Nonlinear conjugate gradient for smooth convex functions*

Sahar Karimi[†] Stephen Vavasis[‡]

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Abstract

The method of nonlinear conjugate gradients (NCG) is widely used in practice for unconstrained optimization, but it satisfies weak complexity bounds at best when applied to smooth convex functions. In contrast, Nesterov's accelerated gradient (AG) method is optimal up to constant factors for this class.

However, when specialized to quadratic function, conjugate gradient is optimal in a strong sense among function-gradient methods. Therefore, there is seemingly a gap in the menu of available algorithms: NCG, the optimal algorithm for quadratic functions that also exhibits good practical performance for general functions, has poor complexity bounds compared to AG.

We propose an NCG method called C+AG ("conjugate plus accelerated gradient") to close this gap, that is, it is optimal for quadratic functions and still satisfies the best possible complexity bound for more general smooth convex functions. It takes conjugate gradient steps until insufficient progress is made, at which time it switches to accelerated gradient steps, and later retries conjugate gradient. The proposed method has the following theoretical properties: (i) It is identical to linear conjugate gradient (and hence terminates finitely) if the objective function is quadratic; (ii) Its running-time bound is $O(\epsilon^{-1/2})$ gradient evaluations for an Lsmooth convex function, where ϵ is the desired residual reduction, (iii) Its runningtime bound is $O(\sqrt{L/\ell} \ln(1/\epsilon))$ if the function is both L-smooth and ℓ -strongly convex. We also conjecture and outline a proof that a variant of the method has the property: (iv) It is n-step quadratically convergent for a function whose second derivative is smooth and invertible at the optimizer. Note that the bounds in (ii) and (iii) match AG and are the best possible, i.e., they match lower bounds up to constant factors for the classes of functions under consideration. On the other hand, (i) and (iv) match NCG.

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[†]Department of Combinatorics & Optimization, University of Waterloo, 200 University Ave. W., Waterloo, ON, N2L 3G1, Canada, sahar.karimi@gmail.com.

[‡]Department of Combinatorics & Optimization, University of Waterloo, 200 University Ave. W., Waterloo, ON, N2L 3G1, Canada, vavasis@uwaterloo.ca.

In computational tests, the function-gradient evaluation count for the C+AG method typically behaves as whichever is better of AG or classical NCG. In some test cases it outperforms both.

1 First-order methods for smooth convex functions

The problem under consideration is minimizing an unconstrained L-smooth convex function $f: \mathbb{R}^n \to \mathbb{R}$. Recall that a convex function is L-smooth if it is differentiable and for all $x, y \in \mathbb{R}^n$,

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) - \nabla f(\boldsymbol{x})^{T} (\boldsymbol{y} - \boldsymbol{x}) \le L \|\boldsymbol{x} - \boldsymbol{y}\|^{2} / 2.$$
(1)

Note that convexity implies that the quantity on the left-hand side of this inequality is nonnegative. We will also sometimes consider ℓ -strongly convex functions, which are defined to be those functions satisfying

$$f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) \ge \ell ||\mathbf{x} - \mathbf{y}||^2 / 2$$
(2)

for all $x, y \in \mathbb{R}^n$ for some modulus $\ell \geq 0$. (This definition presumes differentiability. The class of strongly convex functions includes nondifferentiable functions as well, but those functions are not smooth and are therefore not relevant to this paper.) Note that $\ell = 0$ means simply that f is differentiable and convex.

Nonlinear conjugate gradient (NCG) [21] is perhaps the most widely used first-order method for unconstrained optimization. It is an extension of linear conjugate gradient (LCG) introduced by Hestenes and Stiefel [13] to minimize convex quadratic functions. The smoothness modulus L for a quadratic function $f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}/2 - \mathbf{b}^T \mathbf{x}$, where $A \in \mathbb{R}^{n \times n}$ is positive semidefinite, is the maximum eigenvalue of A. LCG is optimal for quadratic functions in a strong sense that $f(\mathbf{x}_k)$, where k is the kth iterate, is minimized over all choices of \mathbf{x}_k lying in the kth Krylov space leading to the estimate of $k = O(\ln(1/\epsilon)\sqrt{L/\ell})$ iterations to reduce the residual of f by a factor ϵ .

Stated precisely, Daniel [9, Theorem 1.2.2] proved the following bound for the kth iteration of LCG:

$$f(\boldsymbol{x}_k) - f^* \le 4 \left(\frac{1 - \sqrt{\ell/L}}{1 + \sqrt{\ell/L}} \right)^{2k} (f(\boldsymbol{x}_0) - f^*).$$
 (3)

Here and in the remainder of the paper, f^* stands for $\min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x})$ and is assumed to be attained. Therefore, if we define the residual reduction

$$\epsilon_1 := \frac{f(\boldsymbol{x}_k) - f^*}{f(\boldsymbol{x}_0) - f^*},$$

then a rearrangement and application of simple bounds in (3) shows that ϵ_1 reduction is achieved after $k = \ln(4/\epsilon_1) \cdot \sqrt{L/\ell}/2$ iterations.

However, if the class of problems is enlarged to include all smooth, strongly convex functions, then NCG fails to satisfy this complexity bound and could perform even worse

than steepest descent as shown by Nemirovsky and Yudin [18]. Nonetheless, in practice, nonlinear conjugate gradient is difficult to beat even by algorithms with better theoretical guarantees, as observed in our experiments and by others, e.g., Carmon et al. [4].

Several first-order methods have been proposed for smooth strongly convex functions that achieve the running time $O(\ln(1/\epsilon)\sqrt{L/\ell})$ including Nemirovsky and Yudin's [18] method, which requires solution of a two-dimensional subproblem on each iteration, Nesterov's accelerated gradient (AG) [19], and Geometric Descent (GD) [2]. In the case of GD, the bound is on iterations rather than gradient evaluations since each iteration requires additional gradient evaluations for the line search. It is known that $\Omega(\ln(1/\epsilon)\sqrt{L/\ell})$ gradient evaluations are required to reduce the objective function residual by a factor of ϵ ; see, e.g., the book of Nesterov [20] for a discussion of the lower bound result. Since the algorithms mentioned in this paragraph match the lower bound, these algorithms are optimal up to a constant factor. In the case of smooth convex (not strongly convex) functions, AG requires $O(\epsilon^{-1/2})$ iterations.

The precise bound for accelerated gradient for strongly convex functions is stated below in (14), and this bound can be rearranged and estimated as follows. Define the residual reduction

$$\epsilon_2 := rac{f({m x}^k) - f^*}{L\|{m x}_0 - {m x}^*\|^2}.$$

This reduction can be attained after no more than $k = \ln(1/\epsilon_2) \cdot \sqrt{L/\ell}$ iterations.

A technical issue in comparing the bounds is the different definitions of ϵ_1 and ϵ_2 . A standard result of extremal eigenvalues states that

$$\ell \| \boldsymbol{x}_0 - \boldsymbol{x}^* \|^2 / 2 \le f(\boldsymbol{x}_0) - f^* \le L \| \boldsymbol{x}_0 - \boldsymbol{x}^* \|^2 / 2.$$

Therefore, it follows that $\epsilon_2 \leq 2\epsilon_1 \leq (L/\ell)\epsilon_2$. Thus, ϵ_1 tightly controls ϵ_2 , whereas ϵ_2 only loosely controls ϵ_1 , and therefore, the LCG bound is slightly better than the corresponding AG bound in this technical sense.

In practice, conjugate gradient for quadratic functions is typically superior to AG applied to quadratic functions. The reason appears to be not so much the technical reason mentioned in the previous paragraph but the fact that LCG is optimal in a stronger sense than AG: the iterate \boldsymbol{x}_k is the true minimizer of $f(\boldsymbol{x})$ over the kth Krylov space, which is defined to be $\{\boldsymbol{b}, A\boldsymbol{b}, \dots, A^{k-1}\boldsymbol{b}\}$ assuming $\boldsymbol{x}_0 = \boldsymbol{0}$. For quadratic problems in which the eigenvalues lie in a small number of clusters, one expects convergence much faster than $O(\ln(1/\epsilon)\sqrt{L/\ell})$. But even in the case of spread-out eigenvalues, conjugate gradient often bests accelerated gradient. Table 1 shows the results for these algorithms for three 1000×1000 matrices:

$$A_1 = \operatorname{Diag}(\underbrace{1, \dots, 1}_{500}, \underbrace{1000, \dots, 1000}_{500}),$$

$$A_2 = \operatorname{Diag}(\underbrace{1, \dots, 1}_{250}, \underbrace{500, \dots, 500}_{250}, \underbrace{1000, \dots, 1000}_{500}),$$

$$A_3 = \operatorname{Diag}(1, 4, 9, \dots, 1000^2),$$

Table 1: Minimization of $f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x} / 2 - \mathbf{b}^T \mathbf{x}$ for diagonal matrices A_1, A_2, A_3 described in the text with $\mathbf{b}^T = [\sin 1, \sin 2, \dots, \sin 1000]$. Tolerance is $\|\nabla f(\mathbf{x})\| \le 10^{-8}$

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	LCG	C+AG	NCG	AG		
A_1 : # iterations	2	3	2	9167		
A_1 : # function-gradient evaluations	2	27	5	18357		
A_2 : # iterations	3	4	3	10267		
A_2 : # function-gradient evaluations	3	30	7	20557		
A_3 : # iterations	1509	1512	1515	$> 10^6$		
A_3 : # function-gradient evaluations	1509	3065	3036	$> 10^6$		

two of which have clustered eigenvalues, and the third has spread-out eigenvalues.

Note that the three conjugate gradient methods require roughly the same number of iterations, all much less than AG. The function evaluations are: 1 per LCG iteration (i.e., a single matrix-vector multiplication), 2 per C+AG iteration, approximately 2 per NCG iteration, and 1 per AG iteration. The requirement for more than one function evaluation per NCG iteration stems from the need to select a step-size. We return to this point below. Table 1 shows results for the adaptive versions of C+AG and AG for the case that L is not known a priori, discussed in Section 6. Thus, further function-gradient evaluations are needed to estimate L, and the number of function-gradient evaluations is increased accordingly. The reader will note from Table 1 that C+AG required only 2 iterations for A_2 but 27 function evaluations due to the overhead of initially estimating L, and a similar pattern is noted for A_3 . The adaptive estimation doubles the function-gradient evaluations for AG from 1 to 2 per iteration.

In the previous paragraph and for the remainder of this paper, we speak of a "function-gradient evaluation", which means, for a given x, the simultaneous evaluation of f(x) and $\nabla f(x)$. We regard function-gradient evaluation as the atom of work. This metric may be inaccurate in the setting that f(x) can be evaluated much more efficiently than $\nabla f(x)$ for an algorithm that separately uses f and ∇f . However, in most applications evaluating $f, \nabla f$ together is not much more expensive than evaluating either separately. Theoretically, gradient evaluation is never more than a constant factor larger than function evaluation due to the existence of reverse-mode automatic differentiation; see, e.g., [21].

It is also known that NCG is fast for functions that are nearly quadratic. In particular, a classic result of Cohen [5] shows that NCG exhibits *n*-step quadratic convergence near the minimizer provided that the objective function is nearly quadratic and strongly convex in this neighborhood.

Thus, there is seemingly a gap in the menu of available algorithms because NCG, though optimal for quadratic functions and fast for nearly quadratic functions, is not able to achieve reasonable complexity bounds for the larger class of smooth, strongly convex functions. On the other hand, the methods with the good complexity bounds for this class are all suboptimal for quadratic functions.

We propose C+AG to close this gap. The method is based on the following ideas:

- 1. A line-search for NCG described in Section 2 is used that is exact for quadratic functions but could be poor for general functions. Failure of the line-search is caught by the progress measure described in the next item.
- 2. A progress measure described in Section 3 for nonlinear conjugate gradient based on Nesterov's estimate sequence is checked. The progress measure is inexpensive to evaluate on every iteration.
- 3. Restarting in the traditional sense of NCG (i.e., an occasional steepest descent step) is used, as described in Section 4
- 4. On iterations when insufficient progress is made, C+AG switches to AG to guarantee reduction in the progress measure as explained in Section 5.
- 5. C+AG switches from AG back to NCG after a test measuring nearness to a quadratic is satisfied. When CG resumes, the progress measure may be modified to a more elaborate procedure discussed in Appendix A, although this elaborate progress measure is disabled by default.

When applied to a quadratic function, the progress measure is always satisfied (this is proved in Section 3), and hence all steps will be NCG (and therefore LCG) steps. The fact that the C+AG satisfies the $O(\ln(1/\epsilon)\sqrt{L/\ell})$ running-time bound of AG for general convex functions follows because of the progress measure. The conjectured final theoretical property of the method, namely, n-step quadratic convergence, is described in the Appendix B. Computational testing in Section 8 indicates that the running time of the method measured in function-gradient evaluations is roughly equal to whichever of AG or NCG is better for the problem at hand, and in some cases it outperforms both of them.

Both AG and C+AG use prior knowledge of L, ℓ . However, L can be estimated by both methods, and ℓ may be taken to be 0 if no further information is available. Thus, both algorithms are useable, albeit slower, in the absence of prior knowledge of these parameters. We return to this topic in Section 6.

We conclude this introductory section with a few remarks about our previous unpublished manuscript [16]. That work explored connections between AG, GD, and LCG, and proposed a hybrid of NCG and GD. However, that work did not address the number of function-gradient evaluations because the the evaluation count for the line search was not analyzed. Closer to what is proposed here is a hybrid algorithm from the first author's PhD thesis [15]. Compared to the PhD thesis, the proposed algorithm herein has several improvements including the line search and the method for switching from AG to CG as well as additional analysis.

2 NCG and line search

The full C+AG algorithm is presented in Section 7. In this section, we present the NCG portion of C+AG, which is identical to most other NCG routines and is as follows

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\begin{aligned} & \boldsymbol{x}_0 := \boldsymbol{0}; \\ & \boldsymbol{p}_0 := -\nabla f(\boldsymbol{x}_0); \\ & k := 0; \\ & \text{while } \|\nabla f(\boldsymbol{x}_k)\| > \text{tol} \\ & \text{Select } \alpha_k; \\ & \boldsymbol{x}_{k+1} := \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k; \\ & \text{Confirm that } \boldsymbol{x}_{k+1} \text{ satisfies the progress measure.} \\ & \text{Select } \beta_{k+1}; \\ & \boldsymbol{p}_{k+1} := -\nabla f(\boldsymbol{x}_{k+1}) + \beta_{k+1} \boldsymbol{p}_k; \\ & k := k+1; \end{aligned}end while
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For β_{k+1} we use the Hager-Zhang formula [12], which is as follows:

$$\hat{\boldsymbol{y}} := \boldsymbol{g}_{k+1} - \boldsymbol{g}_{k};$$

$$\beta^{1} := \left(\hat{\boldsymbol{y}} - \boldsymbol{p}_{k+1} \cdot \frac{2\|\hat{\boldsymbol{y}}\|^{2}}{\hat{\boldsymbol{y}}^{T} \boldsymbol{p}_{k+1}}\right)^{T} \frac{\boldsymbol{g}_{k+1}}{\hat{\boldsymbol{y}}^{T} \boldsymbol{p}_{k+1}},$$

$$\beta^{2} := \frac{-1}{\|\boldsymbol{p}_{k+1}\| \cdot \min(.01\|\boldsymbol{g}_{0}\|, \|\boldsymbol{g}_{k+1}\|)}.$$

$$\beta_{k+1} := \max(\beta^{1}, \beta^{2}).$$

For α_k , we use the following formulas.

$$\tilde{\boldsymbol{x}} := \boldsymbol{x}_k + \boldsymbol{p}_k / L, \tag{4}$$

$$s := L(\nabla f(\tilde{x}) - \nabla f(x_k)), \tag{5}$$

$$\alpha_k := \frac{-\nabla f(\boldsymbol{x}_k)^T \boldsymbol{p}_k}{\boldsymbol{p}_k^T \boldsymbol{s}}.$$
 (6)

The rationale for this choice of α_k is as follows. In the case that $f(\boldsymbol{x}) = \boldsymbol{x}^T A \boldsymbol{x}/2 - \boldsymbol{b}^T \boldsymbol{x}$ (quadratic), $\nabla f(\boldsymbol{x}_k) = A \boldsymbol{x}_k - \boldsymbol{b}$ and $\nabla f(\tilde{\boldsymbol{x}}) = A \tilde{\boldsymbol{x}} - \boldsymbol{b} = A \boldsymbol{x}_k - \boldsymbol{b} + A \boldsymbol{p}_k/L$, and therefore $\boldsymbol{s} = A \boldsymbol{p}_k$ and $\boldsymbol{p}_k^T \boldsymbol{s} = \boldsymbol{p}_k^T A \boldsymbol{p}_k$. In this case, α_k is the exact minimizer of the univariate quadratic function $\alpha \mapsto f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)$.

In the case of a nonquadratic function, this choice of α_k could be inaccurate, which could lead to a poor choice for \boldsymbol{x}_{k+1} . The progress measure in the next section will catch this failure and select a new search direction \boldsymbol{p}_k in this case.

As for the choice of β_k , we mention that Dai and Yuan [7] carried out an extensive convergence study of different formulas for β_k (not including the Hager-Zhang formula, but covering many others), and in the end, proposed a certain hybrid formula for β_k . Note that Dai and Kou [8] propose another family with the interesting property [8, Theorem 4.2] that convergence is guaranteed for smooth, strongly convex functions, although no rate is derived.

Our experiments (not reported here) suggest that the choice of β_k is not critical to the performance of C+AG. The Dai-Yuan paper points out that certain choices of β_k will lead to nonconvergence if the line-search fails to satisfy the strong Wolfe conditions.

However, our line-search does not satisfy even the weak Wolfe conditions. In other words, the criteria used in the previous literature to distinguish among the choices of formulas for β_k may not be applicable to C+AG.

3 Progress measure

The progress measure is taken from Nesterov's [20] analysis of the AG method. The basis of the progress measure is a sequence of strongly convex quadratic functions $\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), \dots$ called an "estimate sequence" in [20].

The sequence is initialized with

$$\phi_0(\mathbf{x}) := f(\mathbf{x}_0) + \frac{L}{2} ||\mathbf{x} - \mathbf{v}_0||^2,$$
 (7)

where $v_0 := x_0$. Then ϕ_k for $k \ge 1$ is defined in terms of its predecessor via:

$$\phi_{k+1}(\boldsymbol{x}) = (1 - \theta_k)\phi_k(\boldsymbol{x}) + \theta_k \left[f(\bar{\boldsymbol{x}}_k) + \nabla f(\bar{\boldsymbol{x}}_k)^T (\boldsymbol{x} - \bar{\boldsymbol{x}}_k) + \frac{\ell}{2} \|\boldsymbol{x} - \bar{\boldsymbol{x}}_k\|^2 \right].$$
(8)

Here, $\theta_k \in (0,1)$ and $\bar{\boldsymbol{x}}_k \in \mathbb{R}^n$ are detailed below. Note that the Hessian of ϕ_0 and of the square-bracketed quadratic function in (8) are both multiples of I, and therefore inductively the Hessian of ϕ_k is a multiple of I for all k. In other words, for each k there exists $\gamma_k, \boldsymbol{v}_k, \phi_k^*$ such that $\phi_k(\boldsymbol{x}) = \phi_k^* + (\gamma_k/2) \|\boldsymbol{x} - \boldsymbol{v}_k\|^2$, where $\gamma_k > 0$. The formulas for γ_{k+1} , \boldsymbol{v}_{k+1} , ϕ_{k+1}^* are straightforward to obtain from (8) given γ_k , \boldsymbol{v}_k , ϕ_k^* as well as θ_k and $\bar{\boldsymbol{x}}_k$. These formulas appear in [20, p. 73] and are repeated here for the sake of completeness:

$$\gamma_{k+1} := (1 - \theta_k)\gamma_k + \theta_k \ell, \tag{9}$$

$$\boldsymbol{v}_{k+1} := \frac{1}{\gamma_{k+1}} [(1 - \theta_k) \gamma_k \boldsymbol{v}_k + \theta_k \ell \bar{\boldsymbol{x}}_k - \theta_k \nabla f(\bar{\boldsymbol{x}}_k)], \tag{10}$$

$$\phi_{k+1}^* := (1 - \theta_k)\phi_k^* + \theta_k f(\bar{\boldsymbol{x}}_k) - \frac{\theta_k^2}{2\gamma_{k+1}} \|\nabla f(\bar{\boldsymbol{x}}_k)\|^2 + \frac{\theta_k (1 - \theta_k)\gamma_k}{\gamma_{k+1}} (\ell \|\bar{\boldsymbol{x}}_k - \boldsymbol{v}_k\|^2 / 2 + \nabla f(\bar{\boldsymbol{x}}_k)^T (\boldsymbol{v}_k - \bar{\boldsymbol{x}}_k)).$$
(11)

We call the sequence $\bar{x}_0, \bar{x}_1, \ldots$ the *gradient sequence* because the gradient is evaluated at these points.

To complete the formulation of $\phi_k(\cdot)$, we now specify θ_k and \bar{x}_k . Scalar θ_k is selected as the positive root of the quadratic equation

$$L\theta_k^2 + (\gamma_k - \ell)\theta_k - \gamma_k = 0. \tag{12}$$

The fact that $\theta_k \in (0,1)$ is easily seen by observing the sign-change in this quadratic over [0,1]. A consequence of (12) and (9) is the identity

$$\frac{\theta_k^2}{2\gamma_{k+1}} = \frac{1}{2L}.\tag{13}$$

Finally, C+AG has three cases for selecting gradient sequence \bar{x}_k . The first case is $\bar{x}_k := x_k$. The second and third cases are presented later.

The principal theorem assuring progress is Theorem 2.2.2 of Nesterov [20], which we restate here for the sake of completeness. The validity of this theorem does not depend on how the gradient sequence \bar{x}_k is selected in the definition of $\phi_k(\cdot)$.

Theorem 1 (Nesterov) Suppose that for each k = 0, 1, 2, 3, ..., there exists a point \mathbf{x}_k , called the witness, satisfying $f(\mathbf{x}_k) \leq \min_{\mathbf{x}} \phi_k(\mathbf{x}) \equiv \phi_k^*$. Then

$$f(\boldsymbol{x}_k) - f^* \le L \min\left(\left(1 - \sqrt{\ell/L}\right)^k, \frac{4}{(k+2)^2}\right) \|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2.$$
 (14)

The sufficient-progress test used for CG is the condition of the theorem, namely, $f(x_k) \leq \phi_k^*$. That is, in the case of CG, the witness sequence is also the main sequence computed by CG. As long as this test holds, the algorithm continues to take CG steps, and the right-hand side of (14) assures us that the optimal complexity bound is achieved (up to constants) in the case of both smooth convex functions and smooth, strongly convex functions.

The main result of this section is the following theorem, which states that if the objective function is quadratic, then the progress measure is always satisfied by conjugate gradient.

Theorem 2 Assume $\mathbf{v}_0 = \mathbf{x}_0$. If $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$, where A is positive definite, and if the gradient sequence $\bar{\mathbf{x}}_k$ and witness sequence are the same as the CG sequence $\bar{\mathbf{x}}_k := \mathbf{x}_k$, then $f(\mathbf{x}_k) \leq \phi_k^*$ for every iteration k.

Proof. The result clearly holds when k = 0 by (7). Assuming $f(\boldsymbol{x}_k) \leq \phi_k^*$, we now show that $f(\boldsymbol{x}_{k+1}) \leq \phi_{k+1}^*$ For $k \geq 0$,

$$\phi_{k+1}^* = (1 - \theta_k)\phi_k^* + \theta_k f(\boldsymbol{x}_k) - \frac{\theta_k^2}{2\gamma_{k+1}} \|\nabla f(\boldsymbol{x}_k)\|^2 + \frac{\theta_k (1 - \theta_k)\gamma_k}{\gamma_{k+1}} \left(\ell \|\boldsymbol{x}_k - \boldsymbol{v}_k\|^2 + \nabla f(\boldsymbol{x}_k)^T (\boldsymbol{v}_k - \boldsymbol{x}_k)\right)$$
(15)

$$\geq f(\boldsymbol{x}_k) - \frac{\theta_k^2}{2\gamma_{k+1}} \|\nabla f(\boldsymbol{x}_k)\|^2 + \frac{\theta_k (1 - \theta_k)\gamma_k}{\gamma_{k+1}} \left(\nabla f(\boldsymbol{x}_k)^T (\boldsymbol{v}_k - \boldsymbol{x}_k)\right)$$
(16)

$$= f(\boldsymbol{x}_k) - \frac{1}{2L} \|\nabla f(\boldsymbol{x}_k)\|^2 + \frac{\theta_k (1 - \theta_k) \gamma_k}{\gamma_{k+1}} \left(\nabla f(\boldsymbol{x}_k)^T (\boldsymbol{v}_k - \boldsymbol{x}_k)\right). \tag{17}$$

$$= f(\boldsymbol{x}_k) - \frac{1}{2L} \|\nabla f(\boldsymbol{x}_k)\|^2$$
(18)

$$\geq f(\boldsymbol{x}_k - \nabla f(\boldsymbol{x}_k)/L) \tag{19}$$

$$\geq f(\boldsymbol{x}_{k+1}). \tag{20}$$

Here, (15) is a restatement of (11) under the assumption that $\bar{x}_k = x_k$. Line (16) follows from the induction hypothesis. Line (17) follows from (13).

Line (18) follows because, according to the recursive formula (10), \mathbf{v}_k lies in the affine space $\mathbf{x}_0 + \text{span}\{\nabla f(\mathbf{x}_0), \dots, \nabla f(\mathbf{x}_{k-1})\}$. Similarly, \mathbf{x}_k lies in this space. Therefore, $\mathbf{v}_k - \mathbf{x}_k$ lies the kth Krylov subspace span $\{\nabla f(\mathbf{x}_0), \dots, \nabla f(\mathbf{x}_{k-1})\}$. It is well known (see, e.g., [10]) that $\nabla f(\mathbf{x}_k)$ is orthogonal to every vector in this space.

Line (19) is a standard inequality for L-smooth convex functions; see, e.g., p. 57 of [20]. Finally (20) follows because $\mathbf{x}_k - \nabla f(\mathbf{x}_k)/L$ lies in the k+1-dimensional affine space $\mathbf{x}_0 + \operatorname{span}\{\nabla f(\mathbf{x}_0), \dots, \nabla f(\mathbf{x}_k)\}$ while \mathbf{x}_{k+1} minimizes f over the same affine space, another well known property of CG.

We note that this proof yields another proof of Daniel's result that conjugate gradient converges at a linear rate with a factor $1-\operatorname{const}\sqrt{\ell/L}$ per iteration. Specifically, the two bounds are

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}^*) \le \begin{cases} 4\left(\frac{1-\sqrt{\ell/L}}{1+\sqrt{\ell/L}}\right)^{2k} (f(\boldsymbol{x}_0) - f^*) \text{ (Daniel)} \\ \left(1 - \sqrt{\ell/L}\right)^k \cdot L\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2 \text{ (Nesterov + this proof).} \end{cases}$$

We see that the reduction factor is better in Daniel's bound because of the exponent 2k rather than k, which means approximately reduction of $1-2\sqrt{\ell/L}$ per iteration (assuming $\ell \ll L$) instead of $1-\sqrt{\ell/L}$. Furthermore, the multiplicative constant in Daniel's bound is better as noted earlier.

A limitation of this proof is that it requires $v_0 = x_0$. In the case that the CG iterations follow a sequence of AG iterations, this equality will not hold. We return to this point in Appendix A.

4 Restarting CG

The classical method for coping with failure to make progress in nonlinear CG is 'restarting', which means taking a step using the steepest descent direction instead of the conjugate gradient direction. Our proposed C+AG method, when it detects insufficient progress on the kth iteration (i.e., the inequality $f(\mathbf{x}_k) \leq \phi_k^*$ fails to hold), attempts two fall-back solutions. The first fall-back is restarting CG in the traditional manner (steepest descent). It should be noted that this restart does not play a role in the theoretical analysis of the algorithm, but we found that in practice it improves performance (versus immediately proceeding to the second fall-back of the AG method).

The issue of when to restart has received significant attention in the previous literature. One guideline is to restart every n+1 iterations. In more modern codes, restarting is done every kn+1 iterations, where $k \geq 1$ is a constant, e.g., Hager-Zhang's CG-Descent restarts every 6n+1 iterations. We also have implemented this restart in our code, although it is usually not activated because some other test fails first.

Three other conditions for restarting from the previous literature, collectively termed the "Beale-Powell" conditions by Dai and Yuan [6], are

$$|\nabla f(\boldsymbol{x}_{k-1})^T \nabla f(\boldsymbol{x}_k)| \ge c_1 ||\nabla f(\boldsymbol{x}_k)||^2, \quad (BP1)$$

$$\boldsymbol{p}_k^T \nabla f(\boldsymbol{x}_k) \ge -c_2 \|\nabla f(\boldsymbol{x}_k)\|^2, \quad (BP2)$$

$$\boldsymbol{p}_k^T \nabla f(\boldsymbol{x}_k) \le -c_3 \|\nabla f(\boldsymbol{x}_k)\|^2, \quad (BP3)$$

where $c_1 \in (0, \infty)$, $c_2 \in [0, 1]$, and $c_3 \in (1, \infty)$. It should be noted that in exact arithmetic on a quadratic objective function, none of these tests will ever be activated. It should also be noted that Powell [24] as well as Dai and Yuan consider other restart directions (which we have not implemented) besides the steepest descent direction.

We have found that including these tests (BP1)–(BP3) caused the code to take more iterations in the majority of tests (although the difference in iteration counts was never large), so we have turned them off by default. In other words, the default values are $c_1 = \infty$, $c_2 = 0$ (i.e., we restart if p_k is not a descent direction), and $c_3 = \infty$. Presumably this is because there are cases when progress is possible according to our progress measure even though a BP condition fails.

One additional restart condition in our code is that if the denominator of (6) is non-positive, then we restart because this means that calculation of α_k has failed.

A recent paper by Buhler et al. [3] considers nonlinear conjugate gradient for problems in machine learning and in particular the role of (BP) restarts. The motivation for their work is somewhat different from ours: they consider general objective functions, not necessarily smooth convex functions, and therefore accelerated gradient is not available for their class of problems. Their first main concern, costly line search, is not an issue for C+AG since its line search requires only one additional gradient per iteration. Their second main concern, nonconjugacy in search directions, is also less of a concern for C+AG since conjugacy is not an ingredient of the C+AG progress measure. They conclude that (BP1)–(BP3) (and (BP1) in particular) are important for a successful nonlinear CG implementation. The fact that their conclusions differ from ours arises from the different aims of the papers.

5 Switching to AG in the case of lack of progress

If the inequality $f(x_k) \leq \phi_k^*$ fails to hold also for the steepest descent direction described in the previous section, then the second fall-back is to switch to a sequence of AG steps. AG steps continue until the following "almost-quadratic" test is satisfied. Let

$$q_k := -\frac{\nabla f(\bar{\boldsymbol{x}}_k)^T (\nabla f(\bar{\boldsymbol{x}}_k) + \nabla f(\boldsymbol{x}_{k+1}))}{2L}.$$

The termination test for AG is

$$f(\boldsymbol{x}_{k+1}) \le f(\bar{\boldsymbol{x}}_k) + \frac{4}{5}q_k. \tag{24}$$

The rationale for this formula is as follows. One checks with a few lines of algebra that if f were quadratic, then the identity $f(\boldsymbol{x}_{k+1}) = f(\bar{\boldsymbol{x}}_k) + q_k$ holds, assuming that \boldsymbol{x}_{k+1} is defined as $\bar{\boldsymbol{x}}_k - \nabla f(\bar{\boldsymbol{x}}_k)/L$ as in AG (see l. 44 of Algorithm C+AG, Part II below). Thus, (24) tests whether f in the neighborhood of $\bar{\boldsymbol{x}}_k$ is behaving approximately as a quadratic function would behave, which indicates that conjugate gradient might succeed.

Note that (24) involves an extra function-gradient evaluation since an ordinary AG iteration evaluates $f, \nabla f$ at $\bar{\boldsymbol{x}}_k$ but not at \boldsymbol{x}_{k+1} . Therefore, (24) is checked only every 8 iterations to reduce the overhead of the test.

Overall, the C+AG algorithm requires two function-gradient evaluations for a CG step, one to obtain the gradient at x_k and the second to evaluate $\nabla f(\tilde{x})$ in (5). Similarly, the first fall-back requires two function-gradient evaluations. Finally, the accelerated gradient step requires another gradient evaluation. Therefore, the maximum number of function-gradient evaluations on a single iteration before progress is made is five. Therefore, Theorem 1 applies to our algorithm except for a constant factor of 5. In practice, on almost every step, either the CG step succeeds or AG is used, meaning the actual number of function-gradient evaluations per iteration lies between 1 and 2.

6 Estimating L

The C+AG method as described thus far requires knowledge of L and ℓ , the moduli of smoothness and strong convexity respectively. In case these parameters are not known, the method estimates L and simply assumes $\ell = 0$. For many problems (including our examples) $\ell \ll L$, meaning that convergence is governed by the second parenthesized of factor of (14). Thus, taking $\ell = 0$ does not appear to significantly impede convergence.

As for estimating L, we use the following procedure outlined in §10.4.2 of Beck [1]. Starting from an initial guess of L=1, we first decrease L by multiplying by $1/\sqrt{2}$ or increase by multiplying by $\sqrt{2}$ until the condition

$$f(x_0 - \nabla f(x_0)/L) \le f(x_0) - ||\nabla f(x_0)||^2/(2L)$$

is satisfied. This means that C+AG and AG require $O(|\log(L)|)$ iterations for the initial estimate. On subsequent iterations, we re-estimate L on the first iteration of consecutive sequences of CG iterations and on every iteration of AG. On iterations after the first, L cannot decrease; it will either stay the same or increase. Beck proves that using this procedure does not worsen the iteration-complexity of AG when compared to the case that L is known a priori. However, this procedure increases the number of function-gradient evaluations per AG step from one to approximately two. In the case of the conjugate gradient steps, the impact is negligible since only the first in a sequence requires the extra function-gradient evaluation.

It is not necessary to re-estimate L on every CG iteration because the CG step uses L only as the finite-difference step size in its procedure to determine α_k as in (4)–(6). This dependence is mild in the sense that, assuming f is quadratic, (4)–(6) will compute the same (correct) value of α_k regardless of the step size. All computational tests in Tables 1 and 2 use the adaptive version of C+AG described in this section.

There are procedures in the literature for estimating ℓ also, for example, the procedure by Carmon et al. [4]. However, Carmon et al.'s procedure is costly as it involves several trial steps and a guess-and-update procedure for ℓ . Even in the pure quadratic case, estimating ℓ apparently requires multiple steps of the Lanczos method [10] and would be

costly. We have not implemented it since, as mentioned above, taking $\ell=0$ appears to be satisfactory.

7 Pseudocode for C+AG

In this section we present pseudocode for the C+AG algorithm. The pseudocode includes the procedure for estimating L. It does not, however, include the elaborate procedure for finding witnesses after CG is restarted as described in Appendix A. We did not include this in the pseudocode because it is disabled by default as discussed in the appendix. See the concluding remarks of the paper for a downloadable implementation in Matlab, which does include that procedure as an option. The input arguments are f and ∇f , the objective function and gradient, x_0 , the initial guess, gto1, the termination criterion, and L, ℓ , the smoothness modulus and the modulus of strong convexity respectively. Note that $\ell = 0$ is a valid argument, and L = NaN (not a number) is a signal to the algorithm to estimate L.

```
Algorithm 1 ComputeThetaGamma (implementation of (9) and (12))
```

```
Input: L, \ell, \gamma_k
Output: \theta_k, \gamma_{k+1}
Solve L\theta_k^2 + (\gamma_k - \ell)\theta_k - \gamma_k = 0 via the quadratic formula for the positive root \theta_k.
Let \gamma_{k+1} := (1 - \theta_k)\gamma_k + \theta_k \ell
```

Algorithm 2 EstimateLInitial

```
Input: f(\cdot), x_0, f(x_0), \nabla f(x_0), L_{\text{init}}(=1 \text{ by default})
Output: L
L := L_{\text{init}}
for k = 1 : 100 \text{ do}
if f(x_0 - \nabla f(x_0)/L) < f(x_0) - \|\nabla f(x_0)\|^2/(2L) then
L := L/\sqrt{2}
else
return \text{EstimateL}(f(\cdot), x_0, f(x_0), \nabla f(x_0), L)
end if
end for
Throw error: "f may be unbounded below"
```

The mathematical structure of the algorithm has already been described in previous sections, and in this section we will describe a few computational details. The flag onlyAG indicates that the algorithm is currently executing a block of AG statements. As mentioned in Section 5, once AG iterations begin, they continue uninterrupted until (24) holds, and this is checked every 8th iteration.

The variable i_{cg} counts the number of consecutive CG iterations without a restart. A restart means that p_{k+1} is defined to be $-g_k$, i.e., a steepest descent step is taken. The

Algorithm 3 EstimateL

```
Input: f(\cdot), x_0, f(x_0), \nabla f(x_0), L

Output: L

for k = 1 : 60 do

f_1 := f(x_0 - \nabla f(x_0)/L)

if f_1 \ge f(x_0) - \|\nabla f(x_0)\|^2/(2L) and |f_1 - f(x_0)| \ge 10^{-11}|f(x_0)| then

L := \sqrt{2}L

else

return L

end if

end for

Throw error: "Line search failed to determine L; possible incorrect gradient function or excessive roundoff error"
```

Algorithm 4 ComputeVPhiStar (implementation of (10) and (11))

```
Input: \theta_k, \gamma_k, \gamma_{k+1}, \ell, \boldsymbol{v}_k, \phi_k^*, \bar{\boldsymbol{x}}_k, f(\bar{\boldsymbol{x}}_k), \nabla f(\bar{\boldsymbol{x}}_k)

Output: \boldsymbol{v}_{k+1}, \phi_{k+1}^*

Let \boldsymbol{v}_{k+1} := \frac{1}{\gamma_{k+1}}[(1-\theta_k)\gamma_k\boldsymbol{v}_k + \theta_k\ell\bar{\boldsymbol{x}}_k - \theta_k\nabla f(\bar{\boldsymbol{x}}_k)].

Let \phi_{k+1}^* := (1-\theta_k)\phi_k^* + \theta_kf(\bar{\boldsymbol{x}}_k) - \frac{\theta_k^2}{2\gamma_{k+1}}\|\nabla f(\bar{\boldsymbol{x}}_k)\|^2

+ \frac{\theta_k(1-\theta_k)\gamma_k}{\gamma_{k+1}}(\ell\|\bar{\boldsymbol{x}}_k - \boldsymbol{v}_k\|^2/2 + \nabla f(\bar{\boldsymbol{x}}_k)^T(\boldsymbol{v}_k - \bar{\boldsymbol{x}}_k)).
```

Algorithm 5 C+AG (Part I)

```
Input: f(\cdot), \nabla f(\cdot), x_0 \in \mathbb{R}^n, \ell, L, \text{gtol}
Output: x^* such that \|\nabla f(x^*)\| \leq \text{gtol}
  1: f_0 := f(\boldsymbol{x}_0); \ \boldsymbol{g}_0 := \nabla f(\boldsymbol{x}_0); \ \phi_0^* := f_0; \ \boldsymbol{v}_0 := \boldsymbol{x}_0; \ \mathtt{onlyAG} := \mathbf{false};
  2: i_{cg} := 0; i_{ag} := 0; p_0 := -g_0; LNaNFlag := false
  3: if L = \text{NaN then}
               L := \texttt{EstimateLInit}(f(\cdot), \boldsymbol{x}_0, f(\boldsymbol{x}_0), \nabla f(\boldsymbol{x}_0), 1); \ \ell := 0; \ \texttt{LNaNFlag} := \mathbf{true}
  5: end if
  6: \gamma_0 := L;
  7: for k = 0, 1, \dots do
              \theta_k, \gamma_{k+1} := \texttt{ComputeThetaGamma}(L, \ell, \gamma_k)
              for whichsteptype := 1 : 3 do
  9:
                     if whichsteptype \leq 2 then
10:
                            if onlyAG then continue end if
11:
                            if i_{cq} \geq 6n + 1 or whichsteptype = 2 then
12:
13:
                                   p_k := -g_k; i_{cg} := 0
                            end if
14:
                            if i_{cq} = 0 and k > 0 and LNaNFlag then
15:
                                   L := \texttt{EstimateL}(f(\cdot), \boldsymbol{x}_k, f(\boldsymbol{x}_k), \nabla f(\boldsymbol{x}_k), L)
16:
                            end if
17:
                            i_{cq} := i_{cq} + 1; i_{aq} := 0
18:
                            \tilde{\boldsymbol{x}} := \boldsymbol{x}_k + \boldsymbol{p}_k/L; \ f := f(\tilde{\boldsymbol{x}}); \ \tilde{\boldsymbol{g}} := \nabla f(\tilde{\boldsymbol{x}})
19:
                            if \|\tilde{g}\| \leq \text{gtol then return } \tilde{x} \text{ end if }
20:
                            Ap := L(\tilde{\boldsymbol{g}} - \boldsymbol{g}_k); pAp := \boldsymbol{p}_k^T Ap;
21:
                            if \mathbf{g}_k^T \mathbf{p}_k \geq 0 or pAp \leq 0 then continue end if
22:
                            \alpha_k := -\boldsymbol{g}_k^T \boldsymbol{p}_k / \mathtt{pAp}
23:
                            x_{k+1} := x_k + \alpha_k p_k; f_{k+1} := f(x_{k+1}); g_{k+1} := \nabla f(x_{k+1})
24:
                            if ||g_{k+1}|| \leq \text{gtol then return } x_{k+1} \text{ end if }
25:
                            oldsymbol{v}_{k+1}, \phi_{k+1}^* := 	exttt{ComputeVPhiStar}(	heta_k, \gamma_k, \gamma_{k+1}, \ell, oldsymbol{v}_k, \phi_k^*, oldsymbol{x}_k, f_k, oldsymbol{g}_k)
26:
                            if f_{k+1} \leq \phi_{k+1}^* then
27:
                                   \hat{y} := g_{k+1} - g_k
28:
                                  \beta^{1} := \left(\hat{\boldsymbol{y}} - \boldsymbol{p}_{k} \cdot \frac{2\|\hat{\boldsymbol{y}}\|^{2}}{\hat{\boldsymbol{y}}^{T}\boldsymbol{p}_{k}}\right)^{T} \frac{\boldsymbol{g}_{k+1}}{\hat{\boldsymbol{y}}^{T}\boldsymbol{p}_{k}}\beta^{2} := \frac{-1}{\|\boldsymbol{p}_{k}\| \cdot \min(.01\|\boldsymbol{g}_{0}\|,\|\boldsymbol{g}_{k+1}\|)}.
29:
30:
                                   \beta_{k+1} := \max(\beta^1, \beta^2)
31:
32:
                                   \boldsymbol{p}_{k+1} := -\boldsymbol{g}_{k+1} + \beta_{k+1} \boldsymbol{p}_k
                                   break (terminate whichsteptype loop)
33:
34:
                            end if
```

Algorithm 6 C+AG Part II else (whichsteptype = 3) 35: 36: if not onlyAG then onlyAG := true37: $i_{ag} := 0; i_{cg} := 0$ 38: end if 39: $\begin{array}{l} i_{ag} := i_{ag} + 1 \\ \bar{\boldsymbol{x}}_k := \frac{\theta_k \gamma_k \boldsymbol{v}_k + \gamma_{k+1} \boldsymbol{x}_k}{\gamma_k + \theta_k \ell}; \ \bar{f}_k := f(\bar{\boldsymbol{x}}_k); \ \bar{\boldsymbol{g}}_k := \nabla f(\bar{\boldsymbol{x}}_k) \\ \text{if } \|\bar{\boldsymbol{g}}_k\| \leq \text{gtol then return } \bar{\boldsymbol{x}}_k \ \text{end if} \end{array}$ 40: 41: 42: if LNaNFlag then $L := \texttt{EstimateL}(f(\cdot), \boldsymbol{x}_k, f(\boldsymbol{x}_k), \nabla f(\boldsymbol{x}_k), L)$ end if 43: $\boldsymbol{x}_{k+1} := \bar{\boldsymbol{x}}_k - \bar{\boldsymbol{g}}_k / L$ 44: $\boldsymbol{v}_{k+1}, \phi_{k+1}^* := \texttt{ComputeVPhiStar}(\theta_k, \gamma_k, \gamma_{k+1}, \ell, \boldsymbol{v}_k, \phi_k^*, \bar{\boldsymbol{x}}_k, \bar{f}_k, \bar{\boldsymbol{g}}_k)$ 45: if $i_{ag} \equiv 0 \pmod{8}$ and $f(\boldsymbol{x}_{k+1}) \leq f(\bar{\boldsymbol{x}}_k) - \frac{4}{5} \cdot \frac{\bar{\boldsymbol{g}}_k^T(\bar{\boldsymbol{g}}_k + \nabla f(\boldsymbol{x}_{k+1}))}{2L}$ then 46: $f_{k+1} := f(\boldsymbol{x}_{k+1}); \, \boldsymbol{g}_{k+1} := \nabla f(\boldsymbol{x}_{k+1})$ 47: $p_{k+1} := -g_{k+1}$ 48: onlyAG := false49: end if 50: 51: end if end for 52: 53: end for

code forces a restart after 6n + 1 iterations. Such a test is typical in NCG algorithms. The theory for n-step quadratic convergence requires a restart every n + 1 iterations, but well known codes, e.g., CG-Descent [12] often use a longer interval.

The for-loop on l. 9 tries first a CG step and second a steepest descent step in order to make progress. Line 23 computes α_k as discussed in Section 2. The test for sufficient progress in a CG step appears in l. 27. If sufficient progress is attained, then the next CG search direction p_{k+1} is computed.

Line 36 can be reached if both attempts at CG fail to make sufficient progress. It is also reached if the onlyAG flag is set to 'true', meaning that the algorithm is currently inside a block of consecutive AG iterations. The statements beginning with 41 are the formulation of the AG method taken from [20]. Statement 1. 46 implements the test for resuming CG described in Section 5.

8 Computational experiments

In this section we report on computational experiments with C+AG. We compared it to two other codes: AG coded by us based on (2.2.8) of [20] and CG-Descent by Hager and Zhang. We used C version 6.8 of CG-Descent with the Matlab front-end. We used it in memoryless mode, i.e., NCG rather than L-BFGS.

As for our own code C+AG, we discovered via experimentation that the more elaborate calculation of \bar{x}_k described in Appendix A diminished the performance of the code. In

particular, as mentioned the additional overhead of 100% per iteration slowed the code down without improving the iteration count and thus was not used.

To the best of our knowledge, there is no standard benchmark set of smooth convex functions with a known L, ℓ , so instead we constructed our own test set of eight problem instances based on formulations that have occurred in the recent literature in data science.

The convergence criterion is $\|\nabla f(\boldsymbol{x}_k)\| \leq \text{gtol}$, where $\text{gtol} = 10^{-8}$ for the ABPDN and LL problems described below, while $\text{gtol} = 10^{-6}$ for the HR problems. (None of the algorithms were able to converge to 10^{-8} for the HR problems in fewer than $2 \cdot 10^6$ iterations, so we loosened the criterion for that problem.) In the case of CG-Descent, the convergence criterion is based on the ∞ -norm rather than 2-norm. (The ∞ -norm convergence criterion is hardwired into the code, and we did not attempt to rewrite this fairly complex software.) Via some experiments not reported here, we found that stopping when $\|\nabla f(\boldsymbol{x}_k)\|_{\infty} \leq 3 \cdot \text{gtol}/\sqrt{n}$ approximately reproduced the criterion $\|\nabla f(\boldsymbol{x}_k)\| \leq \text{gtol}$ used for the other methods, so this was the termination criterion for CG-Descent.

The reported results for our C+AG routine used $L = \mathbf{NaN}$ and $\ell = 0$ in all cases, in other words, adaptive estimation of L. We assume most users would select this mode since L, ℓ are often not known in advance. For AG, we tested both the known and unknown L, ℓ modes; this is indicated in the table below by "AG" and "AG/EstL."

As mentioned in the introduction, we have reported on function-gradient evaluation counts since that is usually taken as the primary work-unit of first-order methods. We did not report on wall-clock time because CG-Descent, having been written in highly optimized C, has an advantage over AG and C+AG, which are written Matlab.

The first four problems are based on BPDN (basis pursuit denoising), that is, the unconstrained convex optimization problem:

$$\min \frac{1}{2} ||A\boldsymbol{x} - \boldsymbol{b}||^2 + \lambda ||\boldsymbol{x}||_1$$

in which $\lambda > 0$ and $A \in \mathbb{R}^{m \times n}$ has fewer rows than columns, so that the problem is neither strongly convex nor smooth. However, the following approximation (called APBDN) is both smooth and strongly convex on any bounded domain:

$$\min \frac{1}{2} ||Ax - b||^2 + \lambda \sum_{i=1}^{n} \sqrt{x_i^2 + \delta}$$

where $\delta > 0$ is a fixed scalar. It is easy to see that as $\delta \to 0$, the original problem is recovered. As $\delta \to 0$, $\ell \to 0$ and $L \to \infty$, where ℓ, L are the moduli of strong and smooth convexity respectively.

In our tests of ABPDN we took A to be a subset of \sqrt{n} rows of the discrete-cosine transform matrix of size $n \times n$, where n is an even power of 2. (This matrix and its transpose, although dense, can be applied in $O(n \ln n)$ operations.) The subset of rows was selected to be those numbered by the first $m = \sqrt{n}$ prime integers in order to get reproducible pseudorandomness in the choices. Similarly, in order to obtain a pseudorandom \boldsymbol{b} , we selected $\boldsymbol{b} \in \mathbb{R}^m$ according to the formula $b_i = \sin(i^2)$. The value of λ was fixed at 10^{-3} in all tests. Finally, we varied $\delta = 10^{-4}$ and $\delta = 5 \cdot 10^{-6}$ and we tried both n = 65536 and n = 262144 for a total of four test cases.

The ℓ_1 -penalty term in the original BPDN formulation leads to many entries of the solution \boldsymbol{x}^* equal to 0. This is no longer the case for ABPDN since the nondifferentiability at $x_i = 0$ has been smoothed out. However, a simple scaling argument suggests that the threshold for "nearly zero" should be magnitude bounded above by $\sqrt{\delta}$. We determined that our computed solutions for the four ABPDN solutions had between 78% to 82% of entries nearly zero.

The second test case is logistic loss (LL), which is as follows:

$$f(\boldsymbol{x}) = R(A\boldsymbol{x}) + \lambda ||\boldsymbol{x}||^2 / 2,$$

where A is a given $m \times n$ matrix, and $\lambda > 0$ is a regularization parameter. Here, $R(\boldsymbol{v}) = \sum_{i=1}^m r(v_i)$ where $r(v) = \ln(1+e^{-v})$. Row i of A, i=1:n, is of the form $e^T/\sqrt{n} + \boldsymbol{z}_i$, where $\boldsymbol{e} \in \mathbb{R}^n$ is the vector of all 1's and $\boldsymbol{z}_i \sim N(\boldsymbol{0}, \sigma^2 I)$ where $\sigma = 0.4$. We seeded Matlab's random number generator with the same seed on each run for reproducibility. This formulation arises from the problem of identifying the the best halfspace that contains noisy data points. We ran this test with $A \in \mathbb{R}^{6000 \times 3000}$ with two values of λ , namely, $\lambda = 10^{-4}$ and $\lambda = 5 \cdot 10^{-6}$. This function is smooth and strongly convex. The function λ controls the strong convexity.

The third test case is Huber regression (HR). Given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $\mathbf{b} \in \mathbb{R}^m$, Huber regression [14] has been proposed as a means to make linear least-squares regression more robust against outliers. In more detail, a cutoff $\tau > 0$ is selected in order to define the function

$$\zeta(t) = \begin{cases} -\tau^2 - 2\tau t, & t \le -\tau, \\ t^2, & t \in [-\tau, \tau], \\ -\tau^2 + 2\tau t, & t \ge \tau. \end{cases}$$

Note that $\zeta(t)$ is differentiable and convex and behaves like t^2 for small |t| and like O(|t|) for large |t|. Finally, $f(\boldsymbol{x}) = \sum_{i=1}^m \zeta(A(i,:)\boldsymbol{x}-b_i)$. This function is smooth but not strongly convex, i.e., $\ell = 0$. We chose the $(n+1) \times n$ sparse matrix with 1's on the main diagonal and -1's on the first sub diagonal. The vector \boldsymbol{b} was taken to be all 1's except for the final entry, which is -1.1n. (This \boldsymbol{b} is close to $A\boldsymbol{x}$ where $\boldsymbol{x} = [1, 2, \dots, n]^T$; in other words, \boldsymbol{b} is close to a right-hand side that has a 0-residual solution.) We fixed n = 10000. We selected two choices for τ , namely, $\tau = 250$ and $\tau = 1000$.

Our results for the four algorithms on the eight problems are shown in Table 2. We set a limit of 10⁶ function-gradient evaluations for C+AG and AG.

The results in Table 2 show that C+AG outperformed both AG and CG-Descent in most cases. In all cases, C+AG did as about as well as or better than whichever of AG or CG-Descent performed better.

9 Conclusions

We have presented an algorithm called C+AG, which is a variant of nonlinear conjugate gradient tailored to smooth, convex objective functions. It has a guaranteed rate of convergence equal to that of accelerated gradient, which is optimal for the class of

Table 2: Function-gradient evaluation counts for four algorithms in columns 3–6 on eight problems. Bold indicates the best for each row. The second column of the table indicates the percentage of C+AG iterations spent in AG iterations.

Problem	%AG	C+AG	AG	AG/EstL	CG-Descent
ABPDN $(n = 65536, \delta = 10^{-4})$.03%	55,891	518,019	982,919	82,472
ABPDN $(n = 65536, \delta = 5 \cdot 10^{-6})$	14%	226,141	660,355	$> 10^6$	$165,\!207$
ABPDN $(n = 262144, \delta = 10^{-4})$.02%	$80,\!335$	901,418	$> 10^6$	130,040
ABPDN $(n = 262144, \delta = 5 \cdot 10^{-6})$	0%	$483,\!420$	$> 10^6$	$> 10^6$	532,706
$LL(\lambda = 10^{-4})$	0%	148	106,507	$> 10^6$	128
$LL(\lambda = 5 \cdot 10^{-6})$	0%	140	362,236	$> 10^6$	125
$HR(\tau = 250)$	64%	$160,\!115$	$> 10^6$	$> 10^6$	946,488
$HR(\tau = 1000)$	60%	$95,\!416$	$> 10^6$	$> 10^6$	245,376

problems under consideration in the function-gradient evaluation model of computation. The method reduces to linear conjugate gradient in the case that the objective function is quadratic.

The code and all the test cases are implemented in Matlab and available on Github under the project named 'ConjugatePlusAcceleratedGradient'.

The C+AG code outperformed both AG and CG on most test cases tried. One interesting future direction is as follows. The method switches between CG and AG steps depending on the progress measure. A more elegant approach would be a formulation that interpolates continuously between the two steps. Indeed, it is possible (see, e.g., [16]) to write down a single parameterized update step in which one parameter value corresponds to AG and another to CG. But we do not know of a systematic way to select this parameter that leads to a complexity bound.

Another direction to pursue is incorporating restarts into AG. In particular, [22] propose a restart method that appears to work well in practice according to their experiments. Both AG and C+AG could use their restarts, although presumably the former would benefit more than the latter since AG steps are not used as frequently in C+AG compared to pure AG. However, to the best of our knowledge, the restart method is not guaranteed in the sense: It has not been proved that the bounds on AG iteration of Theorem 1 are still valid in the presence of restarts. Since our goal here was to provide a method with the iteration guarantee of AG, we did not incorporate their restarts.

Yet another extension would be to use memory of previous iterates. In the context of NCG, adding memory yields L-BFGS [21]. It is clearly possible to hybridize L-BFGS with AG, and it is likely that the progress measure proposed still holds for L-BFGS in the case that it is applied to a quadratic since L-BFGS reduces to LCG in this case. Note that some authors, e.g. [25], have also proposed adding memory to AG-like methods, so many combinations are possible.

Another interesting direction is to develop a conjugate gradient iteration suitable for constrained convex problems. Conjugate gradient is known to extend to the special case of minimizing a convex quadratic function with a Euclidean-ball constraint; see e.g. Gould et al. [11] and further remarks on the complexity in Paquette and Vavasis [23].

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A Restarting CG after AG

As mentioned in Section 5, if the sufficient-progress test fails for a CG iteration, then the method can fall back to AG iterations. After the AG termination test holds, the method resumes CG, say at iteration m.

An issue with restarting CG is that the sufficient-progress test may not hold for the CG iterations even if the function is purely quadratic on the remaining iterations. This is because the proof of sufficient progress in Theorem 2 assumed that $\mathbf{v}_0 = \mathbf{x}_0$. However, we would not expect the equality $\mathbf{x}_m = \mathbf{v}_m$ to hold, where m is the first iteration of CG, and therefore Theorem 2 does not apply.

We can address this issue with a more elaborate CG sufficient-progress test after resuming CG. The more elaborate test increases the number of function-gradient evaluations per CG iteration from two to four. This extra overhead, according to our experiments, overwhelmed any benefit from the more elaborate procedure.

We did observe the benefit of the elaborate procedure in a contrived test case. In this contrived test, the objective function f is quadratic, and the C+AG code is modified in two ways. First, the initial block of iterations is AG instead of CG, i.e., the only_ag flag is set to true at initialization. Second, instead of setting $v_0 := x_0$, we add random noise to the right-hand side. For this contrived test, indeed we observed for some choices of the random noise that CG was never able to restart unless the elaborate progress measure computation was enabled, and therefore the number of function-gradient evaluations associated with the elaborate procedure was much smaller than without it. However, we did not observe this behavior in any naturally occurring test case.

Therefore, our default setting is not to use the elaborate test. This means that with our default settings, there is no theoretical guarantee that CG iterations can continue indefinitely upon their resumption after AG even if the objective function is purely quadratic on the level set of x_m when CG resumes. However, the other theoretical guarantees of our method (that it has the same complexity as accelerated gradient and that it reduces to CG on a quadratic function) remain.

Despite the fact that the test is turned off by default, it is available in the code and may prove useful, and therefore we describe it here for the sake of completeness. Also, the proof-sketch of n-step quadratic convergence in the next appendix requires that this procedure be used.

Above, we defined m to be the iteration at which CG iterations are resumed. To simplify notation in the remainder of the section, assume m = 0. Thus, we consider

CG starting with $\mathbf{v}_0 \neq \mathbf{x}_0$. As in Theorem 2, we assume the objective function $f(\mathbf{x})$ is quadratic, say $f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}/2 - \mathbf{b}^T \mathbf{x}$. Recall that linear CG generates a sequence of vectors $\mathbf{p}_0, \mathbf{p}_1, \dots$ (see, e.g., [21], §5.1) such that $\mathbf{p}_i^T A \mathbf{p}_j = 0$ whenever $i \neq j$ (called "conjugacy") and such that for all k, span $\{\mathbf{p}_0, \dots, \mathbf{p}_{k-1}\} = \text{span}\{\mathbf{p}_0, A\mathbf{p}_0, \dots, A^{k-1}\mathbf{p}_0\} = \text{span}\{\nabla f(\mathbf{x}_0), \dots, \nabla f(\mathbf{x}_{k-1})\}$, called the kth Krylov space and denoted K_k for $k = 1, 2, \dots$ (where $K_0 := \{\mathbf{0}\}$). Other properties are that \mathbf{x}_k is the minimizer of f over the affine set $\mathbf{x}_0 + K_k$ and the equation $\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k$.

The new progress-checking procedure augments the Krylov space with two additional directions on each iteration to assure that the analogs of (18) and (20), that is, (41) and (43) below, hold for the method. In more detail, it computes additional sequences of vectors $\mathbf{w}_0, \mathbf{w}_1, \mathbf{w}_2, \ldots; \mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \ldots;$ and $\bar{\mathbf{x}}_0, \bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, \ldots;$ and scalars $\bar{\alpha}_0, \bar{\alpha}_1, \bar{\alpha}_2, \ldots; \bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3, \ldots;$ and $\mu_1, \mu_2, \mu_3, \ldots$ whose formulas are forthcoming. Let $\bar{K}_0 := \operatorname{span}\{\mathbf{w}_0\}$ and for $k \geq 1$, $\bar{K}_k := \operatorname{span}\{\mathbf{p}_0, \ldots, \mathbf{p}_{k-1}, \mathbf{w}_k, \mathbf{z}_k\} = K_k \oplus \operatorname{span}\{\mathbf{w}_k, \mathbf{z}_k\}.$ For each $k \geq 1$, define

$$\boldsymbol{u}_k := \bar{\boldsymbol{x}}_{k-1} - \nabla f(\bar{\boldsymbol{x}}_{k-1})/L - \boldsymbol{x}_k, \tag{25}$$

which is not computed by the method but used in its derivation. The construction of these vectors and scalars inductively has the following properties.

- 1. For all $k \geq 0$, $v_k x_k \in \bar{K}_k$. Furthermore, when writing $v_k x_k$ as a linear combination of $p_0, \ldots, p_{k-1}, w_k, z_k$, the coefficients of w_k, z_k are 1,0 respectively. For this property and the next, in the degenerate case that $p_0, \ldots, p_{k-1}, w_k, z_k$ are dependent, this property is understood to mean that there exists a way to write $v_k x_k$ with coefficients 1,0.
- 2. For all $k \geq 1$, $\boldsymbol{u}_k \in \bar{K}_k$. Furthermore, when writing \boldsymbol{u}_k as a linear combination of $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-1}, \boldsymbol{w}_k, \boldsymbol{z}_k$, the coefficients of $\boldsymbol{w}_k, \boldsymbol{z}_k$ are $\mu_k, 1$ respectively.
- 3. For $k \geq 1$, the vectors $p_0, \ldots, p_{k-1}, w_k, z_k$ of \bar{K}_k are conjugate with respect to A.
- 4. For k = 0, define $\bar{\boldsymbol{x}}_0 := \boldsymbol{x}_0 \bar{\alpha}_0 \boldsymbol{w}_0$, and for $k \geq 1$, define $\bar{\boldsymbol{x}}_k := \boldsymbol{x}_k \bar{\alpha}_k \boldsymbol{w}_k \bar{\beta}_k \boldsymbol{z}_k$. Observe that $\bar{\boldsymbol{x}}_k \boldsymbol{x}_k$ lies in \bar{K}_k . Then for all $k \geq 0$, $\bar{\boldsymbol{x}}_k$ is the minimizer of f over $\boldsymbol{x}_k + \bar{K}_k$.
- 5. For all $k \geq 0$, vector \mathbf{v}_{k+1} is computed (as usual) from \mathbf{v}_k according to (10).

To initiate this sequence of properties, let

$$\boldsymbol{w}_0 := \boldsymbol{v}_0 - \boldsymbol{x}_0. \tag{26}$$

This formula implies Property 1 holds. Properties 2–3 do not apply when k = 0. Assure Property 4 by solving a 1-dimensional minimization problem for $\bar{\alpha}_0$, that is,

$$\bar{\alpha}_0 := \underset{\alpha}{\operatorname{argmin}} f(\boldsymbol{x}_0 - \alpha \boldsymbol{w}_0) \tag{27}$$

Finally, Property 5 specifies how v_1 is computed.

Next, for the induction step, assume all the above properties hold for k. Recall that (10) is used to obtain v_{k+1} . Observe from (10) that v_{k+1} is written as a linear combination

$$\mathbf{v}_{k+1} := \sigma \mathbf{v}_k + (1 - \sigma)\bar{\mathbf{x}}_k - \tau \nabla f(\bar{\mathbf{x}}_k), \tag{28}$$

where the scalars σ , τ may be read off from (10). Note: we omit the subscripts k on σ , τ and some other scalars in this discussion for clarity, since k is fixed. In the upcoming formulas, if k = 0, take $\bar{\beta}_0$, \mathbf{p}_{-1} , and \mathbf{z}_0 to be zero. Let us define

$$\boldsymbol{w}_{k+1} := (\sigma - (1 - \sigma)\bar{\alpha}_k)\boldsymbol{w}_k - (1 - \sigma)\bar{\beta}_k\boldsymbol{z}_k + \tau\bar{\alpha}_kA\boldsymbol{w}_k + \tau\bar{\beta}_kA\boldsymbol{z}_k + \delta_1\boldsymbol{p}_{k-1} + \delta_2\boldsymbol{p}_k, \quad (29)$$

$$\boldsymbol{z}_{k+1} := -\bar{\alpha}_k \boldsymbol{w}_k - \bar{\beta}_k \boldsymbol{z}_k + \bar{\alpha}_k A \boldsymbol{w}_k / L + \bar{\beta}_k A \boldsymbol{z}_k / L + \epsilon_1 \boldsymbol{p}_{k-1} + \epsilon_2 \boldsymbol{p}_k - \mu_{k+1} \boldsymbol{w}_{k+1}, \tag{30}$$

where $\delta_1, \delta_2, \epsilon_1, \epsilon_2, \mu_{k+1}$ are yet to be determined. We now establish that these formulas satisfy the above properties.

Starting with Property 1, we have

$$\mathbf{v}_{k+1} - \mathbf{x}_{k+1} = \mathbf{v}_k - \mathbf{x}_k + (1 - \sigma)(\bar{\mathbf{x}}_k - \mathbf{v}_k) - \tau \nabla f(\bar{\mathbf{x}}_k) - \alpha_k \mathbf{p}_k$$

$$= \sigma(\mathbf{v}_k - \mathbf{x}_k) + (1 - \sigma)(\bar{\mathbf{x}}_k - \mathbf{x}_k) - \tau (A\bar{\mathbf{x}}_k - \mathbf{b}) - \alpha_k \mathbf{p}_k$$

$$= \sigma(\mathbf{v}_k - \mathbf{x}_k) + (1 - \sigma)(\bar{\mathbf{x}}_k - \mathbf{x}_k) - \tau (A\mathbf{x}_k - \mathbf{b}) - \tau A(\bar{\mathbf{x}}_k - \mathbf{x}_k) - \alpha_k \mathbf{p}_k.$$
(33)

Here, (31) follows by substituting (28) for v_{k+1} and $x_{k+1} := x_k + \alpha_k p_k$ for x_k ; (32) follows from rearranging and from substituting the definition of f; (33) adds and subtracts $\tau A x_k$.

Consider the terms of (33) separately. The first term $\sigma(\boldsymbol{v}_k - \boldsymbol{x}_k)$ lies in K_k with coefficients of σ , 0 on $\boldsymbol{w}_k, \boldsymbol{z}_k$ respectively by Property 1 inductively. The second term $(1-\sigma)(\bar{\boldsymbol{x}}_k-\boldsymbol{x}_k)$ lies in \bar{K}_k with coefficients $-(1-\sigma)\bar{\alpha}_k, -(1-\sigma)\bar{\beta}_k$ on $\boldsymbol{w}_k, \boldsymbol{z}_k$ respectively by Property 4 inductively. The third term $-\tau(A\boldsymbol{x}_k-\boldsymbol{b})$ lies in span $\{\boldsymbol{p}_0,\ldots,\boldsymbol{p}_k\}$ by the usual properties of CG. The fourth term $-\tau A(\bar{\boldsymbol{x}}_k-\boldsymbol{x}_k)$ lies in $A \operatorname{span}\{\boldsymbol{p}_0,\ldots,\boldsymbol{p}_{k-1},\boldsymbol{w}_k,\boldsymbol{z}_k\}$ span $\{\boldsymbol{p}_1,\ldots,\boldsymbol{p}_k,A\boldsymbol{w}_k,A\boldsymbol{z}_k\}$. In this expansion, the coefficients of $A\boldsymbol{w}_k$ and $A\boldsymbol{z}_k$ are $\tau\bar{\alpha}_k,\tau\bar{\beta}_k$ respectively. Finally, the last term obviously lies in $\operatorname{span}\{\boldsymbol{p}_k\}$. Therefore, if we define \boldsymbol{w}_{k+1} according to (29), then Property 1 holds for k+1.

Next we turn to Property 2. Observe that

$$\boldsymbol{u}_{k+1} = \bar{\boldsymbol{x}}_k - \nabla f(\bar{\boldsymbol{x}}_k) / L - \boldsymbol{x}_{k+1} \tag{34}$$

$$= (\bar{\boldsymbol{x}}_k - \boldsymbol{x}_k) - \alpha_k \boldsymbol{p}_k - (A\boldsymbol{x}_k - \boldsymbol{b})/L - A(\bar{\boldsymbol{x}}_k - \boldsymbol{x}_k)/L. \tag{35}$$

Here, (34) follows from the definition (25) while (35) follows from the substitutions $\nabla f(\bar{\boldsymbol{x}}_k) = A\bar{\boldsymbol{x}}_k - \boldsymbol{b}$ and $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k$ and adding and subtracting $A\boldsymbol{x}_k/L$.

Considering (35) term by term, the first term $(\bar{\boldsymbol{x}}_k - \boldsymbol{x}_k)$ lies in \bar{K}_k with coefficients $-\bar{\alpha}_k, -\bar{\beta}_k$ on $\boldsymbol{w}_k, \boldsymbol{z}_k$ inductively by Property 4. The second term lies in \bar{K}_{k+1} . The third term $-(A\boldsymbol{x}_k - \boldsymbol{b})/L$ lies in span $\{\boldsymbol{p}_0, \dots, \boldsymbol{p}_k\}$. As in the preceding derivation, the fourth term $-A(\bar{\boldsymbol{x}}_k - \boldsymbol{x}_k)/L$ lies in span $\{\boldsymbol{p}_0, \dots, \boldsymbol{p}_k, A\boldsymbol{w}_k, A\boldsymbol{z}_k\}$ with coefficients $\bar{\alpha}_k/L, \bar{\beta}_k/L$ on $A\boldsymbol{w}_k, A\boldsymbol{z}_k$ respectively. Again, we see now that (30) is chosen precisely so that the induction carries through on Property 2.

Now we turn to Property 3. By the induction hypothesis on Property 3, $\boldsymbol{w}_k, \boldsymbol{z}_k$ are conjugate to each other and to $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-1}$. This implies $A\boldsymbol{w}_k, A\boldsymbol{z}_k$ are conjugate to $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-2}$ since for $j = 0, \ldots, k-2$, $\boldsymbol{p}_j^T A(A\boldsymbol{w}_k) = (A\boldsymbol{p}_j)^T A\boldsymbol{w}_k$, and $A\boldsymbol{p}_j \in \text{span}\{\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-1}\}$, and similarly for $A\boldsymbol{z}_k$. Thus, we see term-by-term that every term in the definitions of $\boldsymbol{w}_{k+1}, \boldsymbol{z}_{k+1}$ in (29)–(30) is already conjugate to $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_{k-2}$. Thus, to ensure \boldsymbol{w}_{k+1} is also conjugate to \boldsymbol{p}_{k-1} and \boldsymbol{p}_k , solve a system of two linear equations for the scalars δ_1, δ_2 that appear in (29). (In fact, by conjugacy, the system decouples into two univariate linear equations that are solved via single division operations.) Similarly, to assure \boldsymbol{z}_{k+1} is conjugate to $\boldsymbol{p}_{k-1}, \boldsymbol{p}_k, \boldsymbol{w}_{k+1}$, we solve three linear equations for $\epsilon_1, \epsilon_2, \mu_{k+1}$ from (30), which again decouple into three separate equations.

Next, for Property 4, recall again from the theory of CG that minimizing $f(\boldsymbol{x})$ over $\boldsymbol{x}_{k+1} + \bar{K}_{k+1}$ for which we have a conjugate basis of \bar{K}_k reduces to k+1 uncoupled 1-dimensional minimizations; indeed, this is the main purpose of conjugacy. However, \boldsymbol{x}_{k+1} is already minimal with respect to $\boldsymbol{p}_0, \ldots, \boldsymbol{p}_k$ by the usual properties of CG, so it is necessary to minimize only with respect to $\boldsymbol{w}_{k+1}, \boldsymbol{z}_{k+1}$. Therefore, to obtain $\bar{\boldsymbol{x}}_{k+1}$, one defines

$$\bar{\boldsymbol{x}}_{k+1} := \boldsymbol{x}_{k+1} - \bar{\alpha}_{k+1} \boldsymbol{w}_{k+1} - \bar{\beta}_{k+1} \boldsymbol{z}_{k+1},$$
 (36)

where

$$(\bar{\alpha}_{k+1}, \bar{\beta}_{k+1}) := \underset{\alpha, \beta}{\operatorname{argmin}} f(\boldsymbol{x}_{k+1} - \alpha \boldsymbol{w}_{k+1} - \beta \boldsymbol{z}_{k+1}), \tag{37}$$

a problem that decouples into two simple equations.

Thus, we have established the following result:

Theorem 3 Assume the sequences $\bar{\alpha}_k$'s, $\bar{\beta}_k$'s, μ_k 's, v_k 's, w_k 's, z_k 's, and \bar{x}_k 's are defined by (10) and (26)–(37). Then Properties 1–5 above hold.

Now, finally, we can propose a progress measure assured to hold for quadratic functions, namely, $f(\bar{x}_k) \leq \phi_k^*$. The proof that this holds is a straightforward rewriting of Theorem 2.

Theorem 4 If $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{b}^T \mathbf{x}$, where A is positive definite, then $f(\bar{\mathbf{x}}_k) \leq \phi_k^*$ for every iteration k, where \mathbf{x}_k is the sequence of conjugate gradient iterates and $\bar{\mathbf{x}}_k$ is defined by (36).

Proof. The result clearly holds when k = 0 by (7) and the fact that $f(\bar{x}_0) \leq f(x_0)$ by the minimality of \bar{x}_0 in the line $x_0 + \text{span}\{w_0\}$. Assuming $f(\bar{x}_k) \leq \phi_k^*$, we now show that

 $f(\bar{x}_{k+1}) \le \phi_{k+1}^*$. For $k \ge 0$,

$$\phi_{k+1}^* = (1 - \theta_k)\phi_k^* + \theta_k f(\bar{\boldsymbol{x}}_k) - \frac{\theta_k^2}{2\gamma_{k+1}} \|\nabla f(\bar{\boldsymbol{x}}_k)\|^2 + \frac{\theta_k (1 - \theta_k)\gamma_k}{\gamma_{k+1}} \left(\ell \|\bar{\boldsymbol{x}}_k - \boldsymbol{v}_k\|^2 + \nabla f(\bar{\boldsymbol{x}}_k)^T (\boldsymbol{v}_k - \bar{\boldsymbol{x}}_k)\right)$$
(38)

$$\geq f(\bar{\boldsymbol{x}}_k) - \frac{\theta_k^2}{2\gamma_{k+1}} \|\nabla f(\bar{\boldsymbol{x}}_k)\|^2 + \frac{\theta_k (1 - \theta_k)\gamma_k}{\gamma_{k+1}} \left(\nabla f(\bar{\boldsymbol{x}}_k)^T (\boldsymbol{v}_k - \bar{\boldsymbol{x}}_k)\right)$$
(39)

$$= f(\bar{\boldsymbol{x}}_k) - \frac{1}{2L} \|\nabla f(\bar{\boldsymbol{x}}_k)\|^2 + \frac{\theta_k (1 - \theta_k) \gamma_k}{\gamma_{k+1}} \left(\nabla f(\bar{\boldsymbol{x}}_k)^T (\boldsymbol{v}_k - \bar{\boldsymbol{x}}_k) \right)$$
(40)

$$= f(\bar{x}_k) - \frac{1}{2L} \|\nabla f(\bar{x}_k)\|^2$$
(41)

$$\geq f(\bar{\boldsymbol{x}}_k - \nabla f(\bar{\boldsymbol{x}}_k)/L) \tag{42}$$

$$\geq f(\bar{\boldsymbol{x}}_{k+1}). \tag{43}$$

Here, (38) is a restatement of (11). Line (39) follows from the induction hypothesis. Line (40) follows from (13).

Line (41) follows because, according to the recursive formula (10), \mathbf{v}_k lies in the affine space $\mathbf{x}_k + \bar{K}_k$. Also, $\bar{\mathbf{x}}_k$ lies in this affine space and is optimal for f over this space. Therefore, $\nabla f(\bar{\mathbf{x}}_k)$ is orthogonal to every vector in \bar{K}_k and in particular to $\mathbf{v}_k - \bar{\mathbf{x}}_k$.

Line (42) is the standard inequality for L-smooth convex functions. Finally (43) follows because $\mathbf{x}_k - \nabla f(\mathbf{x}_k)/L = \mathbf{x}_{k+1} + \mathbf{u}_{k+1}$ by (25) and $\mathbf{u}_{k+1} \in \bar{K}_{k+1}$ by Property 2. On the other hand $\bar{\mathbf{x}}_{k+1}$ minimizes f over $\mathbf{x}_{k+1} + \bar{K}_{k+1}$.

This concludes the discussion of how to compute $\bar{\boldsymbol{x}}_{k+1}$ in the case that f is quadratic. In the general case, we do not have a matrix A but only f and ∇f . Therefore, we propose a method to evaluate the quantities in the preceding paragraphs in the general case. Assume inductively that we have $\boldsymbol{w}_k, \boldsymbol{z}_k, \hat{\boldsymbol{w}}_k, \hat{\boldsymbol{z}}_k$, where $\hat{\boldsymbol{w}}_k$ corresponds to $A\boldsymbol{w}_k$ in the above equations and similarly $\hat{\boldsymbol{z}}_k$ corresponds to $A\boldsymbol{z}_k$. Then all the formulas above may be evaluated using these vectors. Note that we already have vectors corresponding to $A\boldsymbol{p}_{k-1}$ and $A\boldsymbol{p}_k$; these are found in (4)–(6). We need these vectors to solve for the scalars $\delta_1, \delta_2, \epsilon_1, \epsilon_2$ assuring conjugacy.

To continue the induction, it is necessary to evaluate $\hat{\boldsymbol{w}}_{k+1}, \hat{\boldsymbol{z}}_{k+1}$ corresponding to $A\boldsymbol{w}_{k+1}, A\boldsymbol{z}_{k+1}$. Multiplying both sides of (29) and (30) by the fictitious A shows that we need to obtain the analog of the product $A(\bar{\alpha}_k A\boldsymbol{w}_k + \bar{\beta}_k A\boldsymbol{z}_k)$. Note that this combination of $A\boldsymbol{w}_k, A\boldsymbol{z}_k$ appears in both right-hand sides of (29) and (30). This may be found by evaluating $\nabla f(\boldsymbol{x}_{k+1} + \bar{\alpha}_k \hat{\boldsymbol{w}}_k + \bar{\beta}_k \hat{\boldsymbol{z}}_k)$ and then subtracting $\nabla f(\boldsymbol{x}_{k+1})$ (which is already evaluated).

We also need to evaluate $f(\bar{x}_{k+1})$ and $\nabla f(\bar{x}_{k+1})$ in order to obtain (25) and check the progress measure $f(\bar{x}_{k+1}) \leq \phi_{k+1}^*$. Thus, the cost of carrying out the method of this section is two extra function-gradient evaluations per iteration. As mentioned earlier, our computational experiments indicate that this 100% overhead is not compensated for by any reduction in iteration count in any test case, and therefore the method described in this section is disabled by default.

B Toward *n*-step quadratic convergence

In previous sections, we showed the proposed C+AG method has the same complexity bound up to a constant factor as accelerated gradient. In this section we suggest that it has an additional complexity bound known to apply to nonlinear conjugate gradient, namely, n-step quadratic convergence. This property is mainly of theoretical interest since n-step quadratic convergence is not usually observed in practice (see, e.g., [21, p. 124]) for larger problems. Therefore, we will provide only a sketch of a possible proof and leave the proof, which is likely to be complicated, to future research.

We propose to follow the proof given by McCormick and Ritter [17] rather than the original proof by Cohen [5]. They argue that classical NCG is n-step quadratically convergent provided that the line-search is sufficiently accurate and provided that the objective function is strongly convex in the neighborhood of the objective function and that its second derivative is Lipschitz continuous. Finally, they assume that nonlinear CG is restarted every n iterations.

In order to apply this result to C+AG, we first need to argue that the sufficient-progress test will not prevent CG iterations. We showed in the last section that for quadratic functions, the sufficient-progress test always holds. A strongly convex function with a Lipschitz second derivative is approximated arbitrarily closely by a quadratic function in a sufficiently small neighborhood of the root. In particular, if we assume that L is strictly larger than the largest eigenvalue of the Hessian in a neighborhood of the root, then inequality (42) is strictly satisfied, and small deviations from a quadratic function are dominated by the residual in (42).

Some other issues with [17] is that their version of NCG implements a step-limiter operation that is not present in our algorithm. It is not clear whether the step-limiter is a requirement for n-step quadratic convergence or merely a device to simplify their analysis. Furthermore, [17] assume the Polak-Ribière choice of β_k [21] rather than the Hager-Zhang step that we used. Note that [17] predates [12] by several decades. We conjecture that the analysis of [17] extends to [12].

The line-search accuracy required by [17] is as follows. On each iteration k, $|\alpha_k - \alpha_k^*| \le O(\|\boldsymbol{p}_k\|)$, where α_k is chosen by C+AG in (4)–(6) and $\alpha_k^* = \operatorname{argmin}\{f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k) : \alpha \in \mathbb{R}\}$. We sketch an argument that could prove $|\alpha_k - \alpha_k^*| \le O(\|\boldsymbol{p}_k\|)$ as follows.

Let $\psi(\alpha) := f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)$. It follows from [17] that $\|\boldsymbol{p}_k\| = \Theta(\|\boldsymbol{x}_k - \boldsymbol{x}^*\|)$. In other words, there is both an upper and lower bound on

$$rac{\|oldsymbol{p}_k\|}{\|oldsymbol{x}_k - oldsymbol{x}^*\|}$$

independent of k. It also follows from their results that $\psi'(0) < 0$. Write $\psi''(\alpha) = s + \epsilon(\alpha)$, where s > 0 is the estimate of ψ'' obtained from (4)–(6), that is $s = L(\psi'(1/L) - \psi'(0))$. It follows by strong convexity and the equation $\|\boldsymbol{p}_k\| = \Theta(\|\boldsymbol{x}_k - \boldsymbol{x}^*\|)$ that $\alpha_k \leq O(1)$ and $\alpha_k^* \leq O(1)$. Again by these same assumptions, we can also derive that $s = \Theta(\|\boldsymbol{p}_k\|^2)$. By the Lipschitz assumption, $\epsilon(\alpha) \leq O(\|\boldsymbol{p}_k\|^3)$ for $\alpha \leq O(1)$.

It also follows from the assumption of strict convexity and proximity to the root $|\psi'(0)| \leq O(\|\boldsymbol{p}_k\|^2)$. The true minimizer α_k^* is the root of ψ' and therefore satisfies the

equation

$$\psi'(0) + \int_0^{\alpha_k^*} (s + \epsilon(\alpha)) d\alpha = 0,$$

i.e.,

$$\psi'(0) + s\alpha_k^* + \int_0^{\alpha_k^*} \epsilon(\alpha) \, d\alpha = 0.$$

The computed minimizer is $\alpha_k = -\psi'(0)/s$. The integral in the previous line is bounded by $O(\|\boldsymbol{p}_k\|^3)$, whereas $-\psi'(0)$ is $O(\|\boldsymbol{p}_k\|^2)$, and $s = \Theta(\|\boldsymbol{p}_k\|^2)$. Therefore, the intermediate value theorem applied to the above univariate equation for α_k^* tells us that $\alpha_k^* = -\psi'(0)/s + O(\|\boldsymbol{p}_k\|) = \alpha_k + O(\|\boldsymbol{p}_k\|)$. This concludes the explanation of accuracy of the line-search.

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