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The modified absolute-value factorization norm for trust-region minimization

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ABSTRACT

A trust-region method for unconstrained minimization, using a trust-region norm based upon a modified absolute-value factorization of the model Hessian, is proposed. It is shown that the resulting trust-region subproblem may be solved using a single factorization. In the convex case, the method reduces to a backtracking Newton linesearch procedure. The resulting software package is available as `HSL_VF06` within the Harwell Subroutine Library. Numerical evidence shows that the approach is effective in the nonconvex case.

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1 Introduction

In this paper, we are concerned with trust-region methods for the unconstrained minimization of a function $f(x)$ of n real variables x. At the k-th iteration of such a method, a *model* $q_k(s)$ of $f(x_k + s)$ is approximately minimized within a *trust region* $\|s\| \leq \Delta_k$ with the aim of improving upon the current estimate of the minimizer x_k. The approximate solution s_k of this trust-region subproblem yields the improved estimate $x_{k+1} = x_k + s_k$ if the reduction in f predicted by this model translates into an significant actual reduction of $f(x_k + s_k)$. If such a reduction is not realized, the trust-region *radius* Δ_k is reduced, and the model resolved. If there is a good agreement between model and function, the radius may be increased. The method is blessed with a powerful convergence theory regardless of which norm defines the trust region, provided that the chosen norm is is uniformly related to the ℓ_2-norm. Little attention has been given to the appropriate choice of norm considering how strongly this choice affects the computation at every iteration of the algorithm. In this paper, we suggest that there is a particular norm which has computational advantages over the ℓ_2- or ℓ_∞-norms which are commonly considered.

2 The subproblem

We consider the quadratic model

$$q(s) = \langle g, s \rangle + \tfrac{1}{2}\langle s, Hs \rangle, \tag{2.1}$$

where g and H are approximations of the gradient and Hessian of $f(x)$, and $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product — for brevity, we have dropped the dependence of these quantities on k. We shall be concerned with elliptical trust regions of the form

$$\|s\|_N \leq \Delta, \quad \text{where} \quad \|s\|_N^2 = \langle s, Ns \rangle \tag{2.2}$$

and N is a real symmetric positive-definite matrix. A global solution to the trust-region subproblem is characterized by the following result.

Theorem 2.1 (Gay, 1981, Sorensen, 1982) Any global minimizer s_* of $q(s)$ subject to $\|s\|_N \leq \Delta$ satisfies the equation

$$H(\lambda_*)s_* = -g, \tag{2.3}$$

where $H(\lambda_*) \equiv H + \lambda N$ is positive semi-definite, $\lambda_* \geq 0$ and $\lambda_*(\|s_*\|_N - \Delta) = 0$. If $H(\lambda_*)$ is positive definite, s_* is unique.

2.1 Notation

Suppose that G is any real symmetric, possibly indefinite, matrix, and that G has a spectral decomposition

$$G = U\Lambda U^T,$$

where Λ is a diagonal matrix of eigenvalues, and U is an orthonormal matrix whose columns are the corresponding eigenvectors. Then we say that the *absolute value* of G is the matrix

$$|G| = U|\Lambda|U^T,$$

where $|\Lambda|$ is the diagonal matrix of absolute values of the eigenvalues of G.

We shall denote the (appropriately dimensioned) identity matrix by I. The square root $D^{\frac{1}{2}}$ of a diagonal matrix D is simply the diagonal matrix whose entries are $\sqrt{d_{ii}}$, while the generalized inverse D^+ is the diagonal matrix whose entries are $1/d_{ii}$ if $d_{ii} \neq 0$ and 0 if $d_{ii} = 0$.

3 The trust-region norm

We suppose, for now, that H is nonsingular. We will relax this assumption in Section 3.4.

3.1 The spectral trust region

We believe that the shape of an ideal trust region should reflect the geometry of the model, and not give undeserved weight to certain directions. Indeed, perhaps the ideal trust region would be in the $|H|$ norm, for which

$$\|s\|^2_{|H|} = \langle s, |H|s\rangle. \tag{3.1}$$

This norm reflects the scaling of the underlying problem — directions for which the model is changing fastest, and thus those for which the model may differ most from the true function, are restricted more than those directions for which the curvature is small. It has a further interesting property, namely, that a single matrix factorization

$$H = U\Lambda U^T \tag{3.2}$$

is needed to solve the problem. For, on writing

$$s_{\rm D} = U^T s \quad \text{and} \quad g_{\rm D} = U^T g,$$

and using the orthonormality of U, the solution of the trust-region subproblem may be expressed as $s = Us_{\rm D}$, where $s_{\rm D}$ solves the *diagonal* trust-region subproblem

$$\underset{s_{\rm D}\in\mathbf{R}^n}{\text{minimize}} \ \ \langle g_{\rm D}, s_{\rm D}\rangle + \tfrac{1}{2}\langle s_{\rm D}, \Lambda s_{\rm D}\rangle \ \ \text{subject to} \ \ \langle s_{\rm D}, |\Lambda| s_{\rm D}\rangle \leq \Delta^2. \tag{3.3}$$

The diagonal trust-region subproblem is, as we shall see, extremely inexpensive to solve. The major drawback of such an approach is, of course, the cost of the spectral factorization (3.2). For problems involving a large number of variables, this decomposition is likely out of the question.

The absolute-value factorization was originally proposed by Greenstadt (1967) in conjunction with linesearch methods for unconstrained minimization.

3.2 The absolute-value trust region

With this in mind, we consider a symmetric, indefinite factorization of the form

$$H = PLBL^T P^T, \tag{3.4}$$

where P is a permutation matrix, L unit lower triangular and B block diagonal, with blocks of size at most two. We shall refer to the blocks as 1 by 1 and 2 by 2 pivots. Notice that the inertia of H — the numbers of positive, negative and zero eigenvalues of H — is trivially obtained by summing the inertia of the pivots. Such a factorization was first proposed by Bunch and Parlett (1971) and later improved by Bunch and Kaufman (1977) and Fletcher (1976) in the dense case and Duff, Reid, Munksgaard and Neilsen (1979) and Duff and Reid (1983) in the sparse case. More recently, Ashcraft, Grimes and Lewis (1995) and Higham (1995) have exposed a potentially serious flaw in the approach in that the norm of the generated factor L may be unbounded relative to $\|H\|$. While, as Higham (1995) has shown that this does not always lead to instability, a more restricted form of pivoting, as typified by the proposal of Ashcraft et al. (1995), may be required to ensure that $\|L\|$ stays bounded. Interestingly, the sparse method proposed by Duff and Reid (1983) and implemented within the Harwell Subroutine Library (1995) code `MA27` already provided a suitably bounded $\|L\|$ and will be suitable for our purposes.

We suggest that a good choice for the trust-region norm is

$$\|s\|_M^2 = \langle s, Ms \rangle, \tag{3.5}$$

where

$$M = PL|B|L^T P^T. \tag{3.6}$$

Observe that $|B|$ is simply computed by taking the absolute values of the 1 by 1 pivots, and by forming an independent spectral decomposition of each of the 2 by 2 pivots and reversing the signs of any resulting negative eigenvalues. By analogy with the Spectral method, writing

$$s_{\text{B}} = L^T P^T s \quad \text{and} \quad g_{\text{B}} = L^{-1} P^T g, \tag{3.7}$$

the solution of the trust-region subproblem may be expressed as $s = PL^{-T}s_{\rm B}$, where $s_{\rm B}$ solves the *block-diagonal* trust-region subproblem

$$\underset{s_{\rm B}\in\mathbf{R}^n}{\text{minimize}} \ \ \langle g_{\rm B}, s_{\rm B}\rangle + \tfrac{1}{2}\langle s_{\rm B}, Bs_{\rm B}\rangle \ \ \text{subject to} \ \ \langle s_{\rm B}, |B|s_{\rm B}\rangle \leq \Delta^2. \tag{3.8}$$

Once again, a single factorization suffices, but this time the factorization may be affordable even when n is large. Note that Gill, Murray, Ponceléon and Saunders (1992) proposed this modified factorization as a preconditioner for iterative methods, while Cheng and Higham (1996) suggest it as an alternative to the modified Cholesky factorizations of Gill and Murray (1974), Gill, Murray and Wright (1981) and Schnabel and Eskow (1991) within linesearch-based methods.

We note, in passing, that others have used the factorization (3.4) to define trust-region norms. Goldfarb (1980) suggests using (3.5), but where (3.6) is replaced by

$$M = PLL^TP^T. \tag{3.9}$$

Following the change of variables (3.7), the resulting block-diagonal trust-region is then of the form

$$\underset{s_{\rm B}\in\mathbf{R}^n}{\text{minimize}} \ \ \langle g_{\rm B}, s_{\rm B}\rangle + \tfrac{1}{2}\langle s_{\rm B}, Bs_{\rm B}\rangle \ \ \text{subject to} \ \ \|s_{\rm B}\| \leq \Delta$$

and its solution is again straightforward to obtain. This idea has recently been further explored by Xu and Zhang (1997). However, we believe that using (3.9) rather than (3.6) does not reflect the proper scaling of the underlying problem. Indeed, if H were a diagonal matrix, (3.5) remains as the ℓ_2 norm regardless of how ill-conditioned H might be.

3.3 Solving the diagonal and block-diagonal trust region subproblems

As the diagonal trust-region subproblem is a special (but not very special) case of the block-diagonal case, here we shall concentrate on the latter. One could simply apply a standard trust-region solver like `GQTPAR` of Moré and Sorensen (1983) to (3.8), but we prefer not to do this as this would, to some extent, ignore the structure in hand.

As B and $|B|$ share eigenvectors, we may write

$$B = Q\Theta Q^T \quad \text{and} \quad |B| = Q|\Theta|Q^T,$$

where each column of Q is nonzero in at most two positions, with entries corresponding to the eigenvectors of the diagonal blocks, and the entries of the diagonal matrix Θ are the corresponding eigenvalues. On defining

$$s_{\rm S} = |\Theta|^{\frac{1}{2}}Q^Ts_{\rm B} \quad \text{and} \quad g_{\rm S} = |\Theta|^{-\frac{1}{2}}Q^Tg_{\rm B},$$

we may solve (3.8) by finding s_{S} to

$$\underset{s_{\mathrm{S}} \in \mathbf{R}^n}{\text{minimize}} \;\; \langle g_{\mathrm{S}}, s_{\mathrm{S}} \rangle + \tfrac{1}{2} \langle s_{\mathrm{S}}, D s_{\mathrm{S}} \rangle \quad \text{subject to} \quad \|s_{\mathrm{S}}\|_2 \leq \Delta, \tag{3.10}$$

and then recover $s_{\mathrm{B}} = Q|\Theta|^{-\frac{1}{2}} s_{\mathrm{S}}$. Significantly, the matrix $D \equiv |\Theta|^{-\frac{1}{2}} \Theta |\Theta|^{-\frac{1}{2}}$ is diagonal with entries ± 1. The required solution must then satisfy

$$(D + \lambda I) s_{\mathrm{S}} = -g_{\mathrm{S}}, \tag{3.11}$$

where the nonnegative Lagrange multiplier λ is sufficiently large to ensure that $D + \lambda I$ is positive semi-definite, and is zero if s_{S} lies within the trust region $\|s_{\mathrm{S}}\|_2 \leq \Delta$.

There are two cases to consider. Firstly, if $D = I$, the solution to (3.11) is

$$s_{\mathrm{S}} = -\frac{1}{1+\lambda} g_{\mathrm{S}}.$$

If $\|g_{\mathrm{S}}\|_2 < \Delta$, the solution to (3.10) is given by $s_{\mathrm{S}} = -g_{\mathrm{B}}$ and $\lambda = 0$. This corresponds to the unconstrained minimizer of the model lying interior to the trust region. If, on the other hand, $\|g_{\mathrm{S}}\|_2 \geq \Delta$, the solution to (3.10) is obtained by finding the value of $\lambda \geq 0$ for which

$$\frac{1}{(1+\lambda)} \|g_{\mathrm{S}}\|_2 = \Delta.$$

This is a linear equation in λ and thus the solution is trivial to obtain; the required s_{S} is

$$s_{\mathrm{S}} = -\frac{\Delta}{\|g_{\mathrm{S}}\|_2} g_{\mathrm{S}}.$$

This corresponds to the case where the model is convex, but the trust region excludes the unconstrained minimizer of the model. Notice, also, in this case, a reduction in the trust region radius following an unsuccessful step merely reduces the length of the step in the direction $-g_{\mathrm{B}}$. Such a strategy is identical in its effect (if not in its motivation) to a backtracking linesearch along the quasi-Newton direction $-H^{-1}g$, and thus there is a strong similarity between trust-region and linesearch methods with this choice of trust region.

Secondly, if H has negative eigenvalues, D will have some diagonal entries of -1. Suppose P_{S} is a permutation matrix which arranges that all the positive diagonals $(+1)$ of D precede its negative diagonals (-1). Then it is easy to show that

$$s_{\mathrm{S}} = -\frac{1}{\lambda^2 - 1} P_{\mathrm{S}}^T \begin{pmatrix} (\lambda - 1) I & 0 \\ 0 & (\lambda + 1) I \end{pmatrix} P_{\mathrm{S}} g_{\mathrm{S}}. \tag{3.12}$$

As H is indefinite, the solution must lie on the trust-region boundary. Thus, we may obtain λ as the root larger than 1 of the quartic equation

$$\langle P_{\mathrm{S}} g_{\mathrm{S}}, \begin{pmatrix} (\lambda - 1)^2 I & 0 \\ 0 & (\lambda + 1)^2 I \end{pmatrix} P_{\mathrm{S}} g_{\mathrm{S}} \rangle = (\lambda^2 - 1)^2 \Delta^2.$$

Although in principle this root may be found explicitly by Ferrari's method (see, for instance, Turnbull, 1939, and Salzer, 1960), Newton's method is equally suitable here. A slight complication may occur when all of the components of $P_{\rm S}g_{\rm S}$ corresponding to the negative diagonals of D are zero. For then (3.12) yields

$$s_{\rm S} = -\frac{1}{\lambda+1} P_{\rm S}^T \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} P_{\rm S} g_{\rm S},$$

and it may be that there is no root larger than 1 of the resulting feasibility equation

$$\langle P_{\rm S} g_{\rm S}, \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} P_{\rm S} g_{\rm S} \rangle = (\lambda+1)^2 \Delta^2.$$

This case corresponds to the "hard" case of Moré and Sorensen (1983), and here, as there, the solution includes a contribution from a suitable eigenvector. In our case, it is of the form

$$s_{\rm S}(\alpha) = -\tfrac{1}{2} P_{\rm S}^T \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} P_{\rm S} g_{\rm S} + \alpha P_{\rm S}^T \begin{pmatrix} 0 \\ u \end{pmatrix},$$

where u is any nonzero vector, and α is chosen as a root of the quadratic equation $\langle s_{\rm S}(\alpha), s_{\rm S}(\alpha) \rangle = \Delta^2$.

3.4 Coping with singularity

Clearly, it is important to deal with any matrix H including those which are, or are close to being, singular. Cheng and Higham (1996) suggest that it suffices to compute the factorization (3.6) and to replace each eigenvalue θ of the block diagonal B with the value

$$\gamma = \begin{cases} \theta & \text{if } \theta \geq \delta \text{ or} \\ \delta & \text{otherwise} \end{cases} \tag{3.13}$$

for some small $\delta > 0$. An alternative, which is closer in spirit both to the absolute value perturbation and to Greenstadt's (1967) perturbation, is to replace each eigenvalue by

$$\gamma = \begin{cases} \theta & \text{if } \theta \geq \delta \text{ or} \\ -\theta & \text{if } \theta \leq -\delta \text{ or} \\ \delta & \text{otherwise.} \end{cases} \tag{3.14}$$

In any event, this does not significantly affect our previous discussion. For, if we let C denote the (possibly) modified block diagonal matrix B, we now use the trust-region norm (3.5) with M defined as

$$M = PLCL^T P^T. \tag{3.15}$$

We shall refer to (3.15) as the *modified absolute-value* factorization. If we make the change of variables (3.7), we must solve the block-diagonal trust-region subproblem

$$\underset{s_{\rm B}\in\mathbf{R}^n}{\text{minimize}} \quad \langle g_{\rm B}, s_{\rm B}\rangle + \tfrac{1}{2}\langle s_{\rm B}, Bs_{\rm B}\rangle \quad \text{subject to} \quad \langle s_{\rm B}, Cs_{\rm B}\rangle \leq \Delta^2. \tag{3.16}$$

It is of little consequence that BC^{-1} no longer necessarily has eigenvalues ± 1, for, as we shall now see, solving the problem (3.16) is also straightforward.

As before, B and C share eigenvectors. We may thus write

$$B = Q\Theta Q^T \quad \text{and} \quad C = Q\Gamma Q^T,$$

where Q is as before, and the entries of the diagonal matrices Θ and Γ are, respectively, the values θ and γ considered in (3.13) or (3.14). Using the transformation

$$s_{\rm S} = \Gamma^{\frac{1}{2}} Q^T s_{\rm B} \quad \text{and} \quad g_{\rm S} = \Gamma^{-\frac{1}{2}} Q^T g_{\rm B},$$

we may recover the solution to (3.16) from $s_{\rm B} = Q\Gamma^{-\frac{1}{2}} s_{\rm S}$, where $s_{\rm S}$ is found to

$$\underset{s_{\rm S}\in\mathbf{R}^n}{\text{minimize}} \quad q_{\rm S}(s_{\rm S}) \equiv \langle g_{\rm S}, s_{\rm S}\rangle + \tfrac{1}{2}\langle s_{\rm S}, Ds_{\rm S}\rangle \quad \text{subject to} \quad \|s_{\rm S}\|_2 \leq \Delta, \tag{3.17}$$

and where $D \equiv \Gamma^{-\frac{1}{2}}\Theta\Gamma^{-\frac{1}{2}}$ is diagonal. Once again, one could simply apply the Moré and Sorensen (1983) algorithm to this problem, but this ignores the facts that the diagonal systems involved are trivial to solve, and that the leftmost eigenvalue of D and a corresponding eigenvector are trivial to obtain. We therefore prefer the following simplification.

If D merely has entries ± 1, the procedure outlined in Section 3.3 is appropriate. So, now suppose that D has a more complicated distribution of values. Then we may apply Algorithm 3.1.

The iteration in Steps 3 to 5 is simply Newton's method to find the appropriate root of the secular equation

$$\frac{1}{\| -(D+\lambda I)^{+} g_{\rm S}\|_2} = \frac{1}{\Delta}$$

(see Hebden, 1973, or Moré and Sorensen, 1983, for details). Step 1 caters for the case where the model is strictly convex, while step 2 is for the more general case where the solution must lie on the trust-region boundary. The precaution in Step 1a is simply to detect the solution when it lies interior to the trust region, while that in Step 2a(i) is to compute the solution in the "hard case" of Moré and Sorensen (1983). The iteration is globally linearly and asymptotically quadratically convergent from the starting values given in Steps 1 and 2. The tolerance ϵ should be set at the level of the machine precision, ϵ_M. We stress that, while this algorithm is appropriate even if D is simply a diagonal matrix with entries ± 1, the procedure outlined in Section 3.3 is more appropriate in this case.

Algorithm 3.1: Newton iteration to solve (3.17)

Let $\epsilon \in (0,1)$.

1. If D is positive definite, set $\lambda = 0$ and $s_{\rm S} = -D^{-1}g_{\rm S}$.

   1a. If $\|s_{\rm S}\|_2 \leq \Delta$, stop.

2. Otherwise, compute the leftmost eigenvalue, θ of D, set $\lambda = -\theta$ and define $g^{\rm n}_{\rm S}$ so that
$$(g^{\rm n}_{\rm S})_i = \begin{cases} (g_{\rm S})_i & \text{if } (D)_{ii} + \lambda = 0 \\ 0 & \text{otherwise.} \end{cases}$$

   2a. If $g^{\rm n}_{\rm S} = 0$, set $s_{\rm S} = -(D + \lambda I)^{+} g_{\rm S}$.

      i. If $\|s_{\rm S}\|_2 \leq \Delta$, compute an eigenvector u corresponding to θ, find the root α of the equation $\|s_{\rm S} + \alpha u\|_2 = \Delta$ which makes the model $q_{\rm S}(s_{\rm S} + \alpha u)$ smallest, replace $s_{\rm S}$ by $s_{\rm S} + \alpha u$, and stop.

   2b. Otherwise, replace λ by $\lambda + \|g^{\rm n}_{\rm S}\|_2/\Delta$, and set $s_{\rm S} = -(D + \lambda I)^{-1} g_{\rm S}$.

3. If
$$|\|s_{\rm S}\|_2 - \Delta| \leq \epsilon\Delta,$$
   stop.

4. Replace λ by $\lambda + \left(\dfrac{\|s_{\rm S}\|_2 - \Delta}{\Delta}\right)\left(\dfrac{\|s_{\rm S}\|_2^2}{\langle s_{\rm S}, (D + \lambda I)^{+} s_{\rm S}\rangle}\right)$.

5. Set $s_{\rm S} = -(D + \lambda I)^{+} g_{\rm S}$ and go to step 3.

3.5 The suitability of the norm

It remains for us to show that the norms defined by the modified absolute-value factorization (3.15) are uniformly related to the ℓ_2-norm, and thus are suitable within a trust-region method. Thus we need to show that there are constants $0 < \gamma_1 < \gamma_2$, independent of the iteration, for which
$$\gamma_1 \|s\|_2^2 \leq \langle s, Ms\rangle \leq \gamma_2 \|s\|_2^2.$$
Equivalently, we need to show that the smallest and largest eigenvalues, $\lambda_{\min}(M)$ and $\lambda_{\max}(M)$, of M are bounded, and bounded away from zero. The analysis here is based upon that given by Higham (1995).

Firstly, by construction, both of (3.13) and (3.14) satisfy the bounds
$$\delta \leq \|C\| = \max(\delta, \|D\|) \leq \max\left(\delta, \|H\|\|(LL^T)^{-1}\|\right).$$

Using Theorem 3.2 of Higham (1995), it then follows that

$$\lambda_{\min}(LL^T)\lambda_{\min}(C) \leq \lambda_{\min}(M) \leq \lambda_{\max}(M) \leq \lambda_{\max}(LL^T)\lambda_{\max}(C),$$

and hence that

$$\delta\lambda_{\min}(LL^T) \leq \lambda_{\min}(M) \leq \lambda_{\max}(M) \leq \lambda_{\max}(LL^T)\max\left(\delta, \|D\| \leq \|H\|\|(LL^T)^{-1}\|\right).$$

But, as Higham then points out, if the largest entry in L is bounded by some β, it is straightforward to bound

$$1 \leq \lambda_{\max}(LL^T) \leq n + \tfrac{1}{2}n(n-1)\beta^2 \quad \text{and} \quad (1+\beta)^{2-2n} \leq \lambda_{\min}(LL^T) \leq 1.$$

Thus so long as L and H are bounded, the norms defined by the modified absolute-value factorization (3.15) are uniformly related to the ℓ_2-norm.

The matrix H will be bounded if, for instance, a Newton (second-order Taylor series) model is used, and if the iterates stay in a bounded set. But now we see the importance of using a factorization which bounds the growth in the elements of L. Ashcraft et al. (1995) show that the original method of Bunch and Parlett (1971) and that of Fletcher (1976) both generate bounded L, as do the sparse methods of Duff and Reid (1983, 1996). However, the more popular Bunch and Kaufman (1977) method and the block version implemented in `LAPACK` may not, and thus must be viewed as untrustworthy for our application.

4 Numerical experiments

The algorithm sketched in Sections 3.3 and 3.4 has been implemented as a Fortran 90 module, `HSL_VF06`, within the Harwell Subroutine Library (HSL) (1998). The factorization (3.4) is performed using the HSL code `MA27` (see, Duff and Reid, 1982). A concise summary of `HSL_VF06` is given as Algorithm 4.1.

Algorithm 4.1: `HSL_VF06`

1. Factorize $H = PLBL^TP^T$, using subroutines `MA27A` and `MA27B`, and $B = Q\Theta Q^T$. Obtain the diagonal matrix Γ from (3.14) with $\delta = \sqrt{\epsilon_M}$, and set $C = Q\Gamma Q^T$ and $D = \Gamma^{-\frac{1}{2}}\Theta\Gamma^{-\frac{1}{2}}$.
2. Solve $PLP^T g_{\rm b} = g$ using `MA27Q`.
3. Obtain $g_{\rm s} = \Gamma^{-\frac{1}{2}}Q^TP^Tg_{\rm b}$
4. Find $s_{\rm S} = \arg\min \langle g_{\rm S}, s_{\rm S}\rangle + \frac{1}{2}\langle s_{\rm S}, Ds_{\rm S}\rangle \quad$ subject to $\quad \|s_{\rm S}\|_2 \leq \Delta$ using Algorithm 3.1, with stopping tolerance $\epsilon = 10n\epsilon_M$.
5. Recover $s_{\rm q} = PQ\Gamma^{\frac{1}{2}}s_{\rm S}$.
6. Solve $PCL^TP^Ts = s_{\rm q}$ using `MA27R`.

In order to demonstrate the potential of our proposal, we have conducted a limited number of numerical tests using `HSL_VF06`. We consider the standard trust-region method for the minimization of an objective $f(x)$ of n real variables x presented as Algorithm 4.2.

We choose the specific values $\epsilon_g = 0.00001$, $\eta_1 = 0.01$, $\eta_2 = 0.95$, $\gamma_1 = 0.5$, and $\gamma_2 = 2$, and set an upper limit of $20n$ iterations. In all cases, the initial trust-region radius is set to $\|M_0\|_\infty$. The step s_k in step 2 is computed using either Algorithm 4.1, or using the algorithm proposed by Gould, Lucidi, Roma and Toint (1997) and implemented as the HSL fortran 90 module `HSL_VF05` using default settings. The latter algorithm is appropriate for general trust-region norms, but is not as efficient as `HSL_VF06` when the absolute-value norm (3.5)–(3.6) is used.

In our tests we compare three choices of norm, namely the ℓ_2 norm, the absolute-value norm, and the norm defined by forming the Schnabel and Eskow (1991) modified Cholesky factorization of H. The latter also uses `MA27`, and is available as part of the LANCELOT nonlinear programming package (see, Conn, Gould and Toint, 1992, Chapter 3). Other norms have been compared by Gould et al. (1997).

All our tests were performed on an IBM RISC System/6000 3BT workstation with 64 Megabytes of RAM; the codes are all double precision Fortran 90, compiled under xlf90 with -O optimization, and IBM library BLAS are used. The test examples we consider are the currently available larger examples from the CUTE test set (see Bongartz, Conn, Gould and Toint, 1995) for which negative curvature is frequently encountered. Tests were terminated if more than thirty CPU minutes elapsed.

Algorithm 4.2: Standard Trust-Region Algorithm

0. An initial point x_0 and an initial trust-region radius Δ_0 are given, as are constants ϵ_g, η_1, η_2, γ_1, and γ_2, which are required to satisfy the conditions
$$0 < \eta_1 \leq \eta_2 < 1 \text{ and } 0 < \gamma_1 < 1 \leq \gamma_2.$$
Set $k = 0$.

1. Stop if $\|\nabla_x f(x_k)\|_2 \leq \epsilon_g$.

2. Define a second-order Taylor series model q_k and a positive-definite preconditioner M_k. Compute a step s_k to "sufficiently reduce the model" q_k within the trust-region $\|s\|_{M_k} \leq \Delta_k$.

3. Compute the ratio
$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{q_k(x_k) - q_k(x_k + s_k)}.$$
If $\rho_k \geq \eta_1$, let $x_{k+1} = x_k + s_k$; otherwise let $x_{k+1} = x_k$.

4. Set
$$\Delta_{k+1} = \begin{cases} \gamma_2 \Delta_k & \text{if } \rho_k \geq \eta_2, \\ \Delta_k & \text{if } \rho_k \in [\eta_1, \eta_2), \\ \gamma_1 \Delta_k & \text{if } \rho_k < \eta_1. \end{cases}$$
Increment k by one and go to Step 1.

The results of our tests are given in Table 4.1. In these tables, in addition to the name and dimension of each example, we give the number of objective function ("#f") and derivative ("#g") values computed, and the total CPU time required in seconds. We indicate those cases where one or other method performs at least 10% better than its competitors by highlighting the relevant figure in bold. A † indicates that convergence to different local minimizers occurred.

The results may effectively be divided into three categories. Into the first category fall problems which appear to be relatively easy, that is those which require few evaluations without a sophisticated trust-region norm. For such problems, the ℓ_2 norm performs best, and the other norms add little while incurring the extra expense of the factorization. The excellent behaviour of the ℓ_2 norm on such problems has already been noted (see, Gould et al., 1997). The second category contains problems for which the Hessian or its factors are relatively dense, and the cost of forming the preconditioner dominates. This category includes problems `EIGENALS`, `MSQRTALS`, `NONCVXU2`, `SPARSINE` and `SPMSRTLS`.

		ℓ_2			modified Cholesky			modified abs-value		
example	n	$\#f$	$\#g$	CPU	$\#f$	$\#g$	CPU	$\#f$	$\#g$	CPU
BROYDN7D †	1000	110	103	7.4	50	35	**4.1**	126	81	10.0
BRYBND	1000	13	13	**0.9**	15	15	2.3	23	15	2.6
CHAINWOO †	1000	915	626	81.8	176	115	**7.9**	175	103	9.5
COSINE	1000	11	11	**0.1**	41	25	1.3	20	14	1.0
CRAGGLVY †	1000	19	19	0.9	23	23	1.4	18	16	1.3
CURLY10	1000	23	21	29.9	57	35	**7.6**	55	33	8.6
CURLY20	1000	21	20	35.8	57	36	27.7	8	8	**6.6**
CURLY30	1000	22	21	46.2	71	42	81.9	12	9	**18.3**
DIXMAANA	1500	13	13	**0.3**	35	23	1.4	8	8	0.7
DIXMAANE	1500	14	14	**1.8**	150	85	7.9	115	76	8.2
DQRTIC	1000	43	43	**0.3**	54	54	1.3	33	32	1.3
EIGENALS	930	66	53	**71.0**	63	47	85.4	> 1800 secs.		
FREUROTH	1000	17	17	**0.4**	86	48	3.5	132	84	7.5
GENHUMPS	1500	14474	13964	1023.0	$> 20n$ its.			10208	9521	**796.4**
GENROSE	1000	721	665	48.1	434	312	**19.3**	1109	776	58.7
MANCINO	100	24	23	**20.2**	77	58	275.9	19	10	37.5
MSQRTALS	1024	35	30	**394.2**	> 1800 secs.			> 1800 secs.		
NCB20B	1000	45	29	141.1	33	20	26.8	21	12	**10.8**
NONCVXUN	1000	> 1800 secs.			$> 20n$ its.			3020	2493	**490.7**
NONCVXU2	1000	272	227	**29.7**	$> 20n$ its.			$> 20n$ its.		
SBRYBND	1000	> 1800 secs.			59	28	9.7	65	28	**5.5**
SCOSINE †	1000	> 1800 secs.			90	70	4.4	70	14	**1.7**
SCURLY10	1000	> 1800 secs.			61	45	10.2	40	6	**2.2**
SCURLY20	1000	> 1800 secs.			75	52	41.3	41	6	**6.3**
SCURLY30	1000	> 1800 secs.			75	52	105.4	45	7	**16.3**
SENSORS †	100	21	20	**8.1**	66	51	32.0	61	39	24.05
SINQUAD	5000	152	99	**21.7**	14	14	100.0	14	14	86.0
SPARSINE	1000	16	16	**36.5**	361	205	1047.5	> 1800 secs.		
SPMSRTLS †	1000	18	16	**2.05**	> 1800 secs.			> 1800 secs.		

Table 4.1: A comparison of trust-region methods using the ℓ_2, modified Cholesky and modified absolute-value norms. See the text for a key to the data.

These indicate the limitations of our approach, and for these problems preconditioners which try to mimic the structure of the Hessian without incurring the cost of the fill-in — such as the limited-memory incomplete Cholesky factorization proposed by Lin and Moré (1997), and the references contained therein — are likely to be preferable. The third category contains the harder, highly nonlinear problems CURLYxx, NONCVXUN, SBRYBND, SCOSINE and SCURLYxx. For these problems, the ℓ_2 norm is ineffective, and some rescaling is necessary. Interestingly, the modified absolute-value preconditioner outperforms the

other sophisticated preconditioner on all but one of these, often by a large margin.

It is interesting to note that the number of "wasted" function evaluations (the difference between $\#g$ and $\#f$ in in Table 4.1) is significantly higher for the new method than for its competitors. There appear to be two reasons for this. Firstly, the initial trust-region radius, $\|M_0\|_\infty$, is often far too large when using the factorization preconditioners, and many iterations are required to cut it to a value for which progress may be made. In our experience, it is usually beneficial to determine a good initial radius, and, given how inexpensive the wasted iterations are in our case — the functions are cheap to evaluate, and the solution of the block-diagonal trust-region problems are, by design, trivial — the cost is not especially high. However, as evaluation costs may be high in general, more sophisticated strategies, such as that by Sartenaer (1997), may be preferred. The second cause of wasted function evaluations happened far less frequently, but occurs following a change in the shape of the trust-region as one or more eigenvalues change sign. In some cases, — the example `SCOSINE` is a point in case — a significant number of radius reductions were required to find a value appropriate for the new geometry. We foresee this as a significant problem, and are currently investigating more sophisticated schemes for trust-region management.

5 Discussion and conclusions

We believe that our results indicate that the modified absolute-value factorization provides a useful norm for trust-region minimization so long as as the factorization is feasible. In particular, for ill-conditioned problems, the norm appears to be especially effective. We do not pretend that (3.15) is uniformly appropriate, but suggest that, at the very least, its use should be considered when a problem is know to be ill-conditioned.

We recognize some potential difficulties with our approach. The attendees at the 1981 NATO Advanced Research Institute on "Nonlinear Optimization" (see Powell, 1982, contributions 1.31–1.35) had much to say about Goldfarb's (1980) proposal, and the comments made there are equally appropriate here. In particular Roger Fletcher (Dundee) expressed concern that the distortion induced by (3.5) and (3.9) may be substantial. We accept that (3.15) may not be as desirable as (3.1), but believe that while (3.1) is out of the question for most large-scale problems, (3.15) is practical, and often useful, for many of them. Fletcher also worried that changes in the pivot ordering during the factorization of a sequence of problems may make it difficult to derive effective methods for adjusting the trust-region radius. Whilst we have observed occasions where pivot-order changes have drastically altered the geometry, and while this sometimes requires a large number of wasted iterations in which the trust-region radius is reduced, for the vast majority of iterations the usual, naive trust-region management seems to be satisfactory. However, we recognize this as a

possible defect, and are currently investigating more sophisticated trust-region adjustment strategies both in this and other contexts.

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