

# REGULARIZED STEP DIRECTIONS IN CONJUGATE GRADIENT MINIMIZATION FOR MACHINE LEARNING

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ABSTRACT. Conjugate gradient minimization methods (CGM) and their accelerated variants are widely used in machine learning applications. We focus on the use of cubic regularization to improve the CGM direction independent of the steplength (learning rate) computation. Using Shanno’s reformulation of CGM as a memoryless BFGS method, we derive new formulas for the regularized step direction, which can be evaluated without additional computational effort. The new step directions are shown to improve iteration counts and runtimes and reduce the need to restart the CGM.

## 1. INTRODUCTION

The unconstrained nonlinear programming problem (NLP) has the form

$$(1) \quad \min_x f(x)$$

where  $x \in \mathbb{R}^n$  and  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ . We assume that  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is smooth and its Hessian is Lipschitz continuous on at least the set  $\{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$ . There are a number of different methods for solving (1) that are usually classified by the amount of derivative information used. For instances where function, gradient, or Hessian evaluations may be unavailable or expensive to evaluate, store, or manipulate, the choice of algorithm may be dictated by what is computationally tractable. Whenever all quantities are readily available, the comparative performance is generally one where there is a trade-off between the number of iterations and the amount of work done per iteration.

In this paper, we focus on conjugate gradient minimization methods (CGM), which are first-order methods for solving (1). These methods are also referred to as *nonlinear conjugate gradient methods* in literature to differentiate them from the classical conjugate gradient methods that were outlined in Hestenes and Stiefel (1952) to solve a linear system of equations. In the context of machine learning, CGM has been successfully used to solve pattern recognition problems (Adeli and Samant (2000), Orozco and García (2003), Khadse et al. (2016a,b)) and in other predictive and classification applications (Saini and Soni (2002), Sözen et al. (2004), Çınar et al. (2009), Azar (2013), Li et al. (2016), Selvamuthu et al. (2019)). It is designed to improve on using only the gradient direction by adding a momentum term: while solving (1), CGM generates a sequence of iterates  $\{x_k\}$  such that

$$(2) \quad \begin{aligned} x_{k+1} &= x_k + \alpha_k \Delta x_k \\ \Delta x_{k+1} &= -\nabla f(x_{k+1}) + \beta_k \Delta x_k, \end{aligned}$$

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where  $\alpha_k$  is the steplength,  $\Delta x_k$  is the step direction, and  $\beta_k$  is a scalar defined as

$$(3) \quad \beta_k = \frac{\nabla f(x_{k+1})^T y_k}{y_k^T \Delta x_k}.$$

Here, we use the standard notation  $y_k := \nabla f(x_{k+1}) - \nabla f(x_k)$ .

If an exact linesearch is used, under the smoothness assumption,  $\alpha_k$  satisfies the first order condition  $\Delta x_k^T \nabla f(x_k + \alpha_k \Delta x_k) = 0$ , or  $\Delta x_k^T \nabla f(x_{k+1}) = 0$ . Under the same assumptions, it can also be shown that  $\Delta x_k^T \nabla f(x_k) = -\nabla f(x_k)^T \nabla f(x_k)$ . Therefore, with exact line search, (3) can be written as

$$(4) \quad \beta_k = \frac{\nabla f(x_{k+1})^T y_k}{\nabla f(x_k)^T \nabla f(x_k)}.$$

This form of  $\beta_k$  gives the Polak-Ribiere formula (Polak and Ribiere (1969)). If  $f$  is quadratic, then (4) further reduces to

$$(5) \quad \beta_k = \frac{\nabla f(x_{k+1})^T \nabla f(x_{k+1})}{\nabla f(x_k)^T \nabla f(x_k)},$$

which is the Fletcher-Reeves formula (Fletcher and Reeves (1964)).

While the momentum term generally yields an improvement over the steepest descent direction, two concerns still remain:

- (1) The step directions can fail to satisfy the conjugacy condition, and
- (2) The step length calculation can be a bottleneck for runtime as it requires multiple function evaluations.

The first concern can have a significant impact on the number of iterations to reach the solution of (1). In fact, it is shown in Powell (1976) and Crowder and Wolfe (1972) that CGM as defined by (2) and (3) exhibits a linear rate of convergence unless restarted every  $n$  iterations with the steepest descent direction. Moreover, in addition to restarting the method every  $n$  iterations, Powell (1977) proposed to use a restart whenever the algorithm moves too far from conjugacy, or more precisely when

$$(6) \quad |\nabla f(x_{k+1})^T \nabla f(x_k)| \geq 0.2 \|\nabla f(x_{k+1})\|^2.$$

In this paper, a restart that occurs after (6) will be called a *Powell restart*. We will show in the numerical results section that nearly all of the problems in our test set require at least one Powell restart and, on average, nearly half of all iterations are Powell restart iterations. Therefore, in order to truly distinguish CGM from steepest descent and improve the rate of convergence, we need a mechanism to improve the step directions. A formal definition of “improvement” will be provided in the next section.

The second concern is about the step length calculation and impacts the amount of effort required per iteration, and, thus, the runtime of the algorithm. An exact line search seeks to find a steplength  $\alpha^*$  which solves

$$(7) \quad \min_{\alpha} \Phi(\alpha) = f(x + \alpha \Delta x)$$

for a given point  $x$  and step direction  $\Delta x$ . For a general nonlinear function  $f$ , this minimization problem in one variable ( $\alpha$ ) is usually “solved” using an iterative approach such as bisection or cubic interpolation, even though these approaches cannot find the exact value of the minimizing  $\alpha$  within a finite number of iterations. For specific forms of  $f$ , such as a strictly convex quadratic function, a formula can be used to directly calculate the minimizing  $\alpha$  without the need for an iterative approach. We should also note that at the solution of the exact line search,  $\Phi'(\alpha) = \nabla f(x + \alpha \Delta x)^T \Delta x = 0$ .

By contrast, an inexact line search only seeks to approximately minimize  $\Phi(\alpha)$ , requiring lower levels of accuracy when the iterates  $x_k$  are away from a stationary point of  $f$ . In order to maintain

theoretical guarantees, most inexact line search techniques rely on guaranteeing *sufficient descent*, that is,  $f(x) - f(x + \alpha\Delta x)$  must be sufficiently large according to some criterion. The Armijo criterion is given by

$$f(x + \alpha\Delta x) < f(x) + \epsilon_1 \alpha \nabla f(x)^T \Delta x,$$

and it is accompanied by the curvature condition

$$-\nabla f(x + \alpha\Delta x)^T \Delta x \leq \epsilon_2 \nabla f(x)^T \Delta x,$$

for constants  $0 < \epsilon_1 < \epsilon_2 < 1$ . The two conditions together are called the *Wolfe conditions*. The curvature condition can also be modified as

$$|\nabla f(x + \alpha\Delta x)^T \Delta x| \leq \epsilon_2 |\nabla f(x)^T \Delta x|$$

to give the *Strong Wolfe conditions*.

While the two best-known forms of CGM are given by (4) and (5) above, they do rely on using an exact line search. This means that when an explicit formula for directly computing the minimizing  $\alpha$  is not available, the function  $f$  and/or its gradient must be evaluated multiple times for an iterative line search within each iteration of the CGM algorithm. Doing so can be costly if  $n$  is large or if the function evaluation is time consuming. For machine learning problems, many gradient-based algorithms choose a fixed step length (also referred to as the learning rate) or use an adaptive approach to setting it. Adagrad (Duchi et al. (2011)), Adadelta (Zeiler (2012)), RMSprop (Hinton et al. (2012)), and Adam (Kingma and Ba (2014)) are examples of adaptive learning rate approaches with good performance, but their use does not currently extend to CGM.

In this paper, we propose a cubic regularization variant of CGM, that combines ideas from Benson and Shanno (2014) and Benson and Shanno (2018) to selectively use cubic regularization when solving (1) and from Shanno (1978b) to recast CGM as “memoryless BFGS” and apply an inexact line search. The resulting approach is shown to reduce the need for Powell restarts and to (approximately) optimize the step direction without the typical overload of additional function evaluations. We show in the numerical results that our implementation improves iteration counts and run time on the CUTER test set (Bongartz et al. (1995)) and on randomly generated machine learning problems. As noted in Griewank (1981) and Benson and Shanno (2014), the approach has an inherent connection to Levenberg-Marquardt’s method (Levenberg (1944), Marquardt (1963)) and is, therefore, related to the scaled conjugate gradient method proposed in Møller (1993) for training neural networks. Scaled CGM is the default training function for Matlab’s pattern recognition neural network function, `patternnet` (MathWorks (2021)).

In the next section, we introduce the central question of our research and set the vocabulary and notation for the remainder of the paper. Given the extensive body of literature our work pulls from, we believe that clarifying our goals and our scope into a single framework is necessary to clearly communicate our proposed approach and put our results into perspective. We then introduce the cubic regularization of CGM, including a review of the memoryless BFGS formulation proposed by Shanno (Shanno (1978b)), the explicit formulae for the regularized step direction, and the corresponding method for choosing the step length. Unlike other applications of cubic regularization, such as Cartis et al. (2011), Benson and Shanno (2014), Benson and Shanno (2018), the regularized step in our framework can be computed without significant overhead beyond that required for (2) with (3). Moreover, we show that the burden of optimizing the step length can be shifted to optimizing the regularization parameter, which does not require as many function or gradient evaluations as solving (7). In Section 3, we present some theoretical results on computational complexity per iteration, as well as global convergence. Numerical results are given in Section 4.

## 2. CUBIC REGULARIZATION FOR CGM

As discussed, CGM is designed to be an “accelerated” version of steepest descent. The momentum term for the step direction is obtained cheaply so as not to increase the computational burden

over the gradient direction, and the local convergence rate is improved from linear to superlinear. However, if the step direction moves away from conjugacy and CGM has to be restarted frequently, CGM will behave more like steepest descent.

The goal of this paper is to propose a regularized method to improve step quality within CGM. Specifically, we aim for this method to

- require fewer iteration counts in computational experiments than its non-regularized version,
- exhibit global convergence with fewer assumptions than its non-regularized version,
- require the same order of computational burden per iteration as its non-regularized version, and
- demonstrate faster overall runtime in computational experiments than its non-regularized version.

In this section, we will present our proposed cubic regularization scheme and its related step length rules. The integration of cubic regularization for CGM will be closer to the approach taken in Benson and Shanno (2014)—we will use the equivalence of cubic regularization to the Levenberg-Marquardt method in order to view it as a regularization of the (approximate) Hessian matrix. (Our previous paper on symmetric rank-1 methods with cubic regularization Benson and Shanno (2018) took the approach of modifying the secant equation, which we are not proposing here but will leave for future work.) Since the formulation of CGM given by (2) and (3) was matrix-free, we will use Shanno’s reformulation of CGM as a memoryless BFGS method (Shanno (1978b)). We start with a brief review of the reformulation and then present the proposed new approach.

**2.1. Memoryless BFGS Formulation of CGM.** It was shown in Shanno (1978b) that a version of CGM is equivalent to a memoryless BFGS method, and we will use that equivalence here to build our cubic regularization approach. First, as a reminder and to set notation, the direction is calculated as

$$\Delta x_k = -H_k \nabla f(x_k),$$

where  $H_k \approx (\nabla^2 f(x_k))^{-1}$ , with  $H_0 = I$  and  $H_{k+1}$  obtained using the BFGS update formula

$$(8) \quad H_{k+1} = H_k - \frac{H_k y_k p_k^T + p_k y_k^T H_k}{p_k^T y_k} + \left(1 + \frac{y_k^T H_k y_k}{p_k^T y_k}\right) \frac{p_k p_k^T}{p_k^T y_k}.$$

Here,  $y_k$  is as before and  $p_k = \alpha_k \Delta x_k$ . A memoryless BFGS method would mean that the updates are not accumulated, that is,  $H_k$  is replaced by  $I$  in the update formula and

$$(9) \quad H_{k+1} = I - \frac{y_k p_k^T + p_k y_k^T}{p_k^T y_k} + \left(1 + \frac{y_k^T y_k}{p_k^T y_k}\right) \frac{p_k p_k^T}{p_k^T y_k}.$$

To derive the equivalence, Shanno (Shanno (1978b)) notes that Perry (Perry (1978)) expressed (2)-(4) in matrix form as

$$(10) \quad \Delta x_{k+1} = - \left( I - \frac{p_k y_k^T}{p_k^T y_k} + \frac{p_k p_k^T}{p_k^T y_k} \right) \nabla f(x_{k+1}).$$

Shanno (Shanno (1978b)) notes that the matrix in this formulation is not symmetric and adds a further correction:

$$\Delta x_{k+1} = - \left( I - \frac{p_k y_k^T}{y_k^T p_k} - \frac{y_k p_k^T}{y_k^T p_k} + \frac{p_k p_k^T}{p_k^T y_k} \right) \nabla f(x_{k+1}).$$

Finally, to ensure that a secant condition is satisfied, the last term in the matrix is re-scaled:

$$(11) \quad \Delta x_{k+1} = - \left[ I - \frac{p_k y_k^T}{y_k^T p_k} - \frac{y_k p_k^T}{y_k^T p_k} + \left(1 + \frac{y_k^T y_k}{p_k^T y_k}\right) \frac{p_k p_k^T}{p_k^T y_k} \right] \nabla f(x_{k+1}).$$

The matrix term is exactly the formula (9) for the memoryless BFGS update.

It is important to note here that, unlike in BFGS, we do not need to store a matrix or a series of updates to calculate  $\Delta x_{k+1}$  using (11). Multiplying  $\nabla f(x_{k+1})$  through the matrix in (11) simply requires dot-products, scalar-vector multiplications, and vector addition and subtraction. As such, each update only requires the storage of 3 vectors of length  $n$  and  $O(n)$  operations.

Furthermore, for an exact line search, (11) reduces to the Polak-Ribiere formula (4), thereby ensuring that our proposed cubic regularization approach remains valid in that case as well. Finally, one advantage of using (11) for CGM is that the criterion  $p_k^T y_k > 0$  is always satisfied, which ensures that the sequence of step directions it produces remain stable and is required for most proofs of global convergence, such as the one proposed by Lenard (1973).

2.1.1. *Initializations and Restarts.* In the first iteration, CGM can be initialized using the gradient. However, a two-step process based on the self-scaling proposed in (Oren and Spedicato (1976)) has demonstrated better stability and improved iteration counts. We will use the same initialization scheme so that

$$(12) \quad \begin{aligned} H_0 &= I \\ H_1 &= \frac{p_0^T y_0}{y_0^T y_0} \left( I - \frac{p_0 y_0^T + y_0 p_0^T}{p_0^T y_0} + \frac{y_0^T y_0 p_0 p_0^T}{p_0^T y_0 p_0^T y_0} \right) + \frac{p_0 p_0^T}{p_0^T y_0}. \end{aligned}$$

As discussed, CGM is restarted every  $n$  iterations (Beale restart) and when condition (6) is satisfied (Powell restart). The Hessian approximation at the most recent restart iteration  $t$  is given by

$$(13) \quad H_t = \frac{p_t^T y_t}{y_t^T y_t} \left( I - \frac{p_t y_t^T + y_t p_t^T}{p_t^T y_t} + \frac{y_t^T y_t p_t p_t^T}{p_t^T y_t p_t^T y_t} \right) + \frac{p_t p_t^T}{p_t^T y_t},$$

which matches the initialization process given by (12).

We incorporate these changes into our approach by replacing  $H_k$  in (8) with  $H_t$  as given in (13) instead of  $I$ . As such, the formula for the step direction is also modified from (11) to

$$(14) \quad \Delta x_{k+1} = - \left[ H_t - \frac{H_t y_k p_k^T + p_k y_k^T H_t}{p_k^T y_k} + \left( 1 + \frac{y_k^T H_t y_k}{p_k^T y_k} \right) \frac{p_k p_k^T}{p_k^T y_k} \right] \nabla f(x_{k+1}).$$

Note that  $H_t \nabla f(x_{k+1})$  and  $H_t y_k$  can be obtained via dot products and scalar-vector multiplications, so there is still no need to compute or store a matrix. With these modifications, the CGM algorithm can be fully described as Algorithm 1.

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Pick a suitable  $x_0$  and  $\epsilon > 0$ .
Let  $\Delta x = -\nabla f(x_0)$ , choose  $\alpha$  to solve (7), and let  $x_1 = x_0 + \alpha \Delta x$ .
Set  $k = 1$  and  $t = 1$ .
while  $\|\nabla f(x^k)\| > \epsilon$  do
  if  $(k - t) \bmod n = 0$  (Beale restart) OR (6) is satisfied (Powell restart) then
     $t \leftarrow k$ 
     $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (13).
  else
     $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (14).
  end
  Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
   $x_{k+1} \leftarrow x_k + \alpha \Delta x$ .
   $k \leftarrow k + 1$ .
end

```

**Algorithm 1:** The memoryless BFGS reformulation of CGM, as given by Shanno (1978b).

**2.2. Cubic Regularization for Quasi-Newton Methods.** The step-direction,  $\Delta x$ , used by a quasi-Newton's method minimizes

$$(15) \quad f_N(x_k + \Delta x) := f(x_k) + \nabla f(x_k)^T \Delta x + \frac{1}{2} \Delta x^T B_k \Delta x,$$

where  $B_k \approx \nabla^2 f(x_k)$  and  $H_k = B_k^{-1}$ .

To obtain the cubic regularization formula, we also define

$$(16) \quad f_M(x_k + \Delta x) := f(x_k) + \nabla f(x_k)^T \Delta x + \frac{1}{2} \Delta x^T B_k \Delta x + \frac{M}{6} \|\Delta x\|^3,$$

where  $M$  is the approximation to the Lipschitz constant for  $\nabla^2 f(x)$ . The cubic step direction is found by solving the problem

$$(17) \quad \Delta x \in \arg \min_s f_M(x^k + s).$$

In Griewank (1981), Nesterov and Polyak (2006), and Cartis et al. (2011), it is shown that for sufficiently large  $M$ ,  $x_k + \Delta x$  will satisfy an Armijo condition and that a line search is not needed when using cubic regularization within a quasi-Newton method or Newton's method. In this new framework, we need to control  $M$  rather than  $\alpha$ . In Cartis et al. (2011), the ARC method starts with a sufficiently large value of  $M$  that is decreased through the iterations and approaches (or is set to) 0 in a neighborhood of the solution. In Benson and Shanno (2014) and Benson and Shanno (2018), the authors proposed setting  $M = 0$  for all iterations where the Hessian or its estimate are positive definite and picking a value of  $M$  using iteration-specific data only as needed.

In order to motivate the selective use of cubic regularization, we observe that determining  $\Delta x$  using (16)-(17) is nontrivial as it involves the solution of an unconstrained NLP. In Cartis et al. (2011), the authors show that it suffices to solve (17) only approximately in order to achieve global convergence.

Moreover, the use of cubic regularization during iterations with negative curvature is based on its equivalence to the Levenberg-Marquardt method. To see the equivalence, let us examine the solution of (17). Note that the first-order necessary conditions for the optimization problem are

$$(18) \quad \nabla f(x_k) + \left( B_k + \frac{M}{2} \|s\| I \right) s = 0.$$

Similarly, the Levenberg-Marquardt method replaces  $B_k$  with  $B_k + \lambda I$  for a sufficiently large  $\lambda > 0$  to satisfy certain descent criteria. (A Levenberg-Marquardt-based variant of CGM was proposed by Møller (1993) as scaled conjugate gradient methods and remains a popular approach for training neural networks.) Note that the step,  $\Delta x$ , obtained by solving

$$(B_k + \lambda I) \Delta x = -\nabla f(x^k),$$

satisfies (18) when

$$M = \frac{2\lambda}{\|\Delta x\|}.$$

(Further details of the equivalence are provided in Benson and Shanno (2014).) Thus, we simply re-interpret the cubic regularization step as coming from a Levenberg-Marquardt regularization of the CGM step with appropriately related values of  $\lambda$  and  $M$ . (A similar insight was mentioned in Weiser et al. (2007) but not explicitly used.) If this direction is not accepted, then we increase  $\lambda$ .

**2.3. Cubic Regularization for CGM.** We posit here that the theoretical difficulties encountered by CGM can be similarly addressed via the cubic regularization approach, without reducing and potentially even improving its overall solution time. In this section, we start by deriving the update formula for an iteration during which cubic regularization is used. Then, we will show the impact of using cubic regularization to reduce the need for restarts in the algorithm. In Section 4, our numerical results show the effectiveness of this approach in practice.

As discussed in the previous section, the use of cubic regularization necessitates that we add a term to the approximate Hessian, that is compute the step direction  $\Delta x_k$  using  $B_{k+1} + \lambda I$ , instead of  $B_{k+1}$ . While the regularization is applied to the approximate Hessian itself, the CGM update formula (8) updates the inverse of the approximate Hessian, that is  $H_{k+1} = (B_{k+1})^{-1}$ . As such, in order to compute the regularized step direction, we need to compute  $(B_{k+1} + \lambda I)^{-1}$ . In previous papers that use regularization with BFGS or with Newton's Method, there is no direct formula for computing this inverse. As such, the solution of multiple linear systems may be required at each iteration until a suitable  $\lambda$  value is found, which means that despite improved step directions that reduce the number of iterations, the effort and time per iteration increase, potentially increasing overall solution time as well.

When applying the regularization to the CG update formula, however, we can derive an explicit formula for  $(B_{k+1} + \lambda I)^{-1}$ . This is a significant advantage for CGM, in that the use of cubic regularization does not incur additional computational burden at each iteration.

We start by showing the formulae for  $B_t$  and  $B_{k+1}$ .

$$(19) \quad B_t = (\hat{H}_t^{-1}) = \begin{pmatrix} y_t^T y_t \\ p_t^T y_t \end{pmatrix} \begin{pmatrix} I - \frac{p_t p_t^T}{p_t^T p_t} + \frac{y_t y_t^T}{y_t^T y_t} \end{pmatrix}$$

$$(20) \quad B_{k+1} = (\hat{H}_{k+1}^{-1}) = B_t - \frac{B_t p_k p_k^T B_t}{p_k^T B_t p_k} + \frac{y_k y_k^T}{p_k^T y_k}$$

Next, we will apply the regularization to  $B_{k+1}$  and take its inverse. To do so, we will first need to compute the inverse of  $B_t + \lambda I$  (henceforth referred to as  $H_t(\lambda)$ ):

$$(21) \quad \begin{aligned} H_t(\lambda) &= (B_t + \lambda I)^{-1} \\ &= \frac{p_t^T y_t}{c} I + \frac{ab}{c(\lambda b + a)} p_t p_t^T - \frac{\lambda}{c(\lambda b + a)} y_t y_t^T - \frac{a}{c(\lambda b + a)} (p_t y_t^T + y_t p_t^T), \end{aligned}$$

where

$$a = \frac{y_t^T y_t}{p_t^T p_t}, \quad b = 2 \frac{y_t^T y_t}{p_t^T y_t} + \lambda, \quad c = y_t^T y_t + \lambda p_t^T y_t.$$

It is easy to verify that when  $\lambda = 0$ , (21) reduces to (13).

We can finally write the formula for computing the inverse of  $B_{k+1} + \lambda I$  (henceforth referred to as  $H_{k+1}$ ):

$$(22) \quad \begin{aligned} H_{k+1}(\lambda) &= (B_{k+1} + \lambda I)^{-1} \\ &= \left( B_t + \lambda I - \frac{B_t p_k p_k^T B_t}{p_k^T B_t p_k} + \frac{y_k y_k^T}{p_k^T y_k} \right)^{-1} \\ &= (B_t + \lambda I)^{-1} \\ &\quad + \frac{p_k^T y_k + y_k^T (B_t + \lambda I)^{-1} y_k}{d} (B_t + \lambda I)^{-1} (B_t p_k) (B_t p_k)^T (B_t + \lambda I)^{-1} \\ &\quad - \frac{p_k^T B_t p_k - (B_t p_k)^T (B_t + \lambda I)^{-1} B_t p_k}{d} (B_t + \lambda I)^{-1} y_k y_k^T (B_t + \lambda I)^{-1} \\ &\quad - \frac{(B_t p_k)^T (B_t + \lambda I)^{-1} y_k}{d} (B_t + \lambda I)^{-1} (B_t p_k) y_k^T (B_t + \lambda I)^{-1} \\ &\quad - \frac{y_k^T (B_t + \lambda I)^{-1} B_t p_k}{d} (B_t + \lambda I)^{-1} y_k (B_t p_k)^T (B_t + \lambda I)^{-1}, \end{aligned}$$

where the denominator  $d$  is given by

$$d = (p_k^T y_k + y_k^T (B_t + \lambda I)^{-1} y_k) (p_k^T B_t p_k - (B_t p_k)^T (B_t + \lambda I)^{-1} (B_t p_k)) + ((B_t p_k)^T (B_t + \lambda I)^{-1} y_k)^2.$$

In order to see that the formula (22) consists of a sum of rank-1 updates to  $H_t(\lambda)$ , we introduce the following intermediate calculation:

$$\tilde{p}_k = (B_t + \lambda I)^{-1} B_t p_k = \frac{y_t^T y_t}{c} p_k + \frac{\lambda a b p_t^T p_k}{c(\lambda b + a)} p_t - \frac{\lambda^2 y_t^T p_k}{c(\lambda b + a)} y_t - \frac{\lambda a y_t^T p_k}{c(\lambda b + a)} p_t - \frac{\lambda a p_t^T p_k}{c(\lambda b + a)} y_t$$

and rewrite (22) as

$$(23) \quad \begin{aligned} H_{k+1}(\lambda) = & H_t(\lambda) - \frac{\tilde{p}_k^T y_k}{d} (\tilde{p}_k y_k^T H_t(\lambda) + H_t(\lambda) y_k \tilde{p}_k^T) \\ & + \frac{p_k^T y_k + y_k^T H_t(\lambda) y_k}{d} \tilde{p}_k \tilde{p}_k^T \\ & - \frac{p_k^T B_t p_k - p_k^T B_t \tilde{p}_k}{d} H_t(\lambda) y_k y_k^T H_t(\lambda), \end{aligned}$$

and  $d$  as

$$d = (p_k^T y_k + y_k^T H_t(\lambda) y_k)(p_k^T B_t p_k - p_k^T B_t \tilde{p}_k) + (y_k^T \tilde{p}_k)^2.$$

When  $\lambda = 0$ , we have that  $\tilde{p}_k = p_k$  and, therefore, (22) reduces to (8).

**2.4. Setting a Value for  $\lambda$ .** Now that we know how to calculate a step direction with cubic regularization, we need to answer two questions:

- (1) When do we apply cubic regularization?
- (2) When applying cubic regularization, how do we choose a value for  $\lambda$ ?

The answer to the first question determines how we answer the second one. As shown above, the computation of the regularized step direction does not require significantly more effort than the unregularized one, so it remains to be seen whether being selective with when to apply the regularization is as important for CGM as it was for Newton's method and quasi-Newton methods.

To start with, we decided to try finding a pair  $(\lambda, \alpha)$  which minimized  $f(x_k + \alpha \Delta x)$ , where  $\Delta x$  was calculated from a regularized step in every iteration. Our preliminary numerical studies showed that this approach reduced the number of iterations for many of the problems, but it significantly worsened the computational effort per iteration by requiring an iterative approach that simultaneously optimized over two variables.

Instead, using Benson and Shanno (2014) as a guide, we pursued the following approach: selectively use cubic regularization whenever the unregularized step direction failed to satisfy the Powell criterion, was not a descent direction, or resulted in a line search failure. The assumption here is that cubic regularization "improves" the step direction in some sense, so it should be deployed when the step direction needs such improvement. In our numerical studies, there were few to no instances of failure to obtain a descent direction or line search failure, so we could not reliably assess the impact of cubic regularization. However, the prevalence of Powell restarts, as will be noted in Section 4, provided a good opportunity to test potential improvements.

When the unregularized step leads to a Powell restart, we will set  $\lambda > 0$  and try a regularized step, with increasing values of  $\lambda$  until it no longer results in a Powell restart. The initial value of  $\lambda$  for a Powell restart is computed as

$$(24) \quad \lambda = 5 \frac{|\nabla f(x_{k+1})^T \nabla f(x_k)|}{\|\nabla f(x_{k+1})\|^2}.$$

and doubled as needed. For each value of  $\lambda$ , we will choose a corresponding optimal  $\alpha$ . We have also added a safeguard to bound the number of  $\lambda$  updates by a constant  $U$ , which helps the numerical stability and convergence results of the algorithm. If the number of updates reaches  $U$ , we perform a restart, however, in our numerical testing, this bound was never invoked.

With all the details complete, we now describe the approach, called *Hybrid Cubic Regularization of CGM*, as Algorithm 2.

### 3. THEORETICAL RESULTS

As stated at the beginning of Section 2, we had four dimensions to our goal of improving step quality within CGM. Two of those goals were theoretical in nature:

- exhibit global convergence with fewer assumptions than its non-regularized version.

```

Pick a suitable  $x_0$ ,  $U$ , and  $\epsilon > 0$ .
Let  $\Delta x = -\nabla f(x_0)$ , choose  $\alpha$  to solve (7), and let  $x_1 = x_0 + \alpha\Delta x$ .
Set  $k = 1$  and  $t = 1$ .
while  $\|\nabla f(x^k)\| > \epsilon$  do
  if  $(k - t) \bmod n = 0$  (Beale restart) then
     $t \leftarrow k$ 
     $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (13).
    Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
  else
    if (6) is satisfied (Cubic Regularization) then
      Reset  $k \leftarrow k - 1$ ,  $u \leftarrow 1$ , and initialize  $\lambda$  using (24).
       $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (23).
      Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
      while (6) is satisfied and  $u < U$  do
         $\lambda \leftarrow 2\lambda$ ,  $u \leftarrow u + 1$ .
         $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (23).
        Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
      end
      if  $u == U$  then
         $t \leftarrow k$ 
         $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (13).
        Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
      end
    else
       $\Delta x \leftarrow -H_k \nabla(x_k)$ , where  $H_k$  is defined by (14).
      Choose  $\alpha$  to solve (7) given  $x_k$  and  $\Delta x$ .
    end
  end
   $x_{k+1} \leftarrow x_k + \alpha\Delta x$ .
   $k \leftarrow k + 1$ .
end

```

**Algorithm 2:** The hybrid cubic regularization of CGM as described in Section 2.3.

- require the same order of computational burden per iteration as its non-regularized version

In this section, we will demonstrate that we have achieved both of these goals. Since we have mentioned the second goal already, we will start with formalizing it first.

**3.1. Computational Burden per Iteration.** We start by showing that the additional work per iteration performed by Algorithm 2 does not grow with the size of the problem.

**Theorem 1.** *Computational effort per iteration for Algorithm 2 is of the same order as the computational effort per iteration for Algorithm 1.*

*Proof.* Proof. The Beale restart and the unregularized steps in Algorithm 2 match those of Algorithm 1. Therefore, we only need to analyze the steps with cubic regularization. We know that we will need to try at most  $U$  different  $\lambda$  values to exit the while-loop in the cubic regularization step with a descent direction that satisfies (6) or with a restart. We can also see that all of the components required to compute  $\Delta x$  with cubic regularization using (23), that is  $H_t(\lambda)$ ,  $\tilde{p}_k$ ,  $B_t$ , and  $d$ , can all be obtained using vector-vector and scalar-vector operations of the form that does not necessitate the calculation or storage of a matrix to obtain  $-H_{k+1}\nabla f(x_k)$ . The vectors

used in these calculations are the same ones as before ( $y_t$ ,  $p_t$ ,  $y_k$ , and  $p_k$ ), which means that the computational burden per iteration of the new approach remains the same as in Algorithm 1.  $\square$

**3.2. Global Convergence.** We now show that Algorithm 2 is globally convergent. If the Powell restart/cubic regularization step is not invoked, Algorithm 2 is equivalent to Algorithm 1, so in that case, we will call on the convergence results shown in Shanno (1978a). Therefore, it suffices to analyze the iterations with cubic regularization.

The key feature of the convergence result in Shanno (1978a) is that the condition number of  $H_k$  remains bounded above under mild assumptions. Since the only change to the algorithm is to replace  $H_k$  with  $H_k(\lambda) = (B_k + \lambda I)^{-1}$  in the cubic regularization step, we need to only examine the condition number of  $H_k(\lambda)$  in order to use the rest of the proofs given in Shanno (1978a). Before we do so, it is important for us to note that the two main assumptions in Shanno (1978a) are that the objective function remains bounded below and that the Hessian estimate remains positive definite.

**Lemma 2.** *Let us denote the condition number of a matrix  $W$  by  $\kappa(W)$ . Then, for  $\lambda > 0$ ,*

$$\kappa((W^{-1} + \lambda I)^{-1}) \leq \kappa(W).$$

*Proof.* Proof. Let  $\chi_{max}$  and  $\chi_{min}$  be the maximum and minimum eigenvalues of  $W$ , respectively. By the assumptions made in Shanno (1978a), we know that  $\chi_{min} > 0$ . Then,

$$\kappa((W^{-1} + \lambda I)^{-1}) = \kappa(W^{-1} + \lambda I) = \frac{(1/\chi_{min}) + \lambda}{(1/\chi_{max}) + \lambda} = \frac{\chi_{max} + \lambda\chi_{min}\chi_{max}}{\chi_{min} + \lambda\chi_{min}\chi_{max}} \leq \frac{\chi_{max}}{\chi_{min}} = \kappa(W).$$

$\square$

While Algorithm 2 only invokes cubic regularization for a Powell restart, it can be modified to include more cases, such as when the search direction fails to be a descent direction, as another reason to invoke it. Doing so would mean that the assumption of the Hessian estimate remaining positive definite is no longer necessary.

With Lemma 1 and the comment above, we can invoke Theorem 7 of Shanno (1978a) to conclude that Algorithm 2 exhibits global convergence.

## 4. NUMERICAL RESULTS

We start this section by describing our testing environment and then we will introduce our numerical results on general unconstrained NLPs from the CUTer test set (Bongartz et al. (1995)) and two types of machine learning problems with randomly generated data.

**4.1. Software and hardware.** The original conjugate gradient method described in Algorithm 1 was implemented by Shanno and Phua in the code Conmin using Fortran4 (Shanno and Phua (1976)). We have reimplemented conjugate gradient method of Conmin in C and connected it to AMPL (Fourer et al. (1993)). In our C implementation, we have omitted the BFGS method also implemented in the original Conmin distribution, and we will call our new code Conmin-CG. The software is available for open source download and use (Buhler (2021)). The cubic regularization scheme proposed in this paper as Algorithm 2 was implemented and tested by modifying this software and is also available at the same link.

Machine learning problems presented an opportunity to compare our method to existing software, and we have chosen ADMM (Boyd et al. (2011a)) as the state-of-the-art for our comparison. The Matlab codes that generate the random problem instances and implement ADMM for the Huber function and for group LASSO were obtained from (Boyd et al. (2011b)). In order to provide a fair comparison to ADMM, we implemented Conmin-CG with and without cubic regularization in Matlab as well. The Matlab routines are also available from Buhler (2021).

In our numerical testing, we used AMPL Version 20210226 and MATLAB R2021a on a Mac running macOS Catalina Version 10.15.7, with a 2.9 GHz Intel Core i7 processor and 8 GB 1600 MHz DDR3 memory.

**4.2. Test set.** The test problems were compiled from the CUTER test set (Bongartz et al. (1995)) as implemented in AMPL (Vanderbei (1997)). We chose 230 unconstrained problems, which included all of the unconstrained problems available from Vanderbei (1997) except for those where the objective function could not be evaluated at the provided or default initial solution, where the initial solution was a stationary point (0 iterations), or where the objective function was unbounded. There are 38 QPs and 192 NLPs in the set. We will focus on the two groups of problems separately in the analysis below.

We have included additional problems from machine learning in our test set. These problems were chosen to satisfy the differentiability requirement for our algorithms. (Subgradient-based approaches for nondifferentiable problems will be considered in future work.) The first class of problems use the Huber loss function as follows:

$$(25) \quad \min_x \sum_{i=1}^m h_i(Ax - b),$$

where  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ , and

$$h_i(z) = \begin{cases} 0.5z_i^2, & \text{for } |z_i| \leq 1 \\ |z_i| - 0.5, & \text{otherwise.} \end{cases}$$

The second class of problems is group LASSO:

$$(26) \quad \min_x \frac{1}{2} \|Ax - b\|_2^2 + \rho \sum_{i=1}^N \|x_i\|_2$$

where  $A$  and  $b$  are as above,  $x_i$  refers to the  $i$ th group of variables, with  $i = 1, \dots, N$ , and  $\rho > 0$  is a penalty parameter. Even though the second norm is nondifferentiable, the only potential issue is if all of the  $x$  values in a group approach 0. In practice, we can keep the group sizes large and easily find randomly generated problem instances where nondifferentiability is not encountered.

To generate random instances of these problems, we used the codes provided in Boyd et al. (2011b). For the Huber loss function (25), we ran 100 instances each for four different problem sizes:  $(m, n) = (5000, 2000)$ ,  $(10000, 2000)$ ,  $(100000, 2000)$ , and  $(100000, 5000)$ . For group LASSO (26), we used 2 or 4 groups, and randomly calculated the size of each group as uniformly distributed between 1 and a parameter  $K$ . We ran 100 instances each of six different scenarios:  $(m, N, K) = (100000, 2, 1000)$ ,  $(1500, 4, 1000)$ ,  $(10000, 4, 1000)$ ,  $(100000, 4, 1000)$ ,  $(100000, 4, 2000)$ , and  $(100000, 4, 5000)$ . (While the group LASSO problem is nondifferentiable when the vector  $x_i = 0$  for group  $i$ , instances with a few large blocks meant that we were less likely to encounter this problem computationally.) The number of variables in each problem,  $n$ , was calculated as the sum of the block sizes. Entries of the feature matrix  $A$  were generated as  $N(0, 1)$ , and then the columns of  $A$  were normalized to have a unit  $l_2$  norm.  $b$  was then generated using  $b = Ax^{\text{true}} + v$  where  $v \sim N(0, 0.1)$ .  $\rho$  was chosen as  $0.001 \|A^T b\|_\infty$ .

**4.3. Do we need Powell restarts?** Of the 192 NLPs in the test set, 187 of them require at least one Powell restart. That is 97.4% - a significant portion. In fact, of the 5 problems that do not use Powell restarts, 4 conclude within the first two iterations without ever reaching a check for the Powell restart and 1 has an objective function that is the weighted sum of a quadratic term and a nonlinear term, where the weight and function values of the nonlinear term are negligible with respect to the quadratic term (and as such, it is effectively a QP). It is, therefore, safe to conclude that every NLP of interest requires at least one Powell restart and focus on these 187 problems in our ongoing analysis.

Of the 187 problems, our main code fails on 30 problems (8 exit due to linesearch failures, 3 exit due to function evaluation errors, and 19 reach the iteration limit of 10,000). The remaining 157 problems are reported as solved and show at least one Powell restart. For each of these problems, we calculated the percentage of Powell restart iterations as

$$\begin{aligned}\phi_i &= \text{Percentage of Powell restart iterations for Problem } i \\ &= \frac{\text{Number of iterations with Powell restarts for Problem } i}{\text{Total number of iterations for Problem } i}.\end{aligned}$$

The average value of  $\phi$  is 45.5%, and its median is 45.7%. Note that we do not test for a Powell restart during an iteration that is already slated for a Beale restart, so the percentage of iterations that satisfy the Powell restart criterion (6) is actually slightly higher at around 55%.

Given the prevalence of Powell restarts, it may be natural to ask how the algorithm performs without them. When Powell restarts are disabled, the code still converges on the same number of problems (27 of the 30 failures remain the same, 3 get resolved, and there are 3 new failures). We get the same iteration count on 13 problems, the code performs better with Powell restarts on 101 problems (80% fewer iterations on average), and the code performs better without Powell restarts on 41 problems (30% fewer iterations on average). Therefore, there is a clear and significant advantage to Powell restarts, but the question remains as to whether or not we need a full restart every time the Powell restart criterion is satisfied.

**4.4. The Impact of Cubic Regularization on the Powell Restart Criterion.** We will now use an example to illustrate the impact of cubic regularization on the satisfaction of the Powell restart criterion (6). More specifically, we will examine how increasing values of  $\lambda$  impact the value of the fraction

$$(27) \quad \frac{|\nabla f(x_{k+1}(\lambda))^T \nabla f(x_k)|}{\|\nabla f(x_{k+1}(\lambda))\|^2}.$$

The example we have chosen is the problem *s206* (Bongartz et al. (1995)):

$$\min_{x_1, x_2} (x_2 - x_1^2)^2 + 100(1 - x_1)^2.$$

Without cubic regularization, Conmin encounters a Powell restart in Iteration 3. The value of the Powell fraction (27) is 23.18, which is much larger than the threshold of 0.2. If we start to apply the cubic regularization with increasing values of  $\lambda$  for this iteration, we get the results shown in Figure 1.

Since the algorithm quickly increases the value of  $\lambda$ , it is hard to visualize a pattern of decrease with the values given in the table. As such, we have also evaluated the Powell fraction for more values of  $\lambda$  between 0 and 600 so that a smooth chart can be produced for Figure 1.

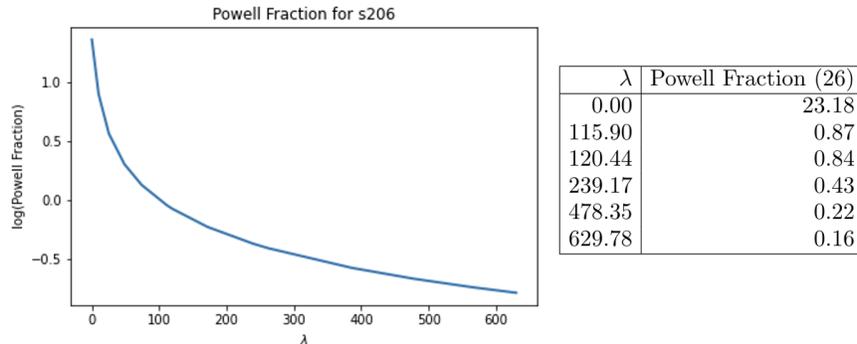


FIGURE 1.  $\lambda$  vs. the log of the Powell fraction in Iteration 3 of solving the problem *s206*. The first two iterations of the problem were solved without cubic regularization.

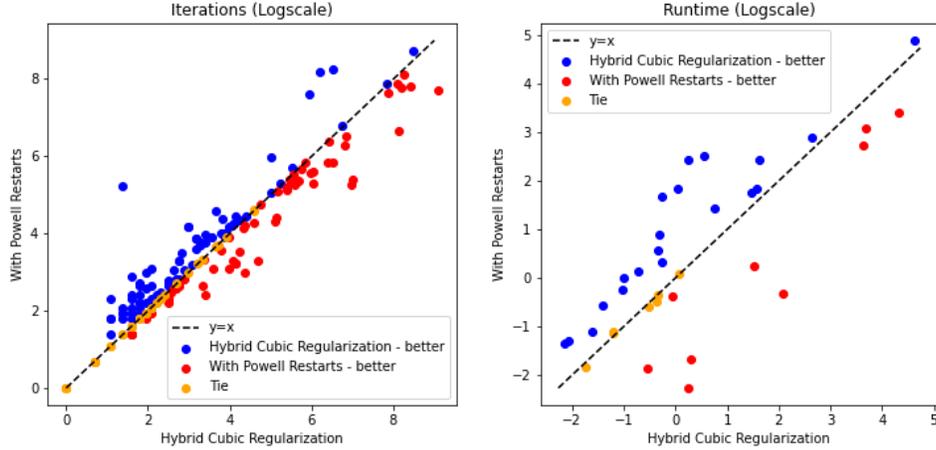


FIGURE 2. Pairwise comparisons of iterations and runtimes for Conmin-CG with Powell restarts and with hybrid cubic regularization. The iterations comparison was conducted on 180 out of the 230 unconstrained problems we solved from the CUTER test set, and the runtimes comparison was conducted on 36 problems on which both solvers exhibited runtimes of at least 0.1 CPU seconds. Blue dots denote the problems where the code with hybrid cubic regularization outperforms the code with Powell restarts, red dots represent the opposite relationship, and orange dots represent a tie (or runtimes within 0.1 of each other). The dotted black line is  $y = x$ .

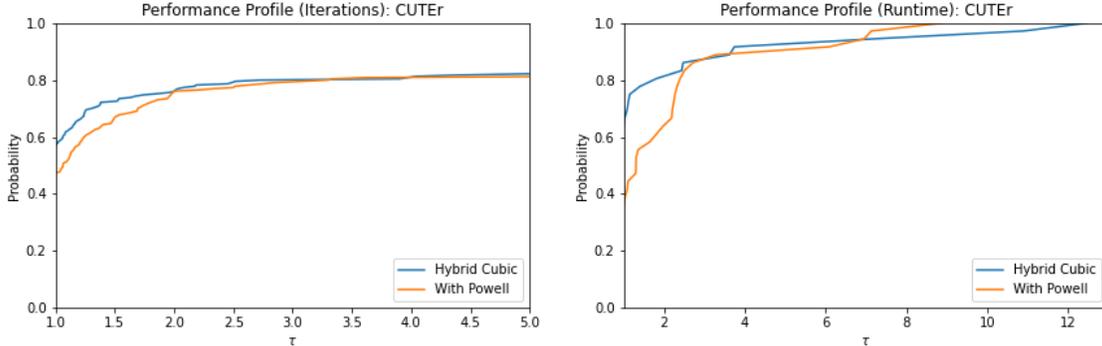


FIGURE 3. Performance profiles of the iterations and runtime results from CUTER test set. The iterations comparison was conducted on all 230 unconstrained problems from the CUTER test set, and the runtimes comparison was conducted on 36 problems on which both solvers exhibited runtimes of at least 0.1 CPU seconds.

**4.5. Numerical comparison.** We start our numerical comparison with general problems of the form (1) from the CUTER test set. Detailed results on these problems are provided in Tables 2-6 in the Appendix. The detailed results include the number of iterations, runtime in CPU seconds, and the objective function value at the reported solution for three algorithms. The first, labeled “With Powell Restarts,” is the algorithm implemented in Conmin-CG and previously presented as Algorithm 1. The second, labeled “No Powell Restarts,” is a modified version of Algorithm 1 with the check for Powell restarts removed, so that only Beale restarts are performed. This algorithm is included in the tables to support the results provided in Section 4.3. The last algorithm, labeled “Hybrid Cubic,” implements Algorithm 2, which uses a hybrid approach where cubic regularization is only invoked when the Powell restart criterion (6) is satisfied.

The results in Tables 2-6 and Figures 2 and 3 show that the hybrid cubic regularization improves the number of iterations and the runtime on the CUTER test set.

- For overall success, we have that “With Powell Restarts” and “Hybrid Cubic” each solve 190 of the 230 problems, a rate of 82.6%. This includes 180 jointly solved problems, 10 problems solved by “With Powell Restarts” only, and 10 problems solved by “Hybrid Cubic” only.
- For iterations, we see in Figures 2 that “Hybrid Cubic” outperforms “With Powell Restarts” on the jointly solved problems. The graph on the left shows a scatterplot where each point represents one problem, with the coordinates equaling iteration counts by the two codes. (The line  $y = x$  is included to help our assessment.) In this graph, there are 81 blue dots representing instances where “Hybrid Cubic” had fewer iterations, 59 red dots where “With Powell Restarts” had fewer iterations, and 40 orange dots where they had the same number of iterations. That means on 121 of the 180 jointly solved problems, or 67.2%, “Hybrid Cubic” exhibits the same or fewer number of iterations as “With Powell Restarts.” The performance profile for iterations, as shown in Figure 3, indicates that “Hybrid Cubic” outperforms “With Powell Restarts” on all 230 problems of the test set.
- It is interesting to note that the improvement becomes slightly more pronounced if we use a typical iteration limit of 1,000 (instead of 10,000). In that case, there are 166 jointly solved problems. “Hybrid Cubic” performs fewer iterations on 76, “With Powell Restarts” performs fewer iterations on 50, and the two codes perform the same number of iterations on 40. That means on 116 of the 166 jointly solved problems, or 69.9%, “Hybrid Cubic” exhibits the same or fewer number of iterations as “With Powell Restarts.”
- There were 14 jointly solved problems where at least one solver performed over 1,000 iterations. On these instances, there is no clearly observed pattern, as such a high iteration typically indicates that the problem is severely ill-conditioned or that  $f(x)$  is highly non-convex. One example is the problem *watson*, with  $n = 31$ , and where

$$f(x) = \sum_{i=1}^{29} \left( \sum_{j=2}^n (j-1) \left(\frac{i}{29}\right)^{j-2} x_j - \left( \sum_{j=1}^n \left(\frac{i}{29}\right)^{j-2} x_j \right)^2 - 1 \right)^2 + x_1^2 + (x_2 - x_1^2 - 1)^2.$$

On this problem, “With Powell Restarts” performs 2248 and “Hybrid Cubic” performs 8919 iterations to reach a solution. Similar behavior is observed on *s371*, which is identical to *watson* but with  $n = 9$ . However, on *dixmaani-dixmaani*, where  $m = 1,000$ ,  $n = 3,000$ , and

$$f(x) = 1.0 + \sum_{i=1}^n \hat{a} \left(\frac{i}{n}\right)^2 x_i^2 + \sum_{i=1}^{n-1} \hat{b} x_i^2 (x_{i+1} + x_{i+1}^2)^2 + \sum_{i=1}^{2m} \hat{c} x_i^2 x_{i+m}^4 + \sum_{i=1}^m \hat{d} \left(\frac{i}{n}\right)^2 x_i x_{i+2m}$$

for different values of  $\hat{a}$ ,  $\hat{b}$ ,  $\hat{c}$ , and  $\hat{d}$ . On these problems, “With Powell Restarts” performs 2,000-6,000 iterations, which is 1,000-3,000 more than “Hybrid Cubic.”

- For the runtimes comparisons, we have taken a subset of the jointly solved problems, namely those that were solved in 0.1 or more CPU seconds by both solvers. (This is to ensure a fair comparison, as smaller runtimes can be easily influenced by other processes running on the same machine and/or exhibit very small differences.) The resulting set consisted of 36 problems, of which “With Powell Restarts” was faster on 13 and “Hybrid Cubic” was faster on 23. This means that “Hybrid Cubic” resulted in faster runtimes on 63.4% of the problems with runtimes of at least 0.1 CPU seconds. The runtime results shown in Figures 2 and 3 support this conclusion.
- For runtime comparison, it may be a good idea to consider small differences as a tie. If runtimes within 0.1 CPU seconds of each other are considered a tie, then “With Powell

Restarts” was faster on 9, “Hybrid Cubic” was faster on 20, and we considered 7 instances as a tie.

Next we will discuss the numerical results from randomly generated data on the Huber loss function (25) and group LASSO (26). In our testing, we compared three codes: Our implementations for “With Powell Restarts” and “Hybrid Cubic” in Matlab, and ADMM as distributed at Boyd et al. (2011b).

- In Table 1, we see that, on the Huber loss function problems, the “Hybrid Cubic” had the shortest average runtime out of the three, while ADMM took the longest to solve. In addition, “Hybrid Cubic” exhibited fewer iterations than its non-regularized version, “With Powell Restarts”. We did not include ADMM iterations, as a comparison may be misleading due to the different nature of iterations for this solver.
- As expected, the results in Table 1 indicate that runtimes increase as problem sizes increase. It can be seen from the last two rows that the increase in runtime per iteration is approximately equal for the two versions of CGM. That is, when  $m$  is fixed at 100,000 and  $n$  is increased by a factor of 2.5, the average runtime per iteration for “With Powell Restarts” goes from 0.409 seconds to 1.163 seconds, a factor of 2.844, while the average runtime per iteration for the “Hybrid Cubic” goes from 0.615 seconds to 1.824 seconds, a factor of 2.966.
- Cubic regularization was invoked in almost every iteration of every instance of the Huber loss function problems. As shown in the previous discussion, the runtime per iteration is higher for “Hybrid Cubic” than for “With Powell Restarts”. Therefore, the overall decrease in runtime from “With Powell Restarts” to “Hybrid Cubic” can be attributed to the significant decrease in the number of iterations.
- By contrast, cubic regularization was invoked on only 202 of the 600 group LASSO problems summarized in Figure 4. On these 202 instances, cubic regularization was typically invoked in 1 iteration.
- For group LASSO problems, ADMM solves 597 of the 600 instances (99.5%) within its default limit of 1000 iterations. “With Powell Restarts” solves 571 (95.2%), and “Hybrid Cubic” solves 576 (96.0%). “Hybrid Cubic” solves 7 problems that “With Powell Restarts” cannot solve. “With Powell Restarts” solves two problems that “Hybrid Cubic” cannot solve.
- Of the 202 instances of group LASSO where cubic regularization is invoked, the two CGM solvers commonly solve 171 instances. On these problems, the two solvers exhibit the same number of iterations on 78 instances. In fact, on 167 of the 171 problems, the improvement in the number of iterations is less than 25%, with the average improvement being 7.5%. Even though there are no instances where the number of iterations is worsened and this small improvement in iterations seems to be fairly uniform across the set, it is not sufficient to offset the additional runtime required by invoking cubic regularization at every iteration.
- As described and shown in Figures 4 and 5, “With Powell Restarts” had a slight advantage over “Hybrid Cubic” in runtime, while ADMM was much slower.

## 5. CONCLUSION

Our goal in this paper was to incorporate cubic regularization selectively into a CGM framework so that the resulting approach would

- require fewer iteration counts in computational experiments than its non-regularized version,
- exhibit global convergence with fewer assumptions than its non-regularized version,
- require the same order of computational burden per iteration as its non-regularized version, and
- demonstrate faster overall runtime in computational experiments than its non-regularized version.

		ADMM	CGM - With Powell Restarts		CGM - Hybrid Cubic	
m	n	Time	Time	Iter	Time	Iter
5000	2000	0.94	0.60	26.48	0.56	13.43
10000	2000	1.60	0.72	16.09	0.54	7
100000	2000	12	3.04	7.43	2.46	4
100000	5000	47.58	11.63	10	9.12	5

TABLE 1. Numerical results for randomly generated data on the Huber loss function (25).  $m$  is the number of rows in the feature matrix  $A$ ,  $n$  is the number of columns in the feature matrix  $A$ ,  $Iter$  is the average iteration count and  $Time$  is the average run time in CPU seconds. Averages are computed over the 100 instances of each problem size.

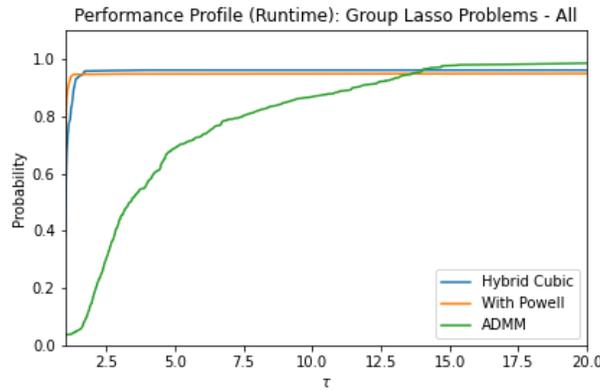


FIGURE 4. Performance profile for runtime on randomly generated data on group LASSO (26). Figure contains results from all 600 instances.

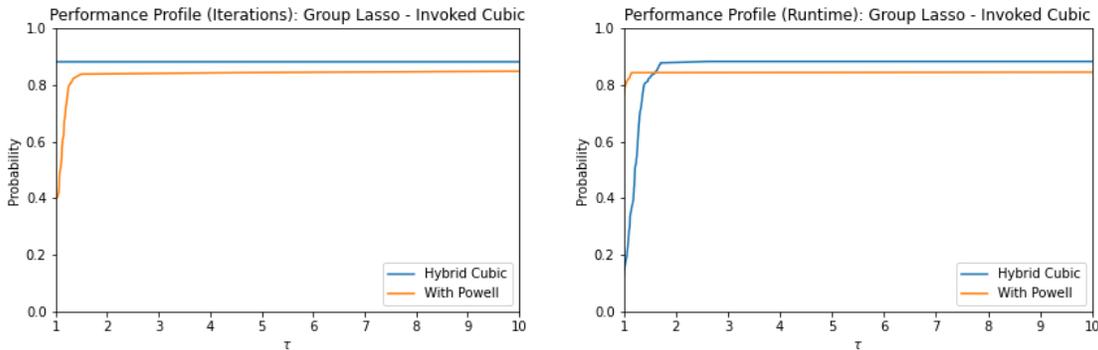


FIGURE 5. Performance profile for iterations and runtime on randomly generated data on group LASSO (26). Figure contains results from only the instances that invoked cubic regularization, 202 out of 600.

Our global convergence results in Section 3 and our numerical results in Section 4 showed that we were able to attain this goal fully.

We have some additional tasks to explore in future work. In our current implementation, we find the optimal  $\alpha$ . However, we wish to explore how these results may be affected with a fixed step size. In addition, we also hope to apply our algorithm to real life datasets. We had used a few datasets

from the UCI machine learning repository (Dua and Graff (2017)), but out of the several we chose, only two invoked cubic regularization. We hope to explore this in more detail and find additional applications for our algorithm. Finally, we plan to extend our work to incorporate subgradients so that we can solve nondifferentiable problems.

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**David F. Shanno** was best known as one of the developers of the widely-used BFGS algorithm for nonlinear optimization and for his contributions to interior-point methods for linear and nonlinear optimization. Shanno studied mathematics and philosophy at Yale University, and received his Ph.D. in mathematics from Carnegie-Mellon University. He taught at the University of Chicago, the University of Arizona, the University of California, Davis, and the Rutgers Center for Operations Research (RUTCOR) before his retirement. Shanno was an associate editor of *Mathematical Programming* and *Journal of Optimization Theory and Applications*, and departmental editor of *Communications of the Association of Computing Machinery*. He was a recipient of the Beale-Orchard-Hays Prize for Excellence in Computational Mathematical Programming and the Operations Research Society of America's Computer Science Technical Section Prize for research excellence in the interface between operations research and computer science. In 2005, Shanno was elected a Fellow of the Institute for Operations Research and the Management Sciences.

**The Story** Sadly, David F. Shanno passed away in July 2019. The research documented in this paper was started by Benson and Shanno in 2015 and was presented at the SIAM Optimization Meeting in 2017. Cassidy Buhler joined the research group after Shanno's passing and led the project to include machine learning applications and comparisons to state-of-the-art software. This work represents the last project that Benson and Shanno completed in their 20-years of collaboration, and the authors hope that it is a tribute to his legacy and a solid foundation for the next generation of researchers.

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## 6. APPENDIX

Numerical results on the unconstrained problems from the CUTer test set (Vanderbei (1997)) are provided in the following tables. Problem names that end in an asterisk are quadratic programming problems.  $n$  is the number of variables in the problem,  $Iter$  is the iteration count,  $Time$  is the run time in CPU seconds, and  $f(x^*)$  is the objective value at the reported solution. (IL) and (E) denote that the solver reached its iteration limit and exited with an error, respectively.

Name	n	With Powell Restarts			No Powell Restarts			Hybrid Cubic		
		Iter	Time	$f(x^*)$	Iter	Time	$f(x^*)$	Iter	Time	$f(x^*)$
aircftb	5	50	<0.1	3.1E-16	53	<0.1	3.8E-15	53	<0.1	5.2E-13
allinitu	4	20	<0.1	5.7E+00	9	<0.1	5.7E+00	7	<0.1	5.7E+00
arglina*	100	1	<0.1	1.0E+02	1	<0.1	1.0E+02	1	<0.1	1.0E+02
arglinb*	10	1	<0.1	4.6E+00	1	<0.1	4.6E+00	1	<0.1	4.6E+00
arglinc*	8	1	<0.1	6.1E+00	1	<0.1	6.1E+00	1	<0.1	6.1E+00
arwhead	5000	8	2.6E-01	-9.6E-10	9	<0.1	-1.4E-09	4	1.2E-01	-2.7E-09
bard	3	17	<0.1	8.2E-03	16	<0.1	8.2E-03	15	<0.1	8.2E-03
bdexp	5000	6	2.5E-01	8.0E-04	3	<0.1	7.3E-121	3	<0.1	7.3E-121
bdqrtic	1000	(E)			(E)			438	4.2E+00	4.0E+03
beale	2	11	<0.1	8.9E-18	11	<0.1	5.5E-19	10	<0.1	6.2E-21
biggs3	3	14	<0.1	1.7E-10	16	<0.1	4.5E-13	28	<0.1	1.1E-11
biggs5	5	84	<0.1	5.7E-03	90	<0.1	5.7E-03	169	<0.1	5.7E-03
biggs6	6	62	<0.1	3.4E-07	110	<0.1	7.2E-09	76	<0.1	3.7E-06
box2	2	5	<0.1	4.2E-15	7	<0.1	1.7E-14	5	<0.1	3.5E-14
box3	3	9	<0.1	4.4E-12	10	<0.1	2.4E-11	12	<0.1	2.9E-11
bratu1d	1001	(E)			(E)			(IL)		
brkmcc	2	4	<0.1	1.7E-01	5	<0.1	1.7E-01	5	<0.1	1.7E-01
browna1	10	7	<0.1	4.6E-16	7	<0.1	1.8E-15	5	<0.1	4.0E-15
brownbs	2	8	<0.1	2.1E-14	11	<0.1	2.4E-22	6	<0.1	2.2E-13
brownden	4	21	<0.1	8.6E+04	37	<0.1	8.6E+04	14	<0.1	8.6E+04
broydn7d	1000	339	3.3E-01	4.0E+02	332	2.0E-01	4.0E+02	345	2.0E-01	4.0E+02
brybnd	5000	12	3.3E-01	1.5E-12	14	3.0E-01	4.1E-12	13	3.0E-01	4.1E-13
chainwoo	1000	167	<0.1	1.0E+00	380	1.7E-01	4.6E+00	217	<0.1	1.0E+00
chnrosnb	50	218	<0.1	1.0E-13	258	<0.1	3.1E-14	232	<0.1	1.1E-13
cliff	2	(E)			(E)			(IL)		
clplatea	4970	877	5.9E+00	-1.3E-02	1306	8.4E+00	-1.3E-02	840	4.3E+00	-1.3E-02
clplateb	4970	538	6.2E+00	-7.0E+00	680	4.4E+00	-7.0E+00	900	4.8E+00	-7.0E+00
clplatec	4970	(IL)			(IL)			(IL)		
cosine	10000	7	7.9E-01	-1.0E+04	(E)			6	3.6E-01	-1.0E+04
cragglyv	5000	80	1.3E+00	1.7E+03	(E)			45	4.6E+00	1.7E+03
cube	2	14	<0.1	2.7E-16	17	<0.1	1.1E-17	16	<0.1	2.1E-20
curly10	10000	(IL)			(IL)			(IL)		
curly20	10000	(IL)			(IL)			(IL)		
curly30	10000	(E)			(E)			(IL)		
deconvu	51	269	<0.1	3.7E-10	321	<0.1	3.7E-10	413	<0.1	7.9E-08
denschna	2	7	<0.1	1.2E-19	7	<0.1	7.1E-15	7	<0.1	7.9E-15
denschnb	2	5	<0.1	1.2E-14	6	<0.1	9.7E-17	5	<0.1	2.3E-24
denschn	2	10	<0.1	2.2E-17	11	<0.1	1.2E-16	8	<0.1	1.9E-19

TABLE 2. Numerical results on the unconstrained problems from the CUTer test set (Vanderbei (1997)).

Name	n	With Powell Restarts			No Powell Restarts			Hybrid Cubic		
		Iter	Time	f(x*)	Iter	Time	f(x*)	Iter	Time	f(x*)
denschnd	3	16	<0.1	3.7E-11	33	<0.1	7.8E-10	12	<0.1	2.4E-09
denschne	3	(E)			(E)			(IL)		
denschnf	2	6	<0.1	3.9E-21	8	<0.1	3.0E-16	4	<0.1	3.0E-16
dixmaana	3000	7	<0.1	1.0E+00	11	<0.1	1.0E+00	5	<0.1	1.0E+00
dixmaanb	3000	7	1.1E-01	1.0E+00	11	<0.1	1.0E+00	4	<0.1	1.0E+00
dixmaanc	3000	8	1.0E-01	1.0E+00	13	<0.1	1.0E+00	5	<0.1	1.0E+00
dixmaand	3000	10	1.7E-01	1.0E+00	16	<0.1	1.0E+00	5	<0.1	1.0E+00
dixmaane	3000	255	3.2E-01	1.0E+00	305	4.7E-01	1.0E+00	256	3.0E-01	1.0E+00
dixmaanf	3000	195	6.1E-01	1.0E+00	248	8.4E-01	1.0E+00	268	7.0E-01	1.0E+00
dixmaang	3000	227	7.0E-01	1.0E+00	239	8.5E-01	1.0E+00	268	7.2E-01	1.0E+00
dixmaanb	3000	181	5.6E-01	1.0E+00	316	1.0E+00	1.0E+00	220	6.0E-01	1.0E+00
dixmaani	3000	6084	1.1E+01	1.0E+00	4793	7.2E+00	1.0E+00	4806	5.0E+00	1.0E+00
dixmaanb	3000	3816	1.2E+01	1.0E+00	1409	4.6E+00	1.0E+00	675	1.7E+00	1.0E+00
dixmaanb	3000	3597	1.1E+01	1.0E+00	663	2.3E+00	1.0E+00	499	1.3E+00	1.0E+00
dixmaanb	3000	2050	6.3E+00	1.0E+00	709	2.3E+00	1.0E+00	380	1.0E+00	1.0E+00
dixon3dq*	10	10	<0.1	2.2E-28	10	<0.1	2.2E-28	10	<0.1	2.4E-28
dqdrtic*	5000	6	<0.1	2.3E-15	6	<0.1	2.3E-15	6	<0.1	2.3E-15
dqdrtic	5000	13	5.7E-01	1.0E-01	164	4.2E-01	9.5E-02	7	2.5E-01	9.5E-03
edensch	2000	17	<0.1	1.2E+04	17	<0.1	1.2E+04	16	<0.1	1.2E+04
eg2	1000	2	<0.1	-1.0E+03	2	<0.1	-1.0E+03	2	<0.1	-1.0E+03
engvall	5000	14	2.8E-01	5.5E+03	21	2.2E-01	5.5E+03	8	1.3E-01	5.5E+03
engval2	3	28	<0.1	5.9E-13	36	<0.1	9.0E-17	29	<0.1	1.5E-13
errinros	50	259	<0.1	4.0E+01	432	<0.1	4.0E+01	394	<0.1	4.0E+01
expfit	2	11	<0.1	2.4E-01	12	<0.1	2.4E-01	5	<0.1	2.4E-01
fletcbv2	100	97	<0.1	-5.1E-01	97	<0.1	-5.1E-01	97	<0.1	-5.1E-01
fletchr	100	302	<0.1	3.5E-13	293	<0.1	1.3E-13	247	<0.1	2.4E-13
floop2hl	650	(IL)			(IL)			(IL)		
floop2hm	650	(IL)			(IL)			(IL)		
floop2th	650	(IL)			(IL)			(IL)		
floop2tl	650	(IL)			(IL)			(IL)		
floop2tm	650	(IL)			(IL)			(IL)		
fminsurf2	1024	223	1.9E-01	1.0E+00	384	3.2E-01	1.0E+00	1106	1.4E+00	1.0E+00
fminsurf	1024	202	1.6E-01	1.0E+00	339	3.5E-01	1.0E+00	420	5.8E-01	1.0E+00
freuroth	5000	22	7.3E-01	6.1E+05	28	3.1E-01	6.1E+05	54	7.9E+00	6.1E+05
genhumps	5	36	<0.1	7.0E-14	34	<0.1	5.5E-13	24	<0.1	3.5E-12
genrose	500	2668	6.8E-01	1.0E+00	3682	5.5E-01	1.0E+00	2572	9.5E-01	1.0E+00
growth	3	196	<0.1	1.0E+00	159	<0.1	1.0E+00	(IL)		
growthls	3	169	<0.1	1.0E+00	177	<0.1	1.0E+00	(IL)		
gulf	3	41	<0.1	4.7E-13	32	<0.1	4.7E-09	41	<0.1	4.9E-10
hairy	2	18	<0.1	2.0E+01	11	<0.1	2.0E+01	5	<0.1	2.0E+01
hatfdd	3	22	<0.1	2.5E-07	26	<0.1	2.5E-07	36	<0.1	2.6E-07
hatfde	3	35	<0.1	4.4E-07	28	<0.1	4.4E-07	44	<0.1	4.4E-07
heart6ls	6	(IL)			(IL)			(IL)		
heart8ls	8	339	<0.1	1.5E-16	382	<0.1	1.5E-12	590	<0.1	5.2E-12
helix	3	21	<0.1	3.6E-17	25	<0.1	2.2E-17	18	<0.1	8.4E-23
hilberta*	10	8	<0.1	5.8E-10	8	<0.1	5.8E-10	8	<0.1	5.8E-10
hilbertb*	50	5	<0.1	2.1E-20	5	<0.1	2.1E-20	5	<0.1	2.1E-20
himmelbb	2	4	<0.1	1.7E-18	5	<0.1	1.7E-16	4	<0.1	5.8E-19
himmelbf	4	44	<0.1	3.2E+02	81	<0.1	3.2E+02	30	<0.1	3.2E+02

TABLE 3. Numerical results on the unconstrained problems from the CUTER test set (Vanderbei (1997)).

Name	n	With Powell Restarts			No Powell Restarts			Hybrid Cubic		
		Iter	Time	f(x*)	Iter	Time	f(x*)	Iter	Time	f(x*)
himmelbg	2	6	<0.1	1.6E-16	7	<0.1	9.4E-20	6	<0.1	1.3E-16
himmelbh	2	5	<0.1	-1.0E+00	5	<0.1	-1.0E+00	5	<0.1	-1.0E+00
humps	2	55	<0.1	2.1E-12	89	<0.1	4.6E-16	48	<0.1	2.2E-12
jensmp	2	15	<0.1	1.2E+02	16	<0.1	1.2E+02	6	<0.1	1.2E+02
kowosb	4	25	<0.1	3.1E-04	45	<0.1	3.1E-04	63	<0.1	3.1E-04
liarwhd	10000	14	1.8E+00	5.5E-15	18	3.3E-01	1.3E-17	12	7.1E-01	2.4E-19
loghairi	2	184	<0.1	1.8E-01	66	<0.1	1.8E-01	4	<0.1	6.2E+00
mancino	100	15	1.6E-01	3.6E-15	15	1.9E-01	5.5E-15	15	1.8E-01	3.9E-15
maratosb	2	(E)			(E)			4	<0.1	-1.0E+00
methanb8	31	2101	<0.1	4.9E-05	1377	<0.1	5.2E-05	2602	1.5E-01	6.9E-05
methanl8	31	(IL)			(IL)			(IL)		
mexhat	2	9	<0.1	-4.0E-02	6	<0.1	-4.0E-02	6	<0.1	-4.0E-02
meyer3	3	(E)			(E)			(IL)		
minsurf	36	13	<0.1	1.0E+00	17	<0.1	1.0E+00	15	<0.1	1.0E+00
msqrtals	1024	3376	2.2E+01	2.7E-08	3658	2.9E+01	1.1E-08	3866	4.0E+01	4.7E-08
msqrtbls	1024	2376	1.6E+01	3.4E-09	2741	2.1E+01	1.7E-08	3630	3.8E+01	6.9E-09
nasty*	2	(E)			(E)			(E)		
ncb20	1010	(E)			(E)			110	6.9E+00	1.7E+03
ncb20b	1000	(E)			(E)			34	7.4E+00	1.7E+03
nlmsurf	15129	2467	1.3E+02	3.9E+01	3857	9.9E+01	3.9E+01	4582	1.0E+02	3.9E+01
noncvxu2	1000	2684	1.1E+00	2.3E+03	2814	9.3E-01	2.3E+03	3325	1.1E+00	2.3E+03
noncvxun	1000	22	<0.1	2.3E+03	20	<0.1	2.3E+03	8	<0.1	2.3E+03
nondia	9999	9	1.2E+00	2.8E-15	8	2.8E-01	3.9E-24	6	4.8E-01	3.2E-12
nondquar	10000	348	1.8E+01	6.4E-05	1523	8.8E+00	6.8E-05	683	1.4E+01	9.5E-05
nonmsqrt	9	670	<0.1	7.5E-01	282	<0.1	7.5E-01	925	<0.1	7.5E-01
osbornea	5	258	<0.1	5.5E-05	289	<0.1	5.5E-05	(IL)		
osborneb	11	162	<0.1	4.0E-02	143	<0.1	4.0E-02	175	<0.1	4.0E-02
palmer1c*	8	(IL)			(E)			(IL)		
palmer1d*	7	(E)			(E)			8357	5.0E-01	6.5E-01
palmer1e	8	(IL)			(IL)			4	<0.1	0.0E+00
palmer2c*	8	(IL)			(IL)			(IL)		
palmer2e	8	(IL)			(IL)			(IL)		
palmer3c*	8	5844	1.0E-01	2.0E-02	(IL)			(IL)		
palmer3e	8	(IL)			9272	1.9E-01	5.1E-05	(IL)		
palmer4c*	8	3319	<0.1	5.0E-02	4021	<0.1	5.1E-02	(IL)		
palmer4e	8	4453	<0.1	1.5E-04	6286	1.3E-01	1.5E-04	(IL)		
palmer5c*	6	6	<0.1	2.1E+00	6	<0.1	2.1E+00	6	<0.1	2.1E+00
palmer5d*	4	9	<0.1	8.7E+01	9	<0.1	8.7E+01	8	<0.1	8.7E+01
palmer6c*	8	2336	<0.1	2.1E-02	6634	1.0E-01	1.9E-02	(IL)		
palmer7c*	8	8231	1.4E-01	6.2E-01	(IL)			(IL)		
palmer8c*	8	1863	<0.1	1.6E-01	4321	<0.1	1.7E-01	(IL)		
penalty1	1000	25	<0.1	9.7E-03	49	<0.1	9.7E-03	25	<0.1	9.7E-03
penalty2	100	86	<0.1	9.7E+04	(E)			63	<0.1	9.7E+04
penalty3	100	(E)			(E)			(IL)		
pfit1	3	40	<0.1	2.9E-04	38	<0.1	2.9E-04	26	<0.1	2.9E-04
pfit1ls	3	40	<0.1	2.9E-04	38	<0.1	2.9E-04	26	<0.1	2.9E-04
pfit2	3	44	<0.1	1.2E-02	50	<0.1	1.2E-02	26	<0.1	1.2E-02
pfit2ls	3	44	<0.1	1.2E-02	50	<0.1	1.2E-02	26	<0.1	1.2E-02

TABLE 4. Numerical results on the unconstrained problems from the CUTEr test set (Vanderbei (1997)).

Name	n	With Powell Restarts			No Powell Restarts			Hybrid Cubic		
		Iter	Time	f(x*)	Iter	Time	f(x*)	Iter	Time	f(x*)
pfit3	3	66	<0.1	8.2E-02	56	<0.1	8.2E-02	20	<0.1	8.2E-02
pfit3ls	3	66	<0.1	8.2E-02	56	<0.1	8.2E-02	20	<0.1	8.2E-02
pfit4	3	(E)			62	<0.1	2.6E-01	19	<0.1	2.6E-01
pfit4ls	3	(E)			62	<0.1	2.6E-01	19	<0.1	2.6E-01
powellsg	4	78	<0.1	2.0E-10	67	<0.1	2.2E-11	70	<0.1	5.6E-10
power*	1000	(IL)			(IL)			(IL)		
quartc	10000	14	2.4E+00	1.6E-01	150	9.9E-01	5.0E-01	6	7.4E-01	7.3E-01
rosenbr	2	27	<0.1	9.4E-18	24	<0.1	7.1E-17	16	<0.1	1.1E-16
s201*	2	2	<0.1	4.7E-27	2	<0.1	4.7E-27	2	<0.1	4.7E-27
s202	2	9	<0.1	4.9E+01	8	<0.1	4.9E+01	7	<0.1	4.9E+01
s204	2	5	<0.1	1.8E-01	5	<0.1	1.8E-01	5	<0.1	1.8E-01
s205	2	9	<0.1	1.1E-16	10	<0.1	1.0E-17	8	<0.1	5.0E-13
s206	2	4	<0.1	1.9E-16	5	<0.1	2.1E-19	5	<0.1	1.9E-24
s207	2	7	<0.1	2.4E-13	8	<0.1	4.3E-14	8	<0.1	2.2E-13
s208	2	27	<0.1	9.4E-18	24	<0.1	7.1E-17	16	<0.1	1.1E-16
s209	2	98	<0.1	1.2E-18	86	<0.1	8.1E-22	39	<0.1	1.8E-19
s210	2	389	<0.1	5.3E-21	372	<0.1	3.6E-20	148	<0.1	1.7E-18
s211	2	14	<0.1	2.7E-16	17	<0.1	1.1E-17	16	<0.1	2.1E-20
s212	2	9	<0.1	6.9E-22	12	<0.1	1.1E-25	8	<0.1	2.2E-15
s213	2	10	<0.1	1.6E-12	14	<0.1	1.1E-09	12	<0.1	1.1E-09
s240*	3	2	<0.1	3.8E-15	2	<0.1	3.8E-15	2	<0.1	3.8E-15
s243	3	9	<0.1	8.0E-01	9	<0.1	8.0E-01	9	<0.1	8.0E-01
s245	3	11	<0.1	1.7E-15	11	<0.1	2.7E-17	30	<0.1	6.1E-14
s246	3	17	<0.1	1.8E-16	18	<0.1	5.5E-18	18	<0.1	4.1E-20
s256	4	78	<0.1	2.0E-10	67	<0.1	2.2E-11	70	<0.1	5.6E-10
s258	4	48	<0.1	6.2E-13	27	<0.1	1.8E-15	24	<0.1	3.1E-17
s260	4	48	<0.1	6.2E-13	27	<0.1	1.8E-15	24	<0.1	3.1E-17
s261	4	27	<0.1	1.2E-09	37	<0.1	6.4E-10	59	<0.1	1.1E-09
s266	5	12	<0.1	1.0E+00	13	<0.1	1.0E+00	10	<0.1	1.0E+00
s267	5	75	<0.1	2.6E-03	68	<0.1	7.7E-09	163	<0.1	5.5E-07
s271*	6	6	<0.1	0.0E+00	6	<0.1	0.0E+00	6	<0.1	0.0E+00
s272	6	34	<0.1	5.7E-03	61	<0.1	5.7E-03	69	<0.1	5.7E-03
s272a	6	67	<0.1	3.4E-02	68	<0.1	3.4E-02	(IL)		
s273	6	11	<0.1	5.3E-18	14	<0.1	6.3E-15	6	<0.1	1.0E-14
s274*	2	2	<0.1	2.6E-24	2	<0.1	2.6E-24	2	<0.1	2.6E-24
s275*	4	3	<0.1	6.0E-12	3	<0.1	6.0E-12	3	<0.1	6.0E-12
s276*	6	3	<0.1	1.5E-12	3	<0.1	1.5E-12	3	<0.1	1.5E-12
s281a*	10	11	<0.1	2.0E-15	11	<0.1	2.0E-15	11	<0.1	1.3E-16
s282	10	212	<0.1	2.7E-15	220	<0.1	1.2E-16	292	<0.1	1.3E-15
s283	10	52	<0.1	1.5E-09	117	<0.1	7.3E-09	49	<0.1	2.4E-09
s286	20	24	<0.1	6.3E-16	27	<0.1	7.2E-14	22	<0.1	1.7E-17
s287	20	54	<0.1	2.4E-17	36	<0.1	9.3E-16	30	<0.1	9.4E-15
s288	20	70	<0.1	3.2E-10	80	<0.1	4.0E-10	58	<0.1	6.9E-10
s289	30	4	<0.1	0.0E+00	4	<0.1	0.0E+00	3	<0.1	0.0E+00
s290*	2	2	<0.1	1.1E-31	2	<0.1	1.1E-31	2	<0.1	3.1E-32
s291*	10	10	<0.1	2.8E-33	10	<0.1	2.8E-33	10	<0.1	5.5E-33
s292*	30	28	<0.1	7.1E-15	28	<0.1	7.1E-15	28	<0.1	7.1E-15
s293*	50	39	<0.1	3.0E-15	39	<0.1	3.0E-15	39	<0.1	3.0E-15

TABLE 5. Numerical results on the unconstrained problems from the CUTEr test set (Vanderbei (1997)).

Name	n	With Powell Restarts			No Powell Restarts			Hybrid Cubic		
		Iter	Time	f(x*)	Iter	Time	f(x*)	Iter	Time	f(x*)
s294	6	50	<0.1	2.2E-15	54	<0.1	2.2E-17	48	<0.1	1.2E-20
s295	10	86	<0.1	1.2E-15	90	<0.1	3.8E-18	81	<0.1	2.0E-14
s296	16	115	<0.1	5.7E-14	134	<0.1	7.6E-15	117	<0.1	1.4E-14
s297	30	203	<0.1	1.6E-13	280	<0.1	1.3E-14	190	<0.1	1.1E-14
s298	50	288	<0.1	1.2E-14	413	<0.1	7.6E-15	317	<0.1	1.7E-14
s299	100	590	<0.1	5.3E-14	809	<0.1	1.1E-14	618	<0.1	3.7E-14
s300*	20	20	<0.1	-2.0E+01	20	<0.1	-2.0E+01	20	<0.1	-2.0E+01
s301*	50	50	<0.1	-5.0E+01	50	<0.1	-5.0E+01	50	<0.1	-5.0E+01
s302*	100	100	<0.1	-1.0E+02	100	<0.1	-1.0E+02	100	<0.1	-1.0E+02
s303	20	15	<0.1	6.7E-30	18	<0.1	3.3E-19	12	<0.1	8.1E-16
s304	50	11	<0.1	7.0E-14	19	<0.1	6.6E-25	9	<0.1	3.3E-24
s305	100	13	<0.1	4.2E-23	30	<0.1	1.6E-15	14	<0.1	3.1E-28
s308	2	7	<0.1	7.7E-01	8	<0.1	7.7E-01	7	<0.1	7.7E-01
s309	2	6	<0.1	2.9E-01	7	<0.1	2.9E-01	7	<0.1	2.9E-01
s311	2	6	<0.1	1.7E-14	7	<0.1	2.1E-23	5	<0.1	1.1E-19
s312	2	33	<0.1	5.9E+00	26	<0.1	5.9E+00	17	<0.1	5.9E+00
s314	2	4	<0.1	1.7E-01	5	<0.1	1.7E-01	5	<0.1	1.7E-01
s333	3	(E)			(E)			3	<0.1	0.0E+00
s334	3	17	<0.1	8.2E-03	16	<0.1	8.2E-03	15	<0.1	8.2E-03
s350	4	25	<0.1	3.1E-04	45	<0.1	3.1E-04	63	<0.1	3.1E-04
s351	4	65	<0.1	3.2E+02	46	<0.1	3.2E+02	54	<0.1	3.2E+02
s352*	4	4	<0.1	9.0E+02	4	<0.1	9.0E+02	4	<0.1	9.0E+02
s370	6	72	<0.1	2.3E-03	80	<0.1	2.3E-03	98	<0.1	2.3E-03
s371	9	771	<0.1	1.8E-06	1838	<0.1	4.0E-06	3361	1.3E-01	5.2E-06
s379	11	159	<0.1	4.0E-02	159	<0.1	4.0E-02	151	<0.1	4.0E-02
s386*	2	2	<0.1	4.7E-27	2	<0.1	4.7E-27	2	<0.1	4.7E-27
sbrybnd	5000	(IL)			(IL)			(IL)		
schmvett	10000	(E)			(E)			(E)		
scosine	10000	(IL)			(IL)			(IL)		
scurlly10	10000	(IL)			(IL)			(IL)		
scurlly20	10000	(IL)			(IL)			(IL)		
scurlly30	10000	(IL)			(IL)			(IL)		
sineval	2	49	<0.1	2.8E-23	50	<0.1	4.3E-22	35	<0.1	5.2E-23
sinquad	10000	194	3.0E+01	4.1E-11	3259	4.0E+01	8.0E-09	1049	7.5E+01	2.6E-05
sisser	2	7	<0.1	2.9E-10	12	<0.1	7.7E-11	4	<0.1	2.7E-10
snail	2	20	<0.1	1.7E-14	69	<0.1	3.1E-23	78	<0.1	2.5E-22
rosenbr	10000	27	4.2E+00	6.7E-15	27	3.4E-01	3.3E-16	109	2.1E+00	5.0E-12
testquad*	1000	(IL)			(IL)			(IL)		
tointgss	10000	6	1.0E+00	1.0E+01	4	2.3E-01	1.0E+01	3	3.7E-01	1.0E+01
tquartic	10000	9	1.4E+00	7.1E-15	10	2.8E-01	4.2E-14	9	7.6E-01	1.8E-12
tridia*	10000	(IL)			4128	1.1E+01	4.8E-15	5118	1.5E+01	4.9E-15
vardim	100	10	<0.1	4.6E-17	21	<0.1	7.5E-18	3	<0.1	7.3E-26
vibrbeam	8	(IL)			(IL)			(IL)		
watson	31	2248	1.0E-01	1.1E-08	4969	2.6E-01	9.5E-09	8919	1.3E+00	9.7E-09
woods	10000	55	5.3E+00	1.8E-15	104	8.9E-01	6.5E-10	44	7.7E-01	6.2E-11
yfitu	3	67	<0.1	6.7E-13	63	<0.1	6.8E-13	78	<0.1	4.1E-06
zangwil2*	2	1	<0.1	-1.8E+01	1	<0.1	-1.8E+01	1	<0.1	-1.8E+01

TABLE 6. Numerical results on the unconstrained problems from the CUTer test set (Vanderbei (1997)).