On Iterated-Subspace Minimization Methods for Nonlinear Optimization

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\textbf{ABSTRACT}

We consider a class of Iterated-Subspace Minimization (ISM) methods for solving large-scale unconstrained minimization problems. At each major iteration of such a method, a low-dimensional manifold, the iterated subspace, is constructed and an approximate minimizer of the objective function in this manifold then determined. The iterated subspace is chosen to contain vectors which ensure global convergence of the overall scheme and may also contain vectors which encourage fast asymptotic convergence. We demonstrate the efficacy of this approach on a collection of large problems and indicate a number of avenues of future research.

\textbf{Keywords}: Unconstrained optimization, large-scale computation, convergence theory.

\textbf{AMS(MOS) subject classifications}: 65K05, 90C30

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Abstract

We consider a class of Iterated-Subspace Minimization (ISM) methods for solving large-scale unconstrained minimization problems. At each major iteration of such a method, a low-dimensional manifold, the iterated subspace, is constructed and an approximate minimizer of the objective function in this manifold then determined. The iterated subspace is chosen to contain vectors which ensure global convergence of the overall scheme and may also contain vectors which encourage fast asymptotic convergence. We demonstrate the efficacy of this approach on a collection of large problems and indicate a number of avenues of future research.

1 Introduction

In this paper, we consider finding a local solution of the unconstrained minimization problem,

\[
\begin{align*}
\text{minimize} & \quad f(x), \\
\text{subject to} & \quad x \in \mathbb{R}^n
\end{align*}
\]

where we assume, for simplicity, that the objective function \( f \in C^2 \). We are particularly interested in the case where \( n \) is sufficiently large that methods appropriate for small problems — such as those which might maintain a dense factorization of a suitable approximation of the Hessian matrix, see, for example, Gill et al. (1981), Dennis and Schnabel (1983) and Fletcher (1987) — are impractical.

We are primarily concerned with the commonly occurring case in which the cost of evaluating the value of the objective function and its derivatives, at a given point \( x \), is less significant than the cost of solving, for instance, the Newton equations. Our experience with the large-scale nonlinear optimization package LANCELOT (see Conn et al., 1992b) has been that it is the linear-algebra cost which tends to dominate when solving a significant number of widely differing application problems (see, Conn et al., 1992c and Conn et al., 1992a). Thus, it would appear desirable in these cases to attempt to reduce the linear-algebra costs, even if this results in an increase in the number of objective function evaluations.

The most common methods for unconstrained minimization either determine a search direction followed by a linesearch or use the trust-region approach (see, for example, Dennis and Schnabel, 1983). In the former case, a simple model of the underlying objective function is constructed in order to determine the search direction. By contrast, in the latter case, an approximate minimizer of the model within a restricted domain (the trust region) is determined. This model minimizer is then used as a prediction of the actual minimizer of the true objective. In a trust-region method, success of this process is measured by
comparing the model and true function values at the predicted minimizer. In linesearch methods, the true function is used to establish a step size. Thus, both of these approaches may be considered to perform their multi-dimensional work with respect to a model whilst probing the true function uni-dimensionally. Of course, the model does make use of the true function and perhaps its derivatives — maybe at more than a single point.

In this paper, we take the view that the above schemes are quite wasteful, given the amount of information that may have been accrued during the (approximate) minimization of the model. In particular, the model may have been sampled in a number of potentially interesting directions, of which only the aggregate direction is normally considered to be of significance.

We also believe that, provided function and derivative values are inexpensive to compute relative to the linear-algebra costs, an (approximate) low-dimensional minimization is a trivial calculation. Indeed, we feel that, quite generally, the small-scale unconstrained minimization problem has effectively been solved in that there is high-quality, robust, general-purpose software easily available for such problems, and that such software is normally capable of solving problems of modest dimensions - say up to 100 variable problems - extremely fast on current workstations provided that function evaluation is cheap. Of course there are, and will continue to be, small-scale problems which are challenging, because they are so nonlinear that algorithms implemented in fixed, finite precision arithmetic are unsuccessful, but in our experience such examples occur rarely in practice. Thus, in this paper, we propose methods which aim to investigate the true objective function in a space larger than the one-dimensional space which is normally associated with linesearch or trust-region methods. We do this knowing that, so long as the space is relatively modest, the approximate multi-dimensional minimization will still be a manageable calculation. Moreover, by carefully choosing the space that we investigate, we hope to reduce significantly the linear-algebra costs while still maintaining global, and fast asymptotic, convergence.

A particular form of this idea has been given by Saad (1990) for the solution of nonlinear systems of equations. Here, a sequence of iterates are generated as least-squares solutions to the equations in suitable Krylov subspaces. The principal difference is that, in Saad’s proposal, the entire Krylov subspace generated is used, while, as we shall see, this is in general quite unnecessary.

Given an initial estimate of the solution to (1.1), $\mathbf{a}^{(0)}$, and an iteration count, $k$, set initially to zero, a prototype algorithm might be as follows:

1. Stop with the solution estimate $\mathbf{a}^{(k)}$ if convergence tests are satisfied.
2. Determine a full-rank subspace matrix $\mathbf{S}^{(k)} \in \mathbb{R}^{n \times s^{(k)}}$, where $s^{(k)} \ll n$.
3. Approximately solve the $s^{(k)}$-dimensional minimization problem

$$\min_{\mathbf{y} \in \mathbb{R}^{s^{(k)}}} f(\mathbf{a}^{(k)} + \mathbf{S}^{(k)}\mathbf{y}),$$

set

$$\mathbf{a}^{(k+1)} = \text{(approx) arg min}_{\mathbf{y} \in \mathbb{R}^{s^{(k)}}} f(\mathbf{a}^{(k)} + \mathbf{S}^{(k)}\mathbf{y}),$$

replace $k$ by $k + 1$ and return to step 1.
We refer to such a method as *Iterated-Subspace Minimization* or ISM for short. This is, of course, a multi-dimensional subspace analog of the unidimensional-subspace linesearch method. We are interested in the following issues.

- What is a good choice for $s^{(k)}$?
- How do we determine the *Iterated-Subspace* matrix $S^{(k)}$?
- What do we mean by “approximate” in the problem (1.3)?
- Are there methods which are particularly appropriate for solving (1.2)?
- What can we say about the convergence of such a method?
- If we can establish convergence, what can we say about its asymptotic rate?

In this paper, we make preliminary attempts to answer all of these questions.

We will use the following notation. Bold lower and upper case roman letters indicate vectors and matrices, respectively, while greek and normal roman letters denote scalars. Script style letters are index sets. A superscript $(k)$ indicates a quantity which occurs at the $k$-th iteration or which is evaluated at $x^{(k)}$.

We let $g(x)$ and $H(x)$, respectively, indicate the gradient, $\nabla_x f(x)$, and Hessian matrix, $\nabla_{xx} f(x)$, of the objective function. We define

$$f_s^{(k)}(y) \overset{\text{def}}{=} f(x^{(k)} + S^{(k)} y),$$

(1.4)

$$g_s^{(k)}(y) \overset{\text{def}}{=} \nabla_y f_s^{(k)}(y) \quad \text{and} \quad H_s^{(k)}(y) \overset{\text{def}}{=} \nabla_{yy} f_s^{(k)}(y),$$

and

$$g_s^{(k)}(y) = S^{(k)T} g(x^{(k)} + S^{(k)} y)$$

(1.5)

and

$$H_s^{(k)}(y) = S^{(k)T} H(x^{(k)} + S^{(k)} y) S^{(k)}.$$  

(1.6)

The paper is organised as follows. In Section 2, we analyse the convergence of the algorithm given in the introduction. We discuss a number of computationally attractive ISM methods in Section 3, and we report on some preliminary numerical experience when solving some relatively large test examples, from the CUTE test suite (see Bongartz et al., 1993). Possible extensions, to the cases where there are linear or nonlinear constraints present, are given in Section 5. We conclude, in Section 6, by offering our perspectives of this and future work.

2 Convergence analysis of a general algorithm

Global convergence of the above scheme can be guaranteed under fairly general assumptions. Suppose that we are able to pick consecutive iterates $x^{(k)}$ and $x^{(k+1)} = x^{(k)} + S^{(k)} y^{(k)}$ for which the Goldstein (1964) conditions

$$f^{(k)} + \beta g^{(k)T} S^{(k)} y^{(k)} \leq f^{(k+1)} \leq f^{(k)} + \alpha g^{(k)T} S^{(k)} y^{(k)},$$

(2.1)

for some $0 < \alpha \leq \beta < 1$, are satisfied, where $y^{(k)}$ is the approximate solution of (1.2). Suppose, furthermore, that

$$\frac{-g^{(k)T} S^{(k)} y^{(k)}}{\|S^{(k)} y^{(k)}\|_2} \geq \epsilon,$$

(2.2)
for some $\epsilon > 0$. Then the ISM algorithm from Section 1 is globally convergent to a stationary point for the problem (1.1) from any starting point so long as $f$ is bounded from below and has a Lipschitz-continuous gradient (see, for example, Dennis and Schnabel, 1983, Theorem 6.3.3). We may rewrite (2.1) as

$$f_s^{(k)}(0) + \beta g_s^{(k)}(0)^T y_s^{(k)} \leq f_s^{(k)}(y_s^{(k)}) \leq f_s^{(k)}(0) + \alpha g_s^{(k)}(0)^T y_s^{(k)}$$

and ensure that (2.2) is satisfied by requiring that

$$-g_s^{(k)}(0)^T y_s^{(k)} \leq \epsilon \|S^{(k)}\|_2.$$  

This is relevant as now the global convergence conditions may be verified in terms of the inner-minimization function $f_s$ and its gradient. Similar global convergence results can be obtained if we replace condition (2.1) by the Armijo (1966) backtracking strategy (see Bertsekas, 1982, Section 1.3). It may, however, be difficult to design general algorithms which ensure that conditions (2.3) and (2.4) are satisfied on exit from the inner minimization. Thus, it may be preferable to impose extra conditions on the iterates generated during the inner minimization to ensure overall global convergence. With this in mind, suppose that we can find any point $y_s^{(k)}$ for which

$$f_s^{(k)}(0) + \beta g_s^{(k)}(0)^T y_s^{(k)} \leq f_s^{(k)}(y_s^{(k)}) \leq f_s^{(k)}(0) + \alpha g_s^{(k)}(0)^T y_s^{(k)}$$

and

$$-g_s^{(k)}(0)^T y_s^{(k)} \geq \epsilon \|S^{(k)}\|_2$$

are satisfied. Suppose, furthermore, that we terminate the inner minimization at a point $y_s^{(k)}$ for which

$$f_s^{(k)}(0) - f_s^{(k)}(y_s^{(k)}) \geq \tau (f_s^{(k)}(0) - f_s^{(k)}(y_s^{(k)})),$$

where $\tau > 0$. Then it is easy to show that this scheme is globally convergent under the same conditions as stated above. The advantage here is that the tests (2.5) and (2.6) need only be satisfied at an intermediate point to ensure convergence. Typically, the first inner-iterate provides such a point for carefully chosen subspaces and minimizers. For example, if the subspace contains the steepest-descent direction and the inner minimization starts by performing a linesearch in this direction, the resulting first inner-iterate satisfies (2.5) and (2.6). Similarly, if the subspace contains a (modified) truncated-Newton direction and the inner minimization starts by performing a linesearch in this direction, the same conclusion is true.

### 3 Computational Variants

We consider it important from a practical point of view to require that $S^{(k)}$ contains at least two components,

- a gradient-related direction, such as $-g^{(k)}$, to encourage global convergence, and
- a Newton-related direction, such as might be computed by a truncated-Newton method, to encourage fast asymptotic convergence, with safeguards to account for indefiniteness.

Of course, these components play a key role in dog-leg trust-region methods (see, for example, Powell, 1970). Additional components have the advantage of enlarging the subspace searched, but the disadvantage of increasing the overheads in solving the $s^{(k)}$-dimensional subspace minimization problem. In this section, we consider various possible ways of choosing the iterated subspace.
3.1 Conjugate gradients

An appealing choice of $S^{(k)}$ may be obtained by picking the columns of $S^{(k)}$ as a set of $H^{(k)}$-conjugate directions, especially if these directions are generated by a (preconditioned) conjugate-gradient (CG) method.

Suppose that $H^{(k)}$ is positive definite. Let $\phi^{(k)}(x^{(k)} + p)$ be the quadratic model,

$$\phi^{(k)}(x^{(k)} + p) = f^{(k)} + p^T g^{(k)} + \frac{1}{2} p^T H^{(k)} p,$$

of $f(x^{(k)} + p)$ about $x^{(k)}$. The preconditioned conjugate-gradient method (see, for example, Hestenes and Stiefel, 1952 and Golub and Loan, 1989, Section 10.3) is an iterative method which may be used to calculate the smallest value of (3.1). It is well known that the solution, $p_n$, to this problem is the Newton direction.

A preconditioner $P^{(k)}$ is usually an easily invertible approximation to $H^{(k)}$. We shall insist that $P^{(k)}$ has a uniformly bounded condition number. The $j$-th step of the preconditioned conjugate-gradient method determines the smallest value of (3.1) in the Krylov subspace spanned by the vectors $\{-(P^{(k)-1}H^{(k)})^jP^{(k)-1}g^{(k)}\}_{j=0}$. Conjugacy properties ensure that each successive step may be accomplished by a univariate minimization of (3.1) in the direction $s_j$; the vectors $\{s_j\}$ are conjugate and are recurred from step to step. Significantly from our point of view, the first such vector, $s_0 = -(P^{(k)-1}g^{(k)})$. In exact arithmetic the method would terminate with the Newton direction, $p_n$, after at most $n$ steps, but numerical rounding errors ensure that the method behaves more like an infinite iteration (see Reid, 1971). Moreover, for the large-scale case, we would be unwilling to consider anywhere close to $n$ iterations. Nonetheless, the method is an effective technique for calculating approximations to the Newton direction, especially if a good preconditioner is used or if low accuracy solutions may be tolerated (see Toint, 1981, Dembo et al., 1982, and Dembo and Steihaug, 1983).

In truncated-Newton methods (see Dembo et al., 1982), the method of conjugate gradients is used to generate approximations to the Newton direction. The resulting search direction, $p_m$, is employed within a linesearch framework for solving unconstrained optimization problems. Significantly, highly accurate approximations to the Newton correction are only needed to accelerate the convergence of the iteration in the neighbourhood of a limit point, and crude improvements upon the steepest-descent direction suffice elsewhere. Furthermore, by monitoring the gradient of the model at each step of the conjugate-gradient method, we can decide when to terminate the iteration.

While such an approach has undoubtedly proved successful in practice, we note that a considerable amount of work is invested, in such a scheme, in calculating an “average” direction and that much of the information gleaned on the way is subsequently ignored. We take the point of view that directions generated by the conjugate-gradient method are of interest for the quadratic model, but might also be locally of interest for the true objective function. We thus propose to construct our iterated subspace from the subspace investigated by the conjugate gradient method.

We intend to include some or all of the following:

- The preconditioned steepest-descent direction, $s_0 = -(P^{(k)-1}g^{(k)})$;
- A number of other conjugate directions, $s_j$, determined by the preconditioned conjugate-gradient method; and
- The overall truncated-Newton direction, $p_m$.

We note that the first of these components is designed to encourage global convergence, while the last will ensure that convergence occurs at a fast asymptotic rate.
3.2 Choice of conjugate directions

Suppose that, in addition to the (preconditioned) steepest-descent and (truncated) Newton directions, we wish to include $q \ H^{(k)}$, conjugate directions in the subspace. The simplest choice is just to take the first $q$ generated (excluding, of course, the steepest-descent direction). However, these may not be those which were most judicious for the quadratic model and another choice may be to take the $q$ which gave the largest decrease in the model. Experiments suggest that this is rarely more successful than the simpler scheme.

Another possibility is to consider including approximations from the extreme eigenspaces, that is the set of eigenvectors which correspond to the smallest and largest eigenvalues (recall $H^{(k)}$ is assumed positive definite). Eigenvectors corresponding to large eigenvalues may be useful as the objective function and CG model differ most significantly in these directions. Those associated with small eigenvalues reflect the space in which the Newton direction is likely to be sensitive and contributions from this space are necessary if rapid progress is to be made. Thus both sets of vectors are reasonable candidates for subspace directions.

Clearly, the calculation of these spaces is generally prohibitively expensive, but they may be approximated by directions generated during the CG process (see, eg, Parlett, 1980, Chapter 13). We might monitor the Rayleigh quotients

$$
\frac{s_j^T H^{(k)} s_j}{s_j^T s_j}
$$

and include the $s_j$ which give rise to the most extreme Rayleigh quotients. Of course, these vectors are not eigenvectors of $H^{(k)}$, but they normally contain significant contributions in the extreme eigenspaces.

3.3 Choice of subspace dimension

The choice of subspace dimension is clearly important. The simplest choice is to fix an upper bound $s$ on this dimension before the computation proceeds (perhaps $s = 10$, see Section 4), and to select $s^{(k)}$ to be the smaller of $s$ and the total number of CG directions sampled during the $k$-th CG iteration — recall that the CG process may be truncated and thus fewer than $s$ directions may have been computed.

A more sophisticated approach is to try to dynamically select the size of subspace based upon the needs of the $k$-th iteration. For instance, if the Hessian is relatively well-conditioned, it is likely that a subspace made up from the steepest-descent and (truncated) Newton directions will suffice. If, on the other hand, the Hessian is ill-conditioned, further subspace directions are likely to prove beneficial.

A simple heuristic would be to monitor the Rayleigh quotient as the CG iteration proceeds. Typically the first search direction, $s_0 = -P^{(k)} g^{(k)}$, for the CG iteration will contain components of all eigenvectors and hence some components of those corresponding to the largest eigenvalues. The influence of the eigenvectors corresponding to the large eigenvalues is reduced in the subsequent directions $s_1, \ldots$, and this is reflected in a reduction in the Rayleigh quotient during these iterations. This effect is reversed after a number of iterations, when the influence of the larger eigenvalues reappears. It would thus seem sensible to record the iteration number, $i^{(k)}$, at which the Rayleigh quotient first starts to increase after its initial sequence of decreases. As we know that we then have sampled eigenvectors in both “large” and “small” eigenspaces, it is appropriate to set $s^{(k)} = i^{(k)}$. 


3.4 The inner minimization

As we have stated, we believe that there are a number of highly effective algorithms for
the unconstrained minimization of a function of several variables. Indeed, it would not
be unreasonable to say that the problem has effectively been solved so long as derivatives
are available. Among the most successful methods are the Newton-like second-derivative
methods and the finite-difference and secant methods which require only gradients (see,
for example, Dennis and Schnabel, 1983, Gill et al., 1981 or Fletcher, 1987).

When considering the minimization of (1.4), we note that the calculation of derivatives
of \( f_s^{(k)} \) requires those of \( f \). We see that the calculation of the second derivatives (1.6)
requires significantly more products involving \( S^{(k)} \) than do the first derivatives (1.5).
Thus, we would prefer to use methods which either only require relatively few Hessian-
vector products, such as (preconditioned and truncated) conjugate-gradient methods, or
secant methods, which build up approximations to the second derivatives from gradients
in the \( s^{(k)} \)-dimensional subspace as they proceed.

The most widely used secant methods are those in the convex Broyden class of positive-
definite approximations, of which the BFGS method has the best reputation (again see,
for example, Dennis and Schnabel, 1983). While there is currently some controversy as to
whether there are better nonconvex secant updates (see for example, Conn et al., 1991,
Khalfan et al., 1993, and Byrd et al., 1993), we feel that convex secant methods are most
natural in a linesearch, as opposed to a trust-region, context. Such methods start with
a positive-definite second-derivative approximation and generate a sequence of matrices
which mimic the curvature in the space of directions searched. Traditionally, the Cholesky
factors of the sequence are updated as the iteration proceeds. We now show that building
a good starting matrix in our case is easy.

Firstly, suppose that \( S^{(k)} \) is made up purely of \( H^{(k)} \)-conjugate directions. Then the
exact second-derivative matrix \( H_s^{(k)} \) is diagonal because of the conjugacy and moreover its
diagonal entries will have been calculated during the conjugate-gradient process. This ma-
trix, then, is a good starting approximation; its Cholesky factors are trivial to determine.
Furthermore, this choice ensures that the first Quasi-Newton search direction is identical
to that generated by minimizing the quadratic model (3.1) in the manifold \( x^{(k)} + S^{(k)} y \)
(see, Gill et al., 1981, section 4.8.3.1).

Now suppose that \( S^{(k)} \) is made by augmenting a set of \( H^{(k)} \)-conjugate directions by
the overall truncated-Newton direction \( p_m \). Then, the exact second-derivative matrix has
an arrowhead structure with the leading \( s^{(k)} - 1 \) by \( s^{(k)} - 1 \) submatrix being diagonal and
the remaining row and column easy to obtain. To be precise, if we denote the residual
\( H^{(k)} p_m + g^{(k)} \) following the truncated conjugate-gradient process by \( r^{(k)} \), the last column
of the required second-derivative matrix is \( S^{(k)} T (r^{(k)} - g^{(k)}) \). Thus, once again this matrix
provides a good starting approximation in that its Cholesky factors are extremely cheap
to compute. Moreover, as before, the first Quasi-Newton direction gives the minimum
of the model (3.1) in the manifold \( x^{(k)} + S^{(k)} y \). Significantly, as the truncated-Newton
direction is in the subspace, this first Quasi-Newton direction is thus the same as the
truncated-Newton direction.

4 Numerical Experiments

We start this section by investigating, from a numerical point of view, the impact of
different subspace sizes on the convergence of the method. As the problem FMINSURF, from
the CUTE collection (see Bongartz et al., 1993), is particularly efficiently solved using ISM
in comparison with the default version of LANCELOT, we examined this problem in detail.
We ran ISM, without preconditioner, but constructing the subspace from a combination of the steepest-descent, truncated-Newton and extreme directions as described above, using a variety of subspace dimensions and illustrate, in Figure 4.1, the effects of the choice of this dimension on the CPU time required to solve the problem. This experiment was performed on an IBM RISC/6000 320h workstation, using optimized (-O) Fortran 77 code and IBM-supplied BLAS.

![Graph](image)

**Figure 4.1:** The impact of varying the subspace dimension on FMINSURF (using an unpre-conditioned ISM in which the subspace is chosen from the the steepest-descent, truncated-Newton and extreme CG directions).

We observe that the CPU time for small subspace dimension is large, but that, for subspaces of dimension between 9 and 40, the time is relatively constant, being within ten percent of the least (s = 11) time. Thus, it appears that for this problem, adding information above the steepest-descent and truncated-Newton directions is beneficial but there is little extra payoff from using more than 11 directions. When we monitored the Rayleigh quotients for this problem, we observed that the quotient decreases for on average 10 CG iterations before increasing for the first time. Thus, unless we insist on at least 10 CG iterations, it is possible that we may not have sampled the complete eigenspace. Similar runs on different problems indicate that this behaviour is quite typical.

We next report the results of running a few variants of our Iterated-Subspace Minimization code on some large or difficult test problems. The simplest variant has the following features.

- The iteration is deemed to have converged when \( \|g^{(k)}\|_2 \) is smaller than \( 10^{-5} \).
- The subspace is constructed from the first \( s^{(k)} - 1 \) conjugate directions plus the truncated-Newton direction. The truncation is performed when the residual (gradient) of the model is smaller than \( \|g^{(k)}\|_2 \min(0.1, \|g^{(k)}\|_2^{0.1}) \) or when more than \( n \) conjugate-gradient iterations were performed.
• \(s^{(k)}\) is the smaller of 10 (as suggested by the above example) and the number of inner iterations required to determine the truncated-Newton direction.

• The model is modified, if necessary, to ensure that it is strictly convex. The modification is carried out as the conjugate-gradient iteration proceeds using the method of Arioli et al. (1993).

• A BFGS linesearch method is used to solve the inner-minimization problem. An Armijo backtracking linesearch is used, starting with a unit step and dividing the step by two until the Armijo sufficient decrease condition is satisfied. If a step of one proves acceptable, but the model has been modified to ensure that it is strictly convex, the step is doubled until an unacceptable stepsize is determined, when the last-found acceptable step is chosen. A maximum of 2 \(s^{(k)}\) BFGS iterations are permitted and the iteration is stopped if \(\|g^{(k)}\|_2\) is smaller than 10\(^{-6}\).

Note that one Hessian evaluation is made for each minimization and one gradient evaluation for each inner iteration. We denote this method by the symbol ISM\((n,f,f)\), where \(n\) means that no preconditioning is used, the first \(f\) that the subspace is constructed from the first CG directions, and the second \(f\) that the maximal subspace dimension \(s\) is fixed (to 10).

We also consider the ISM\((p,f,f)\) method, which is identical to ISM\((n,f,f)\), except that an 11-band modified Cholesky factorization preconditioner is used in the conjugate-gradient calculation. The factorization takes the elements of \(H^{(k)}\) within a band of semi-bandwidth 5 of the diagonal, replacing any other elements by zeros. The resulting band matrix is factorized, modifications being made according to the recipe of Schnabel and Eskow (1991) to ensure that the preconditioner is positive definite with bounded condition number.

We define the methods ISM\((n,e,f)\) and ISM\((p,e,f)\) as the modifications of ISM\((n,f,f)\) and ISM\((p,f,f)\), respectively, where we construct the subspace from a set of extreme \(s^{(k)} - 2\) conjugate directions plus the steepest-descent and truncated-Newton directions. We pick half of the extreme directions to be those whose Rayleigh quotient is largest, while the remainder correspond to the smallest Rayleigh quotients.

We next consider the possibility of generating the subspace dimension automatically, as discussed in Section 3.3. Once the subspace dimension has been determined, we construct the subspace from the set of first or extreme \(s^{(k)} - 2\) conjugate directions plus the steepest-descent and truncated-Newton direction, just as before. This results in four additional variants, namely ISM\((n,f,a)\), ISM\((p,f,a)\), ISM\((n,e,a)\) and ISM\((p,e,a)\).

As a yardstick, we compare the above methods with variants on two other algorithms. The first is the default version of the LANCELOT A nonlinear optimization package (see Conn et al., 1992b) (denoted LAN\((p)\)) in which an 11-band preconditioner is used, together with the same unpreconditioned algorithm (denoted LAN\((n)\)). LANCELOT is a trust-region method in which a gradient and Hessian evaluation are made on every successful iteration. The second algorithm included in our comparison is a truncated-Newton method (see Dembo and Steihaug (1983)). The truncated-Newton search direction is obtained by an inexact minimization of the Newton model using unpreconditioned or preconditioned conjugate gradients. We denote the resulting methods by TN\((n)\) and TN\((p)\), respectively. These variants are obtained from our ISM algorithms by restricting the subspace minimization to a single linesearch along the truncated-Newton direction.

We note that all the algorithms considered in this comparison use exact first and second derivatives.

We selected our 34 test examples as the majority of large and/or difficult unconstrained test examples in the CUTE (see Bongartz et al., 1993) test set. Only problems which took
excessive CPU time (more than 30 minutes), which had multiple local optima, or which were variations on the reported problems, were excluded. All experiments were made on a DEC 3000/400 workstation, using optimized (-O) Fortran 77 code and DEC-supplied BLAS.

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Table 4.1: Cumulative statistics on the performance of all methods

Table 4.1 first reports cumulative statistics on the performance of the considered algorithms, which all succeeded in solving the 34 problems. In this table and the following ones, #f indicates the total number of function evaluations, #cg the total number of CG iterations and time the total CPU time (in seconds). The second column indicates which of the tables in the appendix gives the complete and detailed results for the considered method.

This table shows some interesting results. In particular, it indicates that the automatic choice of the subspace dimension is advantageous on average when preconditioning is not used. A possible explanation is that the automatic subspace selection is more useful if the eigenvalues of the Hessian are not well clustered: the CG procedure might then need more iterations to include the contributions of all relevant extreme eigenvalues. On the other hand, one sees that, on average, the preconditioned ISM variants are all better in CPU time than their unpreconditioned counterparts. Also, there is little difference between the average performance of ISM methods using the first CG directions to define the subspace and those using the extreme ones. It is however misleading in that it seems to suggest that LANCELOT (and, to some extent, truncated-Newton) dominate all ISM methods. Although obviously true on average, this conclusion is exaggerated because of the aggregate nature of the total sums presented in the table. A more disaggregate analysis of what happens problem by problem is thus needed to reveal more specific trends. We thus present in Table 4.2 the number of times that each of the considered method ranks first, second, third, etc. for the different criteria used above. In these rankings, two CPU times are reputed identical if they differ by less than five percent or by less than half a second.

We see in this table that the supremacy of LANCELOT and truncated-Newton in CPU time is not so clear, especially for the preconditioned variants. We also note that the amount of requested CG iterations by the ISM variants is comparable on average to that for LANCELOT, and quite often smaller, but the resulting gain in time is then sometimes lost due to the larger number of objective function evaluations. One should
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Table 4.2: Rankings
also bear in mind, at this point, that LANCELOT is a much more sophisticated code than our ISM variants, because it is designed for solving generally constrained in addition to unconstrained problems and contains a number of safeguards that are not included in the simpler ISM codes. Moreover, there are overheads associated with the interfaces with the SIF input in the ISM codes that are not present in LANCELOT. However, the streamlined character of the ISM variants may be considered to be one of their advantages.

Another interesting observation is that the truncated-Newton methods appear to require more CG iterations than the other methods, and yet their requirements in CPU time is not excessive: this can be explained by the fact that they do not require too many function evaluations and contain little other computational effort.

Finally, we notice that there is little difference in performance between ISM variants that build the subspace from the first CG directions and variants that use the extreme ones. As the former is easier to implement, one might prefer it in practice.

5 Linear and nonlinear constraints

It is straightforward to extend the iterated-subspace minimization philosophy to treat linearly constrained optimization problems of the form

$$\begin{align*}
\text{minimize } & f(x) \quad \text{subject to } \quad l \leq Ax \leq u, \\
& x \in \mathbb{R}^n
\end{align*}$$

(5.1)

where $A$ is an $m$ by $n$ matrix and $l$ and $u$ are $m$-vectors. For suppose $x^{(k)}$ satisfies $l \leq Ax^{(k)} \leq u$. Then we may obtain an improved estimate $x^{(k+1)}$ by applying the following linearly-constrained ISM algorithm:

1. Stop with the solution estimate $x^{(k)}$ if convergence tests are satisfied.

2. Determine a full-rank subspace matrix $S^{(k)} \in \mathbb{R}^{n \times s^{(k)}}$, where $s^{(k)} \ll n$.

3. Approximately solve the $s^{(k)}$-dimensional minimization problem

$$\begin{align*}
\text{minimize } & f(x^{(k)} + S^{(k)}y) \quad \text{subject to } \quad l^{(k)} \leq A^{(k)}y \leq u^{(k)}, \\
& y \in \mathbb{R}^{s^{(k)}}
\end{align*}$$

(5.2)

where $A^{(k)} = AS^{(k)}$, $l^{(k)} = l - Ax^{(k)}$ and $u^{(k)} = u - Ax^{(k)}$, and set

$$x^{(k+1)} = (\text{approx}) \arg \min_{y \in \mathbb{R}^{s^{(k)}}} f(x^{(k)} + S^{(k)}y) \quad \text{subject to } \quad l^{(k)} \leq A^{(k)}y \leq u^{(k)}.$$  

(5.3)

The central issues remain those discussed in Section 1. However, extra care must be exercised when picking the subspace matrix, as it is now desirable for a constrained steepest-descent and (truncated) Newton directions to lie in the subspace. We also now need to use efficient methods for solving small linearly-constrained minimization problems when determining $x^{(k+1)}$, but fortunately the state-of-the-art here is as advanced as it is for unconstrained minimization.

The ISM philosophy does not obviously extend to handle nonlinearly-constrained minimization problems except that, of course, any unconstrained or linearly-constrained subproblems may be treated by existing ISM methods. This may be important for nonlinearly-constrained minimization methods which are based on the sequential minimization of penalty or barrier functions, or their augmented or shifted counterparts.
6 Perspectives and Conclusions

In this paper, we have shown that it is possible to solve large-scale nonlinear optimization problems using methods designed for small-scale problems. These methods may be regarded as a generalization of linesearch-type methods more usually used to solve unconstrained minimization problems. We have indicated that the convergence of our methods depends upon using robust algorithms for the small-dimensional subproblems, and have suggested a number of ways of selecting promising subspaces in which to search. Furthermore, our philosophy extends quite naturally to large-scale linearly-constrained optimization. None the less, we feel that there are a number of important areas for future investigation.

- In our investigations, we found it convenient to use a linesearch (BFGS) method to solve the inner-iteration subproblems. One might, of course, alternatively use a trust-region method to solve the subproblem. However, as the performance of such methods depends upon building a good model within an adequate trust region, and as our ISM method will solve a sequence of subproblems, it may be that a good trust-region radius for one subproblem is poor for the next, and inefficiencies may occur. Thus care may be needed in determining interactions between successive models.

Another important issue is how to pick stopping rules, analogous to (2.5)–(2.7), which are appropriate for trust-region based methods. The main difficulty here is that the initial trust-region radius may interfere with a condition like (2.5).

- While we have suggested a number of methods for computing a good iterated subspace, more work clearly needs to be performed. We believe that we have identified some of the ingredients of a good subspace, but our understanding is far from complete.

- We have suggested that ISM methods are equally appropriate for linearly-constrained problems, but have not addressed the issues related to finding a good iterated subspace in this case. Work progresses in this direction, for both general linear constraints and for problems whose constraints arise from networks.

7 Acknowledgement

Nick Gould would like to thank CERFACS for the facilities which made some of this research possible.

References


A Detailed numerical results

In this appendix, we give comprehensive details of the performance of each of the methods discussed in the main body of the paper on the complete set of test examples. We include these results so that others may, in future, compare new proposals with ours.
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Table A.3: Results for LÀN(n) (unpreconditioned LANCELOT) on large or hard problems. Key: \( n \) = number of variables, \#f = number of function evaluations, \#suc = number of successful iterations, \#cg = total number of CG iterations, time = total CPU time in seconds, \( f \) = smallest function value obtained.
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Table A.4: Results for \( \text{LAN}(p) \) (default preconditioned \text{LANCELOT}) on large or hard problems.

Key: \( n \) = number of variables, \( \#f \) = number of function evaluations, \( \#suc \) = number of successful iterations, \( \#cg \) = total number of CG iterations, \( \text{time} \) = total CPU time in seconds, \( f \) = smallest function value obtained.
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Table A.5: Results for the unpreconditioned truncated-Newton method TN(n) on large or hard problems.

Key: \( n \) = number of variables, \( \#f \) = number of function evaluations, \( \#min \) = number of minimizations, \( \#it \) = total number of iterations, \( \#cg \) = total number of CG iterations, \( time \) = total CPU time in seconds, \( f \) = smallest function value obtained.
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Table A.6: Results for the preconditioned truncated-Newton method TN(p) on large or hard problems.

Key: n = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, time = total CPU time in seconds, f = smallest function value obtained.
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Table A.7: Results for ISM(n,f,f) on large or hard problems, in which no preconditioning is used and the subspace is chosen from the first 10 CG directions.

Key: $n = \text{number of variables}$, $\#f = \text{number of function evaluations}$, $\#\text{min} = \text{number of minimizations}$, $\#\text{its} = \text{total number of iterations}$, $\#\text{cg} = \text{total number of CG iterations}$, $s(k) = \text{average subspace dimension}$, $\text{time} = \text{total CPU time in seconds}$, $f = \text{smallest function value obtained}$. 


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Table A.8: Results for lSM(p,f,f) on large or hard problems, in which preconditioning is used and the subspace is chosen from the first 10 CG directions.

Key: n = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, $s^{(k)}$ = average subspace dimension, time = total CPU time in seconds, f = smallest function value obtained.
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Table A.9: Results for ISM(n,e,f) on large or hard problems, in which no preconditioning is used and the subspace is chosen from 10 extreme CG directions.

Key: $n =$ number of variables, $#f =$ number of function evaluations, $#min =$ number of minimizations, $#its =$ total number of iterations, $#cg =$ total number of CG iterations, $s^{(k)} =$ average subspace dimension, time = total CPU time in seconds, $f =$ smallest function value obtained.
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Table A.10: Results for ISM(p,e,f) on large or hard problems, in which preconditioning is used and the subspace is chosen from the 10 extreme CG directions. Key: $n$ = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, $s^{(k)}$ = average subspace dimension, time = total CPU time in seconds, $f$ = smallest function value obtained.
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Table A.11: Results for ISM(n,f,a) on large or hard problems, in which no preconditioning is used and the subspace dimension is chosen automatically from the first CG directions. Key: n = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, s<sup>(k)</sup> = average subspace dimension, time = total CPU time in seconds, f = smallest function value obtained.
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Table A.12: Results for ISM(p,f,a) on large or hard problems, in which preconditioning is used and the subspace dimension is chosen automatically from the first CG directions. Key: n = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, $s^{(k)}$ = average subspace dimension, time = total CPU time in seconds, f = smallest function value obtained.
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Table A.13: Results for \( ISM(n,e,a) \) on large or hard problems, in which no preconditioning is used and the subspace dimension is chosen automatically from extreme CG directions. Key: \( n \) = number of variables, \( \#f \) = number of function evaluations, \( \#min \) = number of minimizations, \( \#its \) = total number of iterations, \( \#cg \) = total number of CG iterations, \( s^{(k)} \) = average subspace dimension, \( time \) = total CPU time in seconds, \( f \) = smallest function value obtained.
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Table A.14: Results for |SM(p,e,a) on large or hard problems, in which preconditioning is used and the subspace dimension is chosen automatically from extreme CG directions.

Key: n = number of variables, #f = number of function evaluations, #min = number of minimizations, #its = total number of iterations, #cg = total number of CG iterations, $s(k) = $ average subspace dimension, time = total CPU time in seconds, f = smallest function value obtained.