NEW IN Variant TO NONLINEAR SCALING
QUASI-NEWTON ALGORITHMS

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Abstract: New Quasi-Newton methods for unconstrained optimization are proposed which are invariant to a nonlinear scaling of a strictly convex quadratic function. In specific, we examine a logarithmic scaling of some quadratic function and proceed to derive the necessary parameters for obtaining invariance to such nonlinear scalings. The techniques considered in this work have the same convergence properties as the classical BFGS-method, when applied to a quadratic function.

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1. Introduction

The type of problems of interest in this work is of the form

$$\text{minimize } f(x), \text{ where } f : \mathbb{R}^n \rightarrow \mathbb{R}.$$ 

One well-known way to find a solution is by making use of a class of methods widely known as the quasi-Newton methods for unconstrained optimization. Those methods require only the objective function and its first partial derivatives (the gradient) to be derived and encoded. The Hessian matrix is assumed to be unavailable due to its usually complicated derivation and encoding, a process susceptible to error. However, an approximating matrix to the Hessian is rather utilized and updated on a step-wise basis to ensure the incorporation of the latest changes in both function value and the corresponding gradient.
Given $B_i$, the most recent approximation to the Hessian, a new approximating matrix $B_{i+1}$ needs to be built, corresponding to the newly computed iterate $x_{i+1}$. One way to determine a relationship that the new matrix $B_{i+1}$ should satisfy is by using Taylor’s series of first order approximation to the gradient about the newly computed point $x_{i+1}$. This leads to obtaining what is widely known as the Secant equation, \([4]\),

$$B_{i+1} s_i = y_i,$$

where

$$s_i = x_{i+1} - x_i,$$

and

$$y_i = g_{i+1} - g_i.$$

The Secant Equation defines the basis for the derivation of possible updating formulae to find the new Hessian approximation $B_{i+1}$ using simply the old approximation $B_i$ and the corresponding iteration and their respective gradient vectors differences, namely the vectors, $s_i$ and $y_i$. Generally, such an update has the form $B_{i+1} = B_i + C_i$, where $C_i$ is some correction matrix to the Hessian approximation. Alternatively, in many practical situations, it may be preferable to instead utilize $H_{i+1} = H_i + D_i$, where $D_i$ is some correction matrix to the inverse Hessian approximation and $H_{i+1} = B_i^{-1}$.

One particularly successful rank-two formula is the widely recognized BFGS formula. This formula is given by (see \([3]\), \([4]\), \([5]\))

$$B_{i+1}^{BFGS} = B_i + \frac{y_i y_i^T}{s_i s_i^T} - \frac{B_i s_i s_i^T B_i}{s_i^T B_i s_i},$$

$$H_{i+1}^{BFGS} = H_i + \left[1 + \frac{y_i^T H_i y_i}{s_i^T y_i} \right] s_i s_i^T y_i - s_i y_i^T H_i + H_i y_i s_i^T.$$

The BFGS is shown in \([7]\), \([8]\) and \([9]\) to be a least change update from $B_i$ to $B_{i+1}$ under the Frobenius norm. Numerical evidence support the superiority of this formula to other updating formulae especially. This superiority is especially visible in the case of non-exact line search (see, for example, \([4]\), \([5]\)), the thing which makes it an adopted standard.

We examine here the general problem considered in \([2]\) and \([22]\). It is stated as $f = F(q(x))$, $df/dx > 0$ for $x = x_{\text{min}}$, where $x_{\text{min}}$ is the minimizer of $q(x)$ with respect to $x$ and $q(x)$ is a quadratic function. $F$ is some nonlinear scaling of $q(x)$ and for invariancy to nonlinear scaling of the objective function, Spedicato \([22]\) suggested an extra parameter to be included in the quantity $y_i$ as follows.
\[ y_i = g_{i+1} - \delta_i g_i, \text{ where } \delta_i = \rho_{i+1}/\rho_i \text{ and } \rho_j = \frac{d}{dq}F(q)|_{q=q(x_j)}. \] (1)

Alternatively, \( y_i \) may be defined as
\[ y_i = g_{i+1}/\rho_{i+1} - g_i/\rho_i. \]

Invariancy to nonlinear scaling is obtained if the following properties hold true:

i. \( \rho_j > 0 \), for \( x \neq x_{\text{min}} \);

ii. If \( x_{\text{min}} \) is the minimum of \( q(x) \), then it is also a minimum of \( f \).

Similar non-linear scalings of the objective function have been investigated by various authors (see [18]). For example:

a) \( f = \alpha q \), for \( \alpha \in \mathbb{R} \);

b) \( f = -e^{-q} \);

and

c) \( f = q^r \), for \( r \in \mathbb{R} \).

For option (a), the Huang-Oren class ([13], [23]) is obtained naturally. In the second case we have simply \( \frac{df}{dq} = f \). For option (c), \( \frac{df}{dq} \) can be obtained using the method of Fried [10] and of Spedicato [22]. Spedicato noticed that the parameter \( \delta_i = \frac{\rho_{i+1}}{\rho_i} \) is determined using the Chain rule as follows (where \( A \) is the Hessian of \( q(x) \))
\[ G_{i+1} = \left. \frac{d^2 f}{dx^2} \right|_{x=x_{i+1}} = 2A\rho_{i+1} + \left. \frac{d^2 F}{dq^2} \right|_{x=x_{i+1}} g_i g_i^T. \] (2)

Then on the premise of exact line search (\( s_i^T g_i = 0 \)) and upon premultiplying and postmultiplying (2) by the fact that \( s_i = \alpha_i p_i \), where \( p_i \) is a search vector and \( \alpha_i \) is a step length along that search direction obtained by a designated line search algorithm ([11], [12]), we get
\[ s_i^T G_{i+1} s_i = 2s_i^T A s_i \frac{df}{dq} \bigg|_{x=x_{i+1}}. \]

Then, for a quadratic we have
\[ \frac{g_{i+1}}{\rho_{i+1}} - \frac{g}{\rho} = 2As \]
and, therefore, \( \delta_i = \frac{-s_i^T G_{i+1} s_i}{s_i^T g_i} \).
2. Derivation of $\delta_i$ with inaccurate line searches – A logarithmic mode

We consider here the model $F = F(q(x))$, for $F$ being a non-linear scaling of $q$. Spedicato [22] examines the following form for $q$

$$q = c + b^T x + x^T A x,$$

for a positive definite Hessian $A$ and where $b$ is some constant vector and $c$ is some scalar constant.

In this work, we will examine the following two quadratic models

$$q = e_i^T A e_i + c \text{ for } e_i = x - x_{\text{min}}, \quad \text{(model A)}$$

and

$$q = x_i^T A x_i + c, \quad \text{(model B)}$$

where model B is a special case of model A for which $x_{\text{min}} = 0$.

We will examine one particular scaling of $q$ given as

$$f = \ln(q).$$

To proceed with the derivation of $\delta_i$, we start by considering the quantities:

$$g_{i+1} = \rho_{i+1} \nabla q_{x_{i+1}} \text{ or } \nabla q_{i+1} = \frac{g_{i+1}}{\rho_{i+1}}$$

and

$$g_i = \rho_i \nabla q_i \text{ or } \nabla q_i = \frac{g_i}{\rho_i}.$$

From the above, it follows that

$$\frac{\rho_{i+1} g_i}{\rho_i g_{i+1}} = \frac{\nabla q_i}{\nabla q_{i+1}}$$

or, equivalently,

$$\delta_i \frac{g_i}{g_{i+1}} = \frac{\nabla q_i}{\nabla q_{i+1}}. \quad \text{(3)}$$

Using (4), we have (for (model A))

$$\delta_i \frac{s_i^T g_i}{s_i^T g_{i+1}} = \frac{s_i^T \nabla q_i}{s_i^T \nabla q_{i+1}},$$

which gives
\[ \delta_i = \frac{(s_i^T g_i) (s_i^T \nabla g_{i+1})}{(s_i^T g_{i+1}) (s_i^T \nabla q_i)} = \frac{(s_i^T A e_{i+1}) (s_i^T g_i)}{(s_i^T A e_i) (s_i^T g_{i+1})}, \]  
(4)

for \( s_i^T g_{i+1} \neq 0 \) (which is usually true for inexact line searches).

Similarly for (model B), we obtain (using (4)) the following expression for \( \delta_i \):

\[ \delta_i = \frac{(s_i^T A x_{i+1}) (g_i^T s_i)}{(s_i^T A x_i) (s_i^T g_{i+1})} = \frac{(y_i^T x_{i+1}) (g_i^T s_i)}{(y_i^T x_i) (s_i^T g_{i+1})}, \]  
(5)

using \( 2A s_i = y_i \).

In order to complete the derivation of \( \delta_i \) for model A (model B), we need to derive an expression for \( s_i^T A e_i \) and we start by premultiplying \( \delta_i \) by \( \frac{g_{i+1}}{g_i} \):

\[ \frac{g_{i+1} \rho_{i+1}}{g_i \rho_i} = \frac{A e_{i+1}}{A e_i} = \frac{e_{i+1}}{e_i}. \]

We, thus, get:

\[ \delta_i = \frac{\rho_{i+1}}{\rho_i} = \frac{g_{i+1}^T e_{i+1}}{g_i^T e_i}. \]

But

\[ g_i^T e_{i+1} = g_i^T (x_i - x_{min}) + \alpha_i g_i^T p_i \]

and

\[ g_{i+1}^T e_i = g_{i+1}^T (x_i - x_{min}) = g_{i+1}^T e_{i+1} - \alpha_i g_{i+1}^T p_i. \]

Therefore,

\[ \delta_i = \frac{g_{i+1}^T e_{i+1} - s_i^T g_{i+1}}{g_{i+1}^T e_i + s_i^T g_i} = \frac{2\rho_{i+1} e_{i+1}^T A e_{i+1} - s_i^T g_{i+1}}{2\rho_i e_i^T A e_i + s_i^T g_i} = \frac{2\rho_{i+1} q_{i+1} - s_i^T g_{i+1}}{2\rho_i q_i + s_i^T g_i} = \frac{2\rho_{i+1} q_{i+1} - s_i^T (2\rho_{i+1} A e_{i+1})}{2\rho_i q_i + s_i^T (2\rho_i A e_i)}. \]

Hence,

\[ \delta_i = \frac{\rho_{i+1}}{\rho_i} \left( \frac{q_{i+1} - s_i^T A e_{i+1}}{q_i + s_i^T A e_i} \right). \]
or, equivalently,

$$q_{i+1} - q_i = e_i^T A s_i + e_{i+1}^T A s_i,$$

which is true for any quadratic function. But

$$s_i^T A e_{i+1} = s_i^T A e_i + s_i^T A s_i \Rightarrow q_{i+1} - q_i = 2e_i^T A s_i + s_i^T A s_i.$$ 

This gives

$$e_i^T A s_i = \frac{1}{2} (q_{i+1} - q_i - s_i^T A s_i).$$

Using $\nabla q_i = 2A e_i$, we obtain

$$\nabla q_{i+1} - \nabla q_i = 2A e_{i+1} - 2A e_i,$$

which yields $A s_i = \frac{y_i}{2}$.

Therefore,

$$e_i^T A s_i = \frac{1}{2} \left( q_{i+1} - q_i - \frac{s_i^T y_i}{2} \right).$$

(6)

The quantities $q_i$ and $q_{i+1}$ can be determined depending on the nature of the function $f = F(q)$. For example, if $F$ corresponds to the natural logarithm, say (i.e., $f = \ln(q)$), then $q = e^f$, provided $f$ is available. Plugging the quantity in (6) into (5), $\delta_i$ is obtained. If $f$ is not known or it is not possible to determine $q$ using $f$, another derivation can be used instead (see the next section).

3. Another derivation for $\delta_i$

We now give another derivation for $\delta_i$ in the case of $f = \ln(q)$ as follows

$$\delta_i = \frac{g_{i+1}^T}{g_i^T} \left( x_{i+1} - x_{\text{min}} \right) = \frac{2 \rho_{i+1} q_{i+1} - s_i^T g_{i+1}}{2 \rho_i q_i + s_i^T g_i}. \quad \text{(7)}$$

But $\rho = \frac{df}{dq} = \frac{1}{q}$, which, upon substitution, in (7) yields

$$\delta_i = \frac{2 - s_i^T g_{i+1}}{2 + s_i^T g_i}. \quad \text{(8)}$$

For all $\delta_i$ it must be ensured that $\delta_i > 0$ in the actual implementation of the method. If this is not the case, we resort into using $\delta_i = |\delta_i|$. As indicated earlier, our expressions for $\delta_i$ are exact for a quadratic and do not suppose that the line searches are accurate.
We come here to determine $\delta_i$ in an expression which does not involve $q$ for a general $F$. We use
\[ \delta_i = \frac{e^T_{i+1} g_i + 1}{e^T_i g_i}, \]
or
\[ \delta_i = \frac{e^T_{i+1} g_i + 1 + s^T_i g_i + 1}{e^T_i g_i}, \]  
(9)
using the definition of $e_{i+1}$ in (model A).

Now from (5), we have
\[ \delta_i = \left( \frac{e^T_{i+1} g_i + 1 + s^T_i g_i + 1}{e^T_i g_i} \right) \left( \frac{s^T_i g_i}{s^T_i g_i + 1} \right), \]
(10)
using $2A s_i = y_i$ and $y^T_i e_{i+1} = e^T_i y_i + s^T_i y_i$ and, again, the definition of $e_{i+1}$ in (6).

From (10), it follows that
\[ \delta_i = \frac{e^T_i y_i + s^T_i y_i}{\sigma e^T_i y_i}, \text{ where } \sigma = \frac{s^T_i g_i + 1}{s^T_i g_i}. \]

This gives
\[ \delta_i = 1 + \frac{\pi}{\sigma}, \text{ for } \pi = \frac{s^T_i y_i}{e^T_i y_i}. \]
(11)

Now let us define the quantities
\[ \tau = e^T_i y_i, \]
\[ \lambda = e^T_i g_i, \]
\[ \sigma_1 = s^T_i g_i + 1 \]
and
\[ \beta = s^T_i y_i, \]
so that from (10) and (11), we obtain
\[ \frac{\tau + \lambda + \sigma_1}{\lambda} = \frac{\tau + \beta}{\tau \sigma}, \]
from which the following quadratic is achieved
\[ \phi (\tau) = \sigma \tau^2 + (\lambda \sigma + \sigma \sigma_1 - \lambda) \tau - \beta \lambda. \]  
(12)
We are interested in a positive $\delta_i$ and, thus, our aim is to find $\tau$ as the stationary point of $\phi(\tau)$ so that we can determine $\lambda$ from $\phi(\tau)$ for that point using (12). We thus obtain
\[
\tau = -\frac{(\lambda \sigma + \sigma \sigma_1 - \lambda)}{2\sigma}.
\]
(13)
The quantity $\tau$ is a maximum point of $\phi(\tau)$ if and only if $\sigma < 0$ which, in turn, is only true if $s_i^T g_{i+1} > 0$. We are now able to determine $\lambda$ in (11) using (12) and (13).

Since we are only interested in a positive $\delta_i$, we need to determine the conditions under which this is true.

**Corollary 1.** If $H_i$ and $H_{i+1}$ are positive definite, then $\tau$ given by
\[
\tau = -\frac{(|\lambda\sigma + \sigma \sigma_1 - |\lambda|)}{2\sigma},
\]
for $\sigma > 0$, and the following condition holds true
\[
|\lambda\sigma + \sigma \sigma_1 < |\lambda|,
\]
(14)
then $\tau > 0$ and, therefore, $\delta_i > 0$.

The proof is trivial and is, therefore, omitted.

4. Numerical results and conclusions

The comparative tests involve eighteen well-known test functions (see Table 1) obtained from [14], [15], [16], [17]. The comparative performances of the algorithms are assessed by taking into account both the total number of iterations and the number of function evaluations, in addition to computational timings. We define 'iteration' to mean the step carrying a point $x_i$ along the direction $d_i = -H_i g_i$ to a new point $x_{i+1}$, and the number of function calls quoted is that required to reduce the value of $f(x)$ below $1.0^{-10}$. The cubic interpolation technique, fully described in [1], [6] and [7], is used as the linear search routine to obtain the minimum along the search direction $d_i$.

Four algorithms were tested and compared, namely, (i) the standard BFGS algorithm, (ii) the method with the value for $\delta_i$ in (4), (iii) the algorithm defined by the formula in (5) for $\delta_i$ and (iv) the one given by (11). The four algorithms
were compared using twenty six test functions, each tested with several dimensions $n$ ($2 \leq n \leq 100000$), whenever applicable. The total number of problems solved is 886, tested using each of the algorithms (see Table 2). Conditioning was applied to the update matrices involved in the computation of the search directions only initially on the first iteration (see [20] and [21]).

The performance of all the derived algorithms is comparable with some behaving better on certain problems and worse on others. The new algorithms save about 9% on function/gradient evaluations and 8% on the number of iterations, with negligible additional computational overheads. In order to guarantee the convergence of the BFGS and the other tested algorithms, the step size $\alpha_i$ in

$$x_{i+1} = x_i + \alpha_i d_i$$

is deemed acceptable provided it satisfies the Wolfe conditions (see [4], [7], [16], [18], [19], and [24])

$$f(x_i + \alpha_i d_i) - f(x_i) \leq \rho_1 \alpha_i d_i^T g_i,$$  \hspace{1cm} (15)

$$g(x_i + \alpha_i d_i)^T d_i \geq \rho_2 d_i^T g_i,$$  \hspace{1cm} (16)

where $0 < \rho_1 \leq \rho_2 < 1$.

Our numerical results show that algorithm with $\delta_i$ given by (6) beats the other three in the number of function/gradient calls, although the three algorithms perform about the same when compared by the total number of iterations. Its timing is also better than the remaining three tested methods (including the standard BFGS).

Finally, the computational results presented here show that nonlinear scaling methods generally improve the computational efficiency of the BFGS method on large problems and the relative improvement increases monotonically with dimensionality $n$. The effect of changing to inexact line searches is marginal. In conclusion, for this particular set of test functions and for the chosen line search criteria, the new algorithms perform better than the well-known standard BFGS method.

The methods derived in this paper lends themselves to several applications for which the problem under consideration is nonlinearly scaled. Also, the algorithms need to be examined and tested within the context preconditioned Conjugate Gradient (CG) methods (see [3], [25]) to determine their effectiveness, as opposed to the traditional CG approach.
Table 1: Test problems

| problem | function name                  | size   |
|---------|--------------------------------|--------|
| 1       | Extended Rosenbrock            | 100000 |
| 2       | Extended Powell Singular       | 100000 |
| 3       | Trigonometric                  | 100000 |
| 4       | Oren                           | 10000  |
| 5       | Cube                           | 2      |
| 6       | Extended Wood                  | 4-100000 |
| 7       | Beale                          | 2      |
| 8       | Helical Valley                 | 3      |
| 9       | Penalty I                      | 2      |
| 10      | Watson function                | 4      |
| 11      | Variably dimensioned function  | 2-100000 |
| 12      | Generalized Shallow function   | 2-100000 |
| 13      | Wood function                  | 2-100000 |
| 14      | Shallow                        | 2-100000 |
| 15      | Tridiagonal                    | 2-100000 |
| 16      | Helical Valley                 | 2-1000 |
| 17      | Dixon                          | 2-10000 |
| 18      | Oren and Spedicato Power function | 2-10000 |

Table 2: Overall Results (886 problems)

| Method   | Evaluations | Iterations | Time (sec.) | Scores |
|----------|-------------|------------|-------------|--------|
| BFGS     | 86401       | 73090      | 39171.18    | 101    |
|          | 100.0%      | 100.0%     | 100.0%      | 100.0% |
| Alg.(4)  | 80364       | 70404      | 35547.68    | 247    |
|          | 93.01%      | 96.32%     | 90.75%      |        |
| Alg.(5)  | 79164       | 67335      | 34874.71    | 317    |
|          | 91.61%      | 92.12%     | 89.03%      |        |
| Alg.(11) | 86426       | 69262      | 38718.99    | 221    |
|          | 100.1%      | 94.77%     | 98.85%      |        |

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