$ vs. Oracle calls for the student's t (ST) and nonlinear least-squares (NLS) problem and the datasets CIFAR10 and STL10. The plots in each column are generated using the identical initial point $x^0 \sim \mathcal{N}^d(0, 1)$. In each row, the different AA methods and L-BFGS are executed using the same memory parameter $m \in \{5, 10, 15, 20, 30\}$. The x-axes of each plot have the same scaling 0-3,000 (as shown in the bottom row).

discussed in subsection 5.3. We use the LSQR method [29] to solve the AA subproblem (1.3) and to compute $\alpha^k = -H_k^{\dagger} h^{k-\hat{m}} = -(H_k^{\top} H_k)^{-1} H_k^{\top} h^{k-\hat{m}}$. (Here, H_k^{\dagger} represents the Moore-Penrose pseudo-inverse of H_k). The termination condition of LSQR is set to $\|H_k^{\top}(H_k \alpha + h^{k-\hat{m}})\| < 10^{-16}$.

Next, we present the classification models used in our numerical comparison:

• Student's-t Loss with ℓ_2 -Regularization (ST). We consider the following classification problem with student's-t loss, [3, 2],

(5.1)
$$f(x) = \frac{1}{n} \sum_{i=1}^{n} \log\left(1 + (u_i^{\top} x - v_i)^2 / \mu\right) + \frac{\lambda}{2} \|x\|^2$$

The Lipschitz constant of ∇f is given by $L = \frac{2}{\mu n} ||U||^2 + \lambda$ and we set $\mu = 20$. • Nonlinear Least-Squares Problem with ℓ_2 -Regularization (NLS). As a second example, we consider a nonlinear least-squares problem, [50],

(5.2)
$$f(x) = \frac{1}{n} \sum_{i=1}^{n} (\psi(u_i^{\top} x) - v_i)^2 + \frac{\lambda}{2} ||x||^2,$$

where $\psi(z) = 1/(1 + e^{-z})$ is the sigmoid function. The Lipschitz constant of

 ∇f is given by $L = \frac{1}{6n} ||U||^2 + \lambda.$

The initial points for all algorithms and $m \in \{5, 10, 15, 20, 30\}$ are identical for each tested dataset and classification model. Figures 1 and 2 illustrate that AA-R with function value-based globalization (4.1) is a competitive solver. Specifically, Algorithm 4.1 requires the least amount of oracle calls to satisfy the stopping criterion when $m \in \{10, 15, 20, 30\}$. However, in the low memory case m = 5, Algorithm 4.1 and the restarting strategy seem less effective (especially for the nonlinear least-squares problem). The plots in Figures 1–2 generally underline the potential of function valueand descent-based globalization mechanisms for AA schemes. Rejections predominantly occur in the early stage of the iterative process to ensure global convergence and progress of Algorithm 4.1. In addition, transition to a pure AA-R phase with accelerated convergence is maintained — as indicated by our theoretical results.

As the applications tested in this section are nonconvex, we have recorded the smallest eigenvalues of the respective Hessians in the last iterations of AA-R for each of the problems and datasets. We have observed that that these eigenvalues are all approximately equal to $\lambda > 0$ and hence, assumption (A.2) is locally satisfied.

5.2. Descent Properties. In Figure 3, we plot the measure

$$\rho_k := \max\{f(x_{\mathsf{AA}}^k) - f(g(x^k)), 0\} / \|\nabla f(x^{k-\hat{m}})\|^3$$

versus the number of iterations k to further visualize and verify the descent properties derived in Theorem 3.6. If the AA step achieves descent, $f(x_{AA}^k) \leq f(g(x^k))$, then we have $\rho_k = 0$ and we locally expect $\rho_k \approx 0$ for all k sufficiently large. The special marks " \star " in Figure 3 again indicate that an AA step did not pass the descent condition (4.1). Figure 3 illustrates that ρ_k indeed stays zero eventually and that no AA steps are rejected locally. This observation is slightly less pronounced on CIFAR10 when m = 30.

5.3. Ablation Study. Finally, we provide an additional ablation study for the parameters c_1 , c_2 , c_3 , and γ used in Algorithm 4.1 and in the definition of the descent condition (4.1). Based on Theorem 4.1, c_1 , c_2 , c_3 , and γ need to satisfy the conditions $0 < \gamma < \frac{1}{2L}$, c_1 , $c_3 > 0$, and $0 < c_2 < \frac{1}{2mL}$. We compare our default choice with the following extreme sets of parameters:

(5.3)
$$\gamma = \frac{1}{2L}, c_1 = c_2 = c_3 = 0, \text{ and } \gamma = 0, c_1 = c_3 = 10^{10}, c_2 = \frac{1}{2mL}.$$

These two choices correspond to highly strict and loose acceptance criteria for the AA step x_{AA}^k . Since $\nu \in (2,3)$ has only limited influence, we omit an explicit ablation study for ν and use the default value $\nu = 2.1$. Figure 4 demonstrates that Algorithm 4.1 is robust with respect to the choice of c_1, c_2, c_3 , and γ . In particular, performance is only affected marginally when using the more extreme parameters (5.3).

6. Conclusion. In this work, we study descent properties of an Anderson accelerated gradient method with restarting. We first show that the iterates generated by AA-R are equivalent to the iterates generated by GMRES after an additional gradient step within each restarting cycle. Based on the symmetry of the underlying system matrix, we then analyze the error between the iterates generated by GMRES and CR and verify that this error is controllable and related to some higher-order perturbation terms. After connecting CR and CG, the desired descent property for AA-R can be expressed in terms of distances to the respective optimal solution for the iterates generated by CG. We establish such a convergence result for CG utilizing classical techniques. Combining these different observations, we prove that AA-R can decrease



FIG. 3. Plot of $\rho_k = \max\{f(x_{AA}^k) - f(g(x^k)), 0\}/\|\nabla f(x^{k-\hat{m}})\|^3$ vs. Oracle calls for Algorithm 4.1. The marks " \star " indicate rejected AA steps. After the last rejected AA step (red dashed vertical line), ρ_k mostly stays 0, which verifies and illustrates Theorem 3.6. The x-axes of each plot in the rows $m \in \{10, 15, 20, 30\}$ have the same scaling 0–700. For m = 5, the scaling is 0–3,000.

the objective function f locally. These novel findings can be used in the design of effective, function value-based globalization mechanisms for AA-R approaches. We propose one such possible AA-R globalization and conduct numerical experiments on two large-scale learning problems that illustrate our theoretical results.

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Appendix A. Proof of Proposition 3.3.

Proof. We show that Proposition 3.3 is a direct application of [33, Theorem 5.1]. Due to (2.1), the constant κ_g in [33] reduces to $1 - \frac{1}{\kappa_r}$ and we have $\theta_k \leq 1$ and $\beta_k = 1$. Moreover, all the points of interest lie in $\mathbb{B}_r(x^*)$, so all the expansions of the residuals in [33, Section 3] are legitimate. The core estimate (5.18) in [33, Theorem 5.1] then reduces to (3.4). The proof is complete if all assumptions in [33, Theorem 5.1] hold.

Using $x^i \in \mathbb{B}_r(x^*)$, $i = k - \hat{m}, \ldots, k$ and (2.1), it follows

$$\|h^{i} - h^{i-1}\| \ge \|x^{i} - x^{i-1}\| - \|g(x^{i}) - g(x^{i-1})\| \ge \kappa_{r}^{-1}\|x^{i} - x^{i-1}\| \quad \forall i = k - \hat{m} + 1, \dots, k.$$

This is exactly Assumption 2.3 in [33] (see also [33, Remark 2.1]). Next, we verify the sufficient linear independence condition introduced in [33, Lemma 5.2]. Let us



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FIG. 4. Ablation study of Algorithm 4.1 using different c_1 , c_2 , c_3 , and γ . Each plot depicts $(f(x^k) - f^*)/\max\{f^*, 1\}$ vs. Oracle calls for three different runs of Algorithm 4.1. We compare the default parameters with the extreme choices $\gamma = \frac{1}{2L}$, $c_1 = c_2 = c_3 = 0$ and $\gamma = 0$, $c_1 = c_3 = 10^{10}$, $c_2 = \frac{1}{2mL}$. The x-axes of each plot in the rows $m \in \{10, 15, 20, 30\}$ have the same scaling 0–700. For m = 5, the scaling is 0–3,000.

define $\tilde{H}_k = [h^k - h^{k-1}, \ldots, h^{k-\hat{m}+1} - h^{k-\hat{m}}] =: [v^1, \ldots, v^{\hat{m}}]$. We note that there is a fixed nonsingular matrix $P \in \mathbb{R}^{\hat{m} \times \hat{m}}$ such that $\tilde{H}_k = H_k P$ and $\kappa(\tilde{H}_k^\top \tilde{H}_k) \leq \kappa(H_k^\top H_k)\kappa(P^\top P)$. Therefore, by Proposition 3.2 and using $x^i \in U_1$, $i = k - \hat{m}, \ldots, k$, (A.4) implies that the condition number of $\tilde{H}_k^\top \tilde{H}_k$ is bounded by some \tilde{M}^2 . Let $\mathcal{V}_i = \operatorname{span}\{v^1, \ldots, v^i\}$ denote the linear subspace spanned by the first i columns of \tilde{H}_k and let $\tilde{H}_k = Q_k R_k$ be the QR decomposition of \tilde{H}_k . We then have $\kappa(R_k^\top R_k) = \kappa(\tilde{H}_k^\top \tilde{H}_k) \leq \tilde{M}^2$. Furthermore, let $\{r_{ii}\}_{1 \le i \le \hat{m}}$ denote the diagonal entries of R_k . By [33, Proposition 5.2], it follows $r_{11}^2 = \|v_1\|^2$ and $r_{ii}^2 = \|v_i\|^2 \sin^2(v_i, \mathcal{V}_{i-1})$ for all $2 \le i \le \hat{m}$. Since R_k is upper triangular, the diagonal entries r_{ii} , $i = 1, \ldots, \hat{m}$, are exactly the eigenvalues of R_k . Consequently, we obtain

$$(\|v_i\|^2 / \|v_1\|^2) \cdot \sin^2(v_i, \mathcal{V}_{i-1}) = r_{ii}^2 / r_{11}^2 \ge \sigma_{\min}(R_k)^2 / \sigma_{\max}(R_k)^2 \ge 1/\tilde{M}^2.$$

In addition, we have $||v_i||^2 / ||v_1||^2 \le \sigma_{\max}(\tilde{H}_k)^2 / \sigma_{\min}(\tilde{H}_k)^2 \le \tilde{M}^2$. Combining these inequalities, this yields $|\sin(v_i, \mathcal{V}_{i-1})| \ge \tilde{M}^{-2}$ which verifies the last remaining assumption in [33, Lemma 5.2 and Theorem 5.1]. This concludes the proof.

Appendix B. Proof of Theorem 3.15.

Proof. Similar to (3.15) and utilizing the projection $y^{(k+1)}$, we have:

$$\begin{split} \|\bar{y}^{k} - y^{*}\|^{2} - \|y^{k+1} - y^{*}\| &= \|\bar{y}^{k} - y^{(k+1)}\|^{2} - \|y^{k+1} - y^{(k+1)}\|^{2} \\ &= \|\bar{y}^{k} - y^{k+1}\|^{2} + 2\langle \bar{y}^{k} - y^{k+1}, y^{k+1} - y^{(k+1)}\rangle \\ &= \|a_{k}p^{k} - L^{-1}r^{k}\|^{2} + 2\langle a_{k}p^{k} - L^{-1}r^{k}, \gamma_{k}p^{k}\rangle \\ &= a_{k}^{2}\|p^{k}\|^{2} - 2a_{k}L^{-1}\langle p^{k}, r^{k}\rangle + L^{-2}\|r^{k}\|^{2} + 2a_{k}\gamma_{k}\|p^{k}\|^{2} - 2\gamma_{k}L^{-1}\langle p^{k}, r^{k}\rangle \\ &= (a_{k}^{2} + 2a_{k}\gamma_{k})\|p^{k}\|^{2} + \frac{1}{L}[L^{-1} - 2\gamma_{k} - 2a_{k}]\|r^{k}\|^{2} \\ &\geq \left[a_{k}^{2} + 2a_{k}\gamma_{k} - 2\gamma_{k}L^{-1} - 2a_{k}L^{-1} + L^{-2}\right]\|r^{k}\|^{2} \\ &= \left[2\gamma_{k}(a_{k} - L^{-1}) + (a_{k} - L^{-1})^{2}\right]\|r^{k}\|^{2} \geq 0, \end{split}$$

where we have used Property (iii) to show that $\langle p^k, r^k \rangle = ||r^k||^2$, Property (iv) to show that $||p^k||^2 \ge ||r^k||^2$, and Property (ix) to show that $\gamma_k \ge a_k \ge 1/L$.

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