Generalized Implicit-Update in Multi-Step QN Methods

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Abstract

In this paper, we have generalized the implicit update of the Quasi-Newton’s condition. We have here investigated a four; five and n-step update algorithm. We have applied the cases at four and five- step numerically and we have compared these cases with other QN-algorithms. The numerical results of the proposed algorithm show that the new algorithm was better than others.

Generalization of the Implicit-Update in Multi-Step QN Algorithms

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1. Introduction:

One problem, which is more widely used, is QN method, where approximate Hessian or inverse Hessian is updated at each iteration, while the gradients are supplied. The basic requirement for the updating formula is that the QN condition (secant condition i.e $B_{k+1} s_k = y_k$) where $s_k, y_k$ are defined as:

$$s_k = x_{k+1} - x_k, \quad y_k = g_{k+1} - g_k,$$

where $x_k$ is the point at $k$ iteration, $g_k$ is the gradient at $k$ iteration and $B_{k+1}$ is the inverse Hessian.

We consider QN methods for unconstrained optimization problems ($\min f(x), \ x \in \mathbb{R}^n$), where the basic idea behind the QN formulas is to update $B_{k+1}$ from $B_k$ in some computational cheap ways while ensure secant condition, and the computation of the update should be relatively cheap.

2. One Step Method (BFGS Method):

The BFGS method is one of the most efficient QN methods for unconstrained optimization. This algorithm was proposed by Broyden, Fletcher, Goldfarb and Shanno in (1970). BFGS method has a search direction computed by:

$$d_k = -H_k g_k$$

where $H_k$ is a symmetric and positive definite matrix at the $k$-th iteration. The next iterate is given by:

$$x_{k+1} = x_k + \lambda_k d_k$$

where $\lambda_k$ is the step size that satisfies the strong Wolfe condition ($f(x_{k+1}) < f(x_k)$) [Ahmed, 2005].

The approximation matrix is updated by:

$$H_{k+1} = H_k - \frac{H_k s_k s_k^T H_k}{s_k^T H_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} + w_k w_k^T$$

$$= BFGS(H_k, s_k, y_k)$$

where $w_k = (y_k^T H_k y_k) s_k - (y_k^T s_k) H_k y_k$. We call eq.(3) by one step method. [Dai, 2002] and [Nocedal et al., 1987].
2.2 BFGS (One Step Algorithm):

Step 1: Given $x_0 \in R^n$, set $H_0=I$, compute $g_0=\nabla f(x_0)$. If $\|g_0\| \leq 10^{-5}$ then stop, Otherwise, set $k=1$ and continue.

Step 2: Set $d_k = -H_k g_k$.

Step 3: Compute $x_{k+1} = x_k + \lambda_k d_k$.

Step 4: If $\|g_{k+1}\| < \varepsilon$ then stop else continue.

Step 5: Update $H_k$ by the correction matrix to get $H_{k+1}$ defined by:

$$H_{k+1} = H_k - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k} + \frac{s_k s_k^T}{s_k^T y_k} + w_k w_k^T$$

Where

$$w_k = (y_k^T H_k y_k) s_k - (y_k^T s_k) H_k y_k$$

Step 6: Set $k=k+1$ and go to step 2.

3. Implicit update method:

Ford in 2001 developed a two-step implicit algorithm denoted as two-step QN method which are very similar to the standard (one-step) method in very respect, except that the Hessian approximation $H_{k+1}$ in the standard method is constrained to satisfy the relation $(B_{k+1} s_k = y_k)$. Where in the two-step methods, it must satisfy a modified relation of the form:

$$B_{k+1} (s_k - \alpha s_{k-1}) = (y_k - \alpha y_{k-1})$$

(4)

where $\alpha$ is a positive scalar and defined by:

$$\alpha = \hat{\delta}(\hat{\delta}+2)$$

(5)

So we can rewrite (4) by:

$$B_{k+1} r_k = w_k$$

(6)

where

$$r_k = s_k - \hat{\delta}(\hat{\delta}+2) s_{k-1}$$

(7)

and

$$w_k = y_k - \hat{\delta}(\hat{\delta}+2) y_{k-1}$$

(8)
The relation (4) or (6) is dependant on cubic interpolating curve \( \{x(\tau)\} \) and \( \{h(\tau)\} \), where \( \{x(\tau)\} \) interpolates the two latest iterates \( x_{k+1}, x_k \), while \( \{h(\tau)\} \) interpolates the corresponding gradient value \( g(x_{k+1}) \) and \( g(x_k) \) i.e.

\[
x(\tau_j) = x_{i+j-1}, \quad j=0,1
\]

\[
g(\tau_j) = g(x_{i+j-1}), \quad j=0,1
\]

(9) \hspace{1cm} (10)

A Suitable matrix \( B_{k+1} \) satisfying (4) or (6) may then be obtained by using the BFGS formula. [Tharmlikit, 2001].

Now we define \( \delta \) by:

\[
\delta = \tau_1 - \tau_0
\]

\[
= \left\| x(\tau_1) - x(\tau_0) \right\|_M
\]

\[
= \left\| x_{k+1} - x_k \right\|_M
\]

\[
= \left\| s_k \right\|_M
\]

(11)

where \( \left\| s_k \right\|_M = \{s_k^T M s_k\}^{0.5} \) for general \( s_k \). [Ford and Moghrabi, 1993; 1994]

Ford proved that two-step iterations are alternated with standard one-step iterations, so that \( B_k s_{k-1} = y_{k-1} \) on every two-step iteration that satisfies the QN condition of the one-step \( (B_{k+1} s_k = y_k) \): Substitute the value of \( r_k \) and \( w_k \) by (7) and (8) then we obtain:

\[
\hat{B}_{k+1} (s_k - \hat{\delta}(\hat{\delta}+2)s_{k-1}) = y_k - \hat{\delta}(\hat{\delta}+2)y_{k-1}
\]

\[
\hat{B}_{k+1} s_k - \hat{\delta}(\hat{\delta}+2)\hat{B}_{k+1} s_{k-1} = y_k - \hat{\delta}(\hat{\delta}+2)y_{k-1}
\]

\[
\hat{B}_{k+1} s_k = y_k - \hat{\delta}(\hat{\delta}+2)y_{k-1} + \hat{\delta}(\hat{\delta}+2)\hat{B}_{k+1} s_{k-1}
\]

\[
= y_k - \hat{\delta}(\hat{\delta}+2)[y_{k-1} - \hat{B}_{k+1} s_{k-1}]
\]

Since \( \hat{B}_{k+1} s_{k-1} = y_{k-1} \) then

\[
\hat{B}_{k+1} s_k = y_k
\]
4. Ford and Moghrabi (The Two-Step Implicit Update) Algorithm:

Step 1: Given \( x_0 \in R^n \), set \( H_0 = I \), compute \( g_0 = \nabla f(x_0) \). If \( \|g_0\| \leq 10^{-5} \) then stop, Otherwise, set \( k = 1 \) and continue

Step 2: Set \( d_k = -H_k g_k \).

Step 3: Compute \( x_{k+1} = x_k + \lambda_k d_k \).

Step 4: If \( \|g_{k+1}\| < \epsilon \) then stop else continue.

Step 5: If \( k = 1 \) then \( r_k = s_k \) and \( w_k = y_k \), i.e. we use standard BFGS formula,

Else calculate \( \{r_j\}_{j=0}^k \) and compute \( \hat{\delta} \) from Eq.(11) and compute \( r_k \),

\[
w_k = y_k - \hat{\delta}(\hat{\delta} + 2)y_{k-1}
\]

Step 6: Update \( H_k \) by using:

\[
H_{k+1} = H_k - \left(1 + \frac{w_k^T H_k w_k}{r_k^T w_k} \right) \frac{r_k r_k^T}{r_k^T w_k} - \left( \frac{H_k w_k r_k^T + r_k w_k^T H_k}{r_k^T w_k} \right) \]

that satisfying \( H_{k+1} r_k = w_k \)

Step 7: Set \( k = k + 1 \) and go to step 2.

5. The 3-Step Implicit Update Algorithm:

Al-Bayati and Ahmed in 2005 developed a new implicit QN methods which the matrix \( M \) is the result of alternate three-step update of \( B_k \):

The 3-Step Implicit Update (Al-Bayati and Ahmed, 2005) Algorithm:
Step 1: Given $x_0 \in \mathbb{R}^n$, set $H_0 = I$, compute $g_0 = \nabla f(x_0)$. If $||g_0|| \leq 10^{-5}$ then stop, Otherwise, set $k=1$ and continue.

Step 2: Set $d_k = -H_k g_k$.

Step 3: Compute $x_{k+1} = x_k + \lambda_k d_k$.

Step 4: If $||s_k|| < \varepsilon$ then stop else continue.

Step 5: If $k=1$ then $r_k = s_k$ and $w_k = y_k$, i.e. we use standard BFGS formula,

Else calculate $\{r_j\}_{j=0}^1$ and compute $\hat{\delta}$ from Eq.(11) and compute $r_k, w_k$ from

$$r_k = s_k - \left( \frac{\delta}{\delta - 2} \right) s_{k-1} - \left( \frac{\delta}{\delta - 2} \right) s_{k-2}$$

$$w_k = y_k - \left( \frac{\delta}{\delta - 2} \right) y_{k-1} - \left( \frac{\delta}{\delta - 2} \right) y_{k-2}$$

Step 6: Update $H_k$ by using:

$$H_{k+1} = H_k - \left( 1 + \frac{w_k^T H_k w_k}{r_k^T w_k} \right) \begin{pmatrix} r_k^T r_k & r_k^T w_k \\ r_k^T w_k & w_k^T w_k \end{pmatrix} \begin{pmatrix} H_k w_k r_k^T + r_k w_k^T H_k \\ r_k^T w_k \end{pmatrix}$$

that satisfying $H_{k+1} r_k = w_k$

Step 7: Set $k=k+1$ and go to step 2.

6. Generalized Implicit-Update in QN Methods:

Here we extended the three-step update to the four-step update by using four terms and we extended the four-step update to the five-step update by using five terms and hence we generalize the process to n-terms as the following:

6.1 4-Step Implicit Update Forms:
Let \( \psi = \frac{\hat{\sigma} + 2}{\hat{\sigma}} \), then:

\[
\hat{B}_{k+1}(s_k - \psi s_{k-1} - \psi s_{k-2} - \psi s_{k-3} - \psi s_{k-4}) = y_k - \psi y_{k-1} - \psi y_{k-2} - \psi y_{k-3} - \psi y_{k-4}
\]

\[
\hat{B}_{k+1} s_k - \psi \hat{B}_{k+1} s_{k-1} - \psi \hat{B}_{k+1} s_{k-2} - \psi \hat{B}_{k+1} s_{k-3} - \psi \hat{B}_{k+1} s_{k-4} = y_k - \psi y_{k-1} - \psi y_{k-2} - \psi y_{k-3} - \psi y_{k-4}
\]

\[
\hat{B}_{k+1} s_k = y_k - \psi (y_{k-1} - \hat{B}_{k+1} s_{k-1}) - \psi (y_{k-2} - \hat{B}_{k+1} s_{k-2}) - \psi (y_{k-3} - \hat{B}_{k+1} s_{k-3}) - \psi (y_{k-4} - \hat{B}_{k+1} s_{k-4})
\]

Since \((\hat{B}_{k+1} s_{k-1} = y_{k-1})\) then

\[
\hat{B}_{k+1} s_k = y_k
\]

### 6.2 5-Step Implicit Update Forms:

Let \( \psi = \frac{\hat{\sigma} + 2}{\hat{\sigma}} \), then:

\[
\hat{B}_{k+1}(s_k - \psi s_{k-1} - \psi s_{k-2} - \psi s_{k-3} - \psi s_{k-4}) = y_k - \psi y_{k-1} - \psi y_{k-2} - \psi y_{k-3} - \psi y_{k-4}
\]

\[
\hat{B}_{k+1} s_k - \psi \hat{B}_{k+1} s_{k-1} - \psi \hat{B}_{k+1} s_{k-2} - \psi \hat{B}_{k+1} s_{k-3} - \psi \hat{B}_{k+1} s_{k-4} = y_k - \psi y_{k-1} - \psi y_{k-2} - \psi y_{k-3} - \psi y_{k-4}
\]

\[
\hat{B}_{k+1} s_k = y_k - \psi (y_{k-1} - \hat{B}_{k+1} s_{k-1}) - \psi (y_{k-2} - \hat{B}_{k+1} s_{k-2}) - \psi (y_{k-3} - \hat{B}_{k+1} s_{k-3}) - \psi (y_{k-4} - \hat{B}_{k+1} s_{k-4})
\]

Since \((\hat{B}_{k+1} s_{k-1} = y_{k-1})\) then

\[
\hat{B}_{k+1} s_k = y_k
\]
Note:

6.3 N-Step Implicit Update Forms:
We prove that N-step implicit form by using mathematical induction:
Assume that we extended all-step to (n-1)-step as:
\[
\hat{B}_{k+1}(s_k - \psi s_{k-1} - \psi s_{k-2} - \ldots - \psi s_{k-(n-1)}) = y_k - \psi y'_{k-1} - \psi y'_{k-2} - \ldots - \psi y'_{k-(n-1)}
\]
\[
\hat{B}_{k+1} s_k - \psi \hat{B}_{k+1} s_{k-1} - \psi \hat{B}_{k+1} s_{k-2} - \ldots - \psi \hat{B}_{k+1} s_{k-(n-1)}
\]
\[
= y_k - \psi y'_{k-1} - \psi y'_{k-2} - \ldots - \psi y'_{k-(n-1)}
\]
\[
\hat{B}_{k+1} s_k = y_k - \psi (y_{k-1} - \hat{B}_{k+1} s_{k-1}) - \psi (y_{k-2} - \hat{B}_{k+1} s_{k-2})
\]
\[-\ldots - \psi (y_{k-(n-1)} - \hat{B}_{k+1} s_{k-(n-1)})
\]
Since \((\hat{B}_{k+1} s_{k-(n-1)} = y_{k-(n-1)})\) then
\[
\hat{B}_{k+1} s_k = y_k
\]

7. The Generalized N-Step Algorithm:
Step 1: Given \(x_0 \in \mathbb{R}^n\), set \(H_0=I\), compute \(g_0=\nabla f(x_0)\). If \(\|g_0\| \leq 10^{-5}\) then stop, Otherwise, set \(k=1\) and continue
Step 2: Set \(d_k = -H_k g_k\).
Step 3: Compute \(x_{k+1} = x_k + \lambda_k d_k\).
Step 4: If \(\|g_{k+1}\| < \varepsilon\) then stop else continue.
Step 5: If \(k=1\) then \(r_k = s_k\) and \(w_k = y_k\), i.e. we use standard BFGS formula,

Else calculate \(\{r_{j}\}_{j=0}^{y}\) and compute \(\delta\) from Eq.(11) and compute \(r_k, w_k\) from
\[ r_k = s_k - \sum_{j=1}^{n-1} \psi_j s_{k-j} - \sum_{j=2}^{n-1} \psi_j s_{k-j} \]

\[ w_k = y_k - \sum_{j=1}^{n-1} \psi_j y_{k-j} - \sum_{j=2}^{n-1} \psi_j y_{k-j} \]

Where: \( \psi = \frac{(\hat{\delta} + 2)}{\hat{\delta}} \)

Step 6: Update \( H_k \) by using:

\[
H_{k+1} = H_k - \left( 1 + \frac{w_k^T H_k w_k}{r_k^T r_k} \right) \left( \frac{r_k^T}{r_k^T w_k} \right) \left( \frac{H_k w_k r_k^T + r_k w_k^T H_k}{r_k^T r_k} \right)
\]

that satisfying \( H_{k+1} r_k = w_k \)

Step 7: Set \( k = k + 1 \) and go to step 2.

8. Numerical Results:

In order to assess the performance of the new implicit N-step QN methods for the cases N=4, N=5, we tested these cases by using (5) nonlinear test functions with dimension N=100.

All results are obtained using Pentium 3. All programs are written in FORTRAN 90 language and for all cases the stopping criterion taken to be \( \|s_{k+1}\| < \varepsilon \), where \( \varepsilon = 10^{-5} \).

The comparative performance for all of these methods are evaluated by considering NOF, NOI, where NOF is the number of function evaluations and NOI is the number of iterations.

All the methods, in this search use the same exact line search strategy which is the quadratic interpolation technique directly adapted from [Bunday, 1984].

In table (1), we have compared our new methods 4-step and 5-step with BFGS and 3-step methods. The numerical results of the proposed methods show that the new methods were better than others (i.e. when the steps are increasing, the results be good).
Table (1)
Comparison Among the BFGS; 2-step; 3-Step; 4-Step and 5-Step Methods at N=100

| Test | BFGS NOF(NOI) | 2-step NOF(NOI) | 3-step NOF(NOI) | 4-step NOF(NOI) | 5-step NOF(NOI) |
|------|----------------|-----------------|-----------------|-----------------|-----------------|
| 1    | 122 (44)       | 280 (111)       | 198 (37)        | 177 (40)        | 125 (39)        |
| 2    | 310 (92)       | 334 (98)        | 299 (81)        | 253 (76)        | 222 (69)        |
| 3    | 27 (9)         | 33 (12)         | 24 (10)         | 25 (12)         | 20 (9)          |
| 4    | 62 (33)        | 82 (45)         | 67 (37)         | 53 (31)         | 48 (29)         |
| 5    | 113 (44)       | 263 (116)       | 60 (19)         | 65 (17)         | 23 (19)         |
| Total| 634 (222)      | 992 (382)       | 648 (184)       | 573 (176)       | 438 (165)       |

9. Appendix:

1- Generalized Powell Function:

\[ f = \sum_{i=1}^{n/4} [(x_{4i-3} - 10x_{4i-2})^2 + 5(x_{4i-1} - x_{4i})^2 + (x_{4i-2} - 2x_{4i-1})^4 + 10(x_{4i-3} - x_{4i})^4], \]

\[ x_0 = (3, -1, 0, 1; ...)^T. \]

2- Generalized Rosenbrock Function:

\[ f = \sum_{i=1}^{n/2} [100(x_{2i} - x_{2i-1})^2 + (1 - x_{2i-1})^2], \quad x_0 = (-1, 2, 1; ...)^T. \]

3- Generalized Sum of Quadratics Function:

\[ f = \sum_{i=1}^{n} (x_i - i)^4, \quad x_0 = (2; ...)^T. \]

4- Generalized Dixon Function:

\[ f = \sum_{i=1}^{n} [(1 - x_i)^2 + (1 - x_n)^2 + \sum_{i=1}^{n-1} (x_i^2 - x_{i-1})^2], \quad x_0 = (-1; ...)^T. \]
5- Generalized Cubic Function:
\[ f = \sum_{i=1}^{n/2} [100(x_{2i} - x_{2i-1})^2 + (1 - x_{2i-1})^2], \quad x_0 = (-1.2, 1; \ldots)^T \]

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