

A New Transformed VM-algorithm for Unconstrained Optimization

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Abstract

The Broyden class of Quasi-Newton updates is an approximation for the inverse Hessian matrix, are transformed to the standard BFGS update, which makes it possible to generalize the well-known t-BFGS formula. One of the variants, the simpler of them, is given in this study and does not require any additional matrix storage by vector multiplications. Experimental results indicate that the new proposed algorithm was more efficient than the standard BFGS algorithm.

خوارزمية جديدة محولة للمتري المتغير في الأمثلية غير المقيدة

الملخص

Broyden

t-BFGS

BFGS

BFGS

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1. Introduction :

Consider the unconstrained optimization problem :

$$\min \{f(x) \mid x \in R^n\} \quad \text{.....(1)}$$

where f is a continuously differentiable function of n variables .Quasi-Newton methods for solving (1) often needed the new search direction d_k at each iteration by :

$$d_k = -H_k g_k \quad \text{.....(2)}$$

where $g_k = \nabla f(x_k)$ is the gradient of f evaluated at the current iterate x_k [11]. One then computes the next iterate by

$$x_{k+1} = x_k + \alpha_k d_k \quad \text{.....(3)}$$

where the step size α_k satisfies the Wolfe – conditions

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta_1 \alpha_k d_k^T g_k \quad \text{.....(4)}$$

$$g(x_k + \alpha_k d_k)^T d_k \geq \delta_2 d_k^T g_k \quad \text{.....(5)}$$

where $0 < \delta_1 < 1/2$ and $\delta_1 < \delta_2 < 1$, and H_{k+1} is an approximation to $\{\nabla^2 f(x_k)\}^{-1}$.The matrix H_{k+1} satisfies the actual quasi-Newton condition

$$H_{k+1} y_k = \rho_k v_k \quad \text{.....(6)}$$

where $y_k = g_{k+1} - g_k$, $v_k = x_{k+1} - x_k$, ρ_k is a scalar, for Exact QN condition $\rho_k = 1$ see [1] .

To simplify the notation, we now omit the index k and replace the index $k+1$ by $+$.

The following lemma (1.1) is given in [6].

Lemma (1.1): The BFGS update can be written in the form

$$H_+ = \gamma V^T H V + \frac{\rho}{b} v v^T \quad \text{.....(7)}$$

where

$$V = I - \frac{1}{b} y v^T \quad \text{.....(8)}$$

and where $y = g_+ - g$, $v = x_+ - x$ and $a = y^T H y$, $b = y^T v$, ρ is scalar.

In [6] The scaled Broyden class of updates of H with positive value of parameter η can be written in the form :

$$\frac{1}{\gamma} H_+^{Broyden} = H + \frac{w}{b} v v^T - \frac{\eta}{b} (H y v^T + v y^T H) + \frac{\eta - 1}{b} H y y^T H \quad \text{.....(9)}$$

where

$$w = \frac{\rho}{\gamma} + \frac{a}{b} \eta \quad \text{.....(10)}$$

2.A new transformed BFGS update

The matrices storage free BFGS method is an adaptation of the BFGS method. By Malik et al. [8] is almost identical to that of standard BFGS method and the only difference is in the matrix update.

Motivated by the work of Barzilai & Borwein [3] and Birgin & Martinez [4], we use the scalar parameter

$$\lambda_+ = \frac{v^T v}{v^T y} \quad \text{.....(11)}$$

This parameter is the inverse of the Rayleigh quotient $v^T \nabla^2 f v / v^T v$, which lies between the largest and the smallest eigenvalues of the average Hessian $\nabla^2 f$. Rigorous analysis of methods exclusively based on this approximation may be found in [1,5,9,10].

Considering $H = \lambda_+ I$, ($B = H^{-1} = (1/\lambda_+)I$) see [2,1], as an approximation to the Hessian of f at x_k , where $\lambda = v^T v / v^T y$. In [3] the updated matrix H_+ is defined by

$$H_+^{t-BFGS} = \mathcal{W}^T(\lambda_+ I) \mathcal{V} + \frac{\rho}{b} v v^T \quad \text{where } V = I - \frac{1}{b} y v^T \quad \text{.....(12)}$$

using $H = \lambda_+ I$ and from (9) we get :

$$\frac{1}{\gamma} H_+ = \lambda_+ I + \frac{w}{b} v v^T - \frac{\eta}{b} ((\lambda_+ I) y v^T + v y^T (\lambda_+ I)) + \frac{\eta - 1}{b} (\lambda_+ I) y y^T (\lambda_+ I) \quad \text{.....(13)}$$

Although we use the unit values of γ and ρ in almost all cases, we will consider also non-unit values in case of VM methods. First we give the simple variant of this transformations. We denote

$$\mu = \eta + (1 - \eta) \frac{\rho}{\gamma} \frac{\bar{b}}{\bar{a}} \quad \text{.....(14)}$$

Theorem (2.1) :

If $\rho > 0, \gamma > 0, w \neq 0$, & $\alpha^* = (\eta + \sqrt{\mu}) / w$ in eq.(13), can be expressed in the following new formula :

$$\frac{1}{\gamma} H_+ = \frac{\rho}{\gamma} \frac{\eta}{\bar{b}} v v^T + V (\lambda_+ I) V^T, \quad \bar{v} = v - \alpha (\lambda_+ I) y, V = I - \frac{\sqrt{\mu}}{\bar{b}} v y^T \quad \text{.....(15)}$$

Proof : Setting $v = \bar{v} + \xi (\lambda_+ I) y, \xi \in R$, in (13) we obtain

$$\frac{1}{\gamma} H_+ = \lambda_+ I + \frac{\bar{w}}{\bar{b}} v v^T - \frac{\xi - \bar{w} \eta}{\bar{b}} ((\lambda_+ I) y v^T + \bar{v} y^T (\lambda_+ I)) + \left(\frac{\eta - 1}{\bar{a}} + \frac{\xi^2 \bar{w} - 2\xi \eta}{\bar{b}} \right) (\lambda_+ I) y y^T (\lambda_+ I)$$

The last term vanishes for $\xi^2 \bar{w} - 2\xi\eta + (\bar{b} / \bar{a})(\eta - 1) = 0$, i.e. for

$\xi = (\eta + \sqrt{\mu}) / \bar{w} = \alpha^*$, then $\xi \bar{w} - \eta = +\sqrt{\mu}$ and

$$\frac{1}{\gamma} H_+ = H + \frac{\bar{w} \bar{v} \bar{v}^T}{b} + \frac{+\sqrt{\mu}}{b} ((\lambda I) y \bar{v}^T + \bar{v} y^T (\lambda I)) \quad \dots\dots\dots(16)$$

$$\frac{1}{\gamma} H_+ = V(\lambda_+ I) V^T + \left(\bar{w} - \frac{\bar{a}}{b} \mu \right) \frac{\bar{v} \bar{v}^T}{b} \quad \dots\dots\dots(17)$$

In view of

$$\bar{w} - \frac{\bar{a}}{b} \mu = \frac{\rho}{\gamma} + \frac{\bar{a}}{b} \eta - \frac{\bar{a}}{b} \eta - \frac{\rho}{\gamma} (1 - \eta) = \frac{\rho}{\gamma} \eta \quad \dots\dots\dots(18)$$

and hence eq. (15). is obtained and the proof is completed.

Note that we prefer the minus sign in α and V , to get $\alpha = 0$ and

$\bar{v} = v$ when $\eta = 1$, (t-BFGS).

Algorithm (2.1): [new t-BFGS]

Step 0 : Choose an initial point $x_1 \in R^n$, set $k = 1$.

Step 1 : If the hybrid stopping criterion is satisfied stop :

ITERM=1- if $|x_{k+1} - x_k|$ was less than or equal to $1.0D-16$,

ITERM=2- if $|f_{k+1} - f_k|$ was less than or equal to $1.0D-14$,

ITERM=3- if f_{k+1} is less than or equal to $1.0D-16$,

ITERM= 4- if $\|g_k\|$ is less than or equal to $1.0D-6$,

ITERM= 6 if termination criterion was not satisfied, but

solution is probably acceptable,

ITERM=12- if NOF exceeded 1000,

ITERM < 0- if the method failed.

Step 2 : Solve $d_+ = -H_+ g_+$ to obtain a search direction d where λ is

defined by (11).

Step 3 : Find a step size α_k which satisfy the rule (4) and (5) to generate

a new iteration point by $x_+ = x + \alpha d$.

Step 4 : Calculate the new updating formula H_+ by

$$H_+ = \frac{\eta}{b} \bar{v} \bar{v}^T + V(\lambda_+ I) V^T, \bar{v} \text{ \& } V \text{ are defined in (15) .}$$

Step 5 : Set $k = k + 1$ and go to step 1 .

3. The global convergence property of the new algorithm :

We assume that f is strongly convex and Lipschitz continuous on the level set

$$L_0 = \{x \in R^n : f(x) \leq f(x_0)\}. \quad \dots\dots\dots(19)$$

That is, there exists constants $\mu > 0$ and L such that

$$(\nabla f(x) - \nabla f(y))^T (x - y) \geq \mu \|x - y\|^2 \quad \dots\dots\dots(20)$$

and

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|, \quad \dots\dots\dots(21)$$

for all x and y from L_0 (see [12]).

Shanno [13,14] proved that the conjugate gradient methods are exactly the BFGS quasi-Newton method, where at every step the approximation to the inverse Hessian is restarted as the identity matrix. Now we extend this result for the scaled conjugate gradient.

The direction d_+ can be computed as :

$$d_+ = - \left\{ \lambda_+ I - \lambda_+ \frac{\bar{y} \bar{v}^T + \bar{v} \bar{y}^T}{\bar{y}^T \bar{v}} + \left[1 + \lambda_+ \frac{\bar{y}^T \bar{y}}{\bar{y}^T \bar{v}} \right] \frac{\bar{v} \bar{v}^T}{\bar{y}^T \bar{v}} \right\} g_+ \quad \dots\dots\dots(22)$$

$$= -\lambda_+ I + \lambda_+ \left(\frac{\bar{g}_+^T \bar{v}}{\bar{y}^T \bar{v}} \right) \bar{y} - \left[\left(1 + \lambda_+ \frac{\bar{y}^T \bar{y}}{\bar{y}^T \bar{v}} \right) \frac{\bar{g}_+^T \bar{v}}{\bar{y}^T \bar{v}} - \lambda_+ \left(\frac{\bar{g}_+^T \bar{y}}{\bar{y}^T \bar{v}} \right) \bar{v} \right] \bar{v} \quad \dots\dots\dots(23)$$

If $\bar{g}_+^T \bar{v} = 0$, then (15) is reduced to:

$$d_+ = -\lambda_+ g_+ + \lambda_+ \frac{\bar{g}_+^T \bar{y}}{\bar{y}^T \bar{v}} \bar{v} \quad \dots\dots\dots(24)$$

$\lim_{k \rightarrow \infty} \alpha^* = 0$ because $\alpha^* = (\eta - \sqrt{\mu})/w$, then (24) is reduced to :

$$d_+ = -\lambda_+ g_+ + \lambda_+ \frac{\bar{g}_+^T \bar{y}}{\bar{y}^T \bar{v}} \bar{v} \quad \dots\dots\dots(25)$$

Thus, the effect is simply multiplying the Hestenes and Stiefel [13] search direction by a positive scalar.

Theorem (3.1) : Suppose that α in (3) satisfies the Wolfe condition (4) and (5), then the direction d_+ given by (23) is a descent direction.

Proof. Multiplying (23) by g_+^T , we have

$$g_+^T d_+ = \frac{1}{(y^T \bar{v})^2} \left[-\lambda_+ \|g_+\|^2 (y^T \bar{v})^2 + 2\lambda_+ (g_+^T y)(g_+^T \bar{v})(y^T \bar{v}) - (g_+^T \bar{v})^2 (y^T \bar{v}) - \lambda_+ (y^T y)(g_+^T \bar{v})^2 \right]$$

Applying the inequality $u^T v \leq \frac{1}{2}(\|u\|^2 + \|v\|^2)$ to the second term of the right hand side of the above equality, with $u = (\bar{v}^T y)g_+$ and $v = (g_+^T \bar{v})y$ we get :

$$g_+^T d_+ \leq - \frac{(g_+^T \bar{v})^2}{y^T \bar{v}}. \quad \text{.....(26)}$$

On the other hand, by the strong convexity property (20), we have

$$y^T \bar{v} \geq \mu \left\| \bar{v} \right\|^2. \quad \text{.....(27)}$$

Now, by Wolfe condition (5) and (27). We have, $g_+^T d_+ < 0$ for every $k = 0, 1, 2, \dots$, and hence the theorem is proved.

4.Numerical Results :

In this section, we have reported the numerical results for the new formula (15). We tested, using the collection of problems, for general sparse and separable unconstrained optimization test problems from [7]. We have in this paper used the dimension of the problem (N), $N=10,100,500,1000$. Algorithms use a line search technique [6] which satisfy Wolfe - condition as in which $\delta_1 = 0.0001, \delta_2 = 0.2$. We will test the following two VM-algorithms.

1. Standard BFGS algorithm.
2. New t-BFGS algorithm.

Tables of numerical results show the computational results , where the columns have the following meanings :

Problem : the name of the test problem .

NOI : number of iterations .

NOF : number of function evaluations .

f : value of the objective function at the point x .

g : gradient of the objective function at the point x .

ITERM : the hybrid stopping criterion

From Table (4-1), we have observed that the average performances of the new formula (15) are better than the standard BFGS and for our selected unconstrained minimization are test problems.

Table (4-1)

Comparison results of all the two algorithms as a total of (15) test functions.

	Standard BFGS algorithm		
N	NOI	NOF	TIME
10	3885	7703	0:00:00.08
100	5463	10332	0:00:00.67
500	3778	8164	0:00:02.20
1000	3747	8001	0:00:04.63
Total	16873	34200	0:00:07.58
	New t-BFGS algorithm with $\eta = 0.5$		
N	NOI	NOF	TIME
10	3005	7253	0:00:00.06
100	4161	9594	0:00:00.53
500	2987	7824	0:00:01.92
1000	2814	7647	0:00:03.94
Total	12967	32318	0:00:06.45
	New t-BFGS algorithm with $\eta = 0.8$		
N	NOI	NOF	TIME
10	3041	7296	0:00:00.06
100	4150	9553	0:00:00.53
500	2997	7830	0:00:01.92
1000	2844	7634	0:00:03.94
Total	13032	32313	0:00:06.45

The details of these test results are fully described in the subsequent tables.

Table (4-2)

Algorithm	standard BFGS algorithm with N=10				
Problem	NOI	NOF	F	g	ITERM
1	398	1001	22.3407562	0.163E+01	12
2	654	1001	0.121328883E-03	0.125E-01	12
3	656	1000	0.921077850	0.620E-02	12
4	106	153	0.799804276E-10	0.702E-05	2
5	139	179	0.160886197E-09	0.788E-05	2
6	69	112	3.01929454	0.965E-06	4
7	423	1000	11.4354732	0.217E+01	12
8	57	92	-133.510600	0.233E-05	2
9	374	1002	1.05358706	0.316E-01	12
10	13	23	0.944550269E-13	0.428E-06	4
11	500	1001	0.105143334E-03	0.167E-02	12
12	262	698	1.92460901	0.698E-04	2
13	74	123	-8.05139211	0.877E-06	4
14	74	145	-0.385263183E-01	0.836E-06	4
15	86	173	-0.251419625E-01	0.968E-06	4
Total	3885	7703			

TIME= 0:00:00.08

Table (4-3)

Algorithm	Standard BFGS algorithm with N=100				
Problem	NOI	NOF	F	g	ITERM
1	357	1000	375.772751	0.416E+01	12
2	675	1000	0.417037296E-03	0.229E-01	12
3	642	1000	25.2065330	0.110E-01	12
4	94	126	0.736274182E-10	0.347E-05	2
5	195	259	0.353606890E-08	0.233E-04	2
6	84	145	33.3754297	0.800E-06	4
7	490	725	1039.41617	0.274E-04	2
8	56	57	-98.8560279	0.562E-06	4
9	350	1001	18.9030005	0.500E+00	12
10	7	14	0.512511155E-13	0.667E-07	4
11	500	1001	0.110666145E-05	0.118E-04	12
12	334	1002	2.39784602	0.109E+00	12
13	578	1000	-49.9997833	0.285E-04	12
14	501	1001	-0.133766122E-02	0.207E-01	12
15	600	1001	0.908528629E-02	0.334E-01	12
Total	5463	10332			

TIME= 0:00:00.67

Table (4-4)

Algorithm	Standard BFGS algorithm with N=500				
Problem	NOI	NOF	F	g	ITERM
1	313	1000	1950.53768	0.506E+01	12
2	654	1000	0.190687684E-03	0.178E-01	12
3	615	1000	133.781367	0.107E-01	12
4	143	179	0.407524183E-10	0.174E-05	2
5	224	298	0.116517131E-08	0.108E-04	2
6	88	151	168.291764	0.134E-05	2
7	83	196	163899.853	0.740E-03	2
8	34	54	90.9672145	0.713E-06	4
9	406	1002	97.5181572	0.102E+01	12
10	6	12	0.315195199E-13	0.251E-06	4
11	132	265	0.101551041E-07	0.100E-05	4
12	334	1002	2.66906251	0.436E-01	12
13	390	1001	-218.394928	0.162E+01	12
14	335	1002	0.311487476	0.209E-01	12
15	334	1002	0.120585472	0.261E-01	12
Total	4091	9164			

TIME= 0:00:02.18

Table (4-5)

Algorithm	Standard BFGS algorithm with N=1000				
Problem	NOI	NOF	F	g	ITERM
1	318	1002	3920.15325	0.250E+01	12
2	645	1000	0.134675134E-03	0.171E-01	12
3	592	1001	269.500609	0.302E-01	12
4	151	190	0.658806352E-10	0.233E-05	2
5	229	300	0.142991691E-08	0.119E-04	2
6	90	151	336.937181	0.225E-05	2
7	106	265	761774.954	0.242E-02	2
8	34	55	316.436141	0.433E-06	4
9	468	1002	196.256249	0.228E+01	12
10	5	10	0.783883858E-11	0.252E-06	4
11	10	21	0.129032045E-08	0.992E-06	4
12	334	1002	2.68842398	0.300E-01	12
13	414	1000	-423.279033	0.514E+01	12
14	335	1002	0.336253881	0.155E-01	12
15	334	1002	0.128686577	0.194E-01	12
Total	4065	9003			

TIME= 0:00:04.63

Table (4-6)

Algorithm	New t-BFGS algorithm with $\eta = 0.5$ and N=10				
Problem	NOI	NOF	F	g	ITERM
1	254	1002	18.8964532	0.776E+00	12
2	500	1000	0.737373717E-04	0.151E-01	12
3	444	1001	0.920973871	0.217E-02	12
4	36	67	0.291424252E-11	0.984E-06	4
5	64	103	0.272817745E-11	0.976E-06	4
6	32	66	3.01929454	0.910E-06	4
7	334	1001	11.1394527	0.120E+01	12
8	33	71	-133.510600	0.102E-05	2
9	340	1002	1.05910329	0.245E+00	12
10	11	22	0.125965391E-12	0.416E-06	4
11	500	1001	0.105143334E-03	0.167E-02	12
12	283	567	1.92460901	0.839E-06	4
13	31	63	-8.05139211	0.274E-06	4
14	57	114	-0.385263183E-01	0.799E-06	4
15	86	173	-0.251419625E-01	0.968E-06	4
Total	3005	7253			

TIME= 0:00:00.06

Table (4-7)

Algorithm	New t-BFGS algorithm with $\eta = 0.5$ and N=100				
Problem	NOI	NOF	F	g	ITERM
1	229	1001	374.048162	0.217E+01	12
2	500	1000	0.903159788E-04	0.175E-01	12
3	479	1001	25.2062519	0.464E-02	12
4	41	77	0.319582393E-11	0.362E-06	4
5	100	186	0.156921851E-10	0.983E-06	4
6	56	119	33.3754297	0.935E-06	4
7	154	382	1057.85018	0.257E-04	2
8	55	57	-98.8560279	0.848E-06	4
9	337	1002	16.3828346	0.257E+01	12
10	7	14	0.348235823E-12	0.173E-06	4
11	500	1001	0.110666145E-05	0.118E-04	12
12	334	1002	2.39784602	0.109E+00	12
13	369	751	-49.9997833	0.499E-05	2
14	500	1000	-0.217226015E-02	0.204E-01	12
15	500	1001	0.142511903E-01	0.206E+00	12
Total	4161	9594			

TIME= 0:00:00.53

Table (4-8)

Algorithm	New t-BFGS algorithm with $\eta = 0.5$ and N=500				
Problem	NOI	NOF	F	g	ITERM
1	2	21	320193.528	0.197E+06	-6
2	500	1000	0.170900860E-03	0.220E-01	12
3	420	1000	133.781141	0.565E-02	12
4	39	75	0.201232571E-10	0.330E-06	4
5	87	171	0.307767517E-10	0.823E-06	4
6	55	119	168.291764	0.125E-05	2
7	44	134	163899.853	0.613E-03	2
8	20	41	90.9672145	0.780E-06	4
9	330	1000	77.7916010	0.325E+01	12
10	6	12	0.142795749E-12	0.534E-06	4
11	132	265	0.101551041E-07	0.100E-05	4
12	334	1002	2.66906251	0.436E-01	12
13	352	1002	-218.905261	0.149E+00	12
14	334	1001	0.310280282	0.209E-01	12
15	334	1002	0.120585472	0.261E-01	12
Total	2989	7845			

TIME= 0:00:01.92

Table (4-9)

Algorithm	New t-BFGS algorithm with $\eta = 0.5$ and N=1000				
Problem	NOI	NOF	F	g	ITERM
1	2	21	450850.163	0.256E+06	-6
2	500	1000	0.182658186E-03	0.269E-01	12
3	411	1000	269.499613	0.311E-02	12
4	40	80	0.616107780E-11	0.295E-06	4
5	99	186	0.181714799E-10	0.987E-06	4
6	56	121	336.937181	0.947E-06	4
7	53	170	761774.954	0.252E-02	2
8	27	53	316.436141	0.251E-05	2
9	286	1000	148.400432	0.163E+02	12
10	5	10	0.242975595E-10	0.443E-06	4
11	10	21	0.129032045E-08	0.992E-06	4
12	334	1002	2.68842398	0.300E-01	12
13	325	1001	-427.103778	0.147E+01	12
14	334	1001	0.335617639	0.154E-01	12
15	334	1002	0.128686577	0.194E-01	12
Total	2816	7668			

TIME= 0:00:03.94

Table (4-10)

Algorithm	New t-BFGS algorithm with $\eta = 0.8$ and N=10				
Problem	NOI	NOF	F	g	ITERM
1	254	1002	18.8964532	0.776E+00	12
2	500	1000	0.737373717E-04	0.151E-01	12
3	460	1000	0.920954442	0.133E-02	12
4	38	70	0.151059113E-11	0.926E-06	4
5	60	102	0.320279426E-11	0.829E-06	4
6	32	66	3.01929454	0.782E-06	4
7	334	1001	11.1394527	0.120E+01	12
8	37	78	-133.510600	0.128E-05	2
9	340	1002	1.05910329	0.245E+00	12
10	10	20	0.293070019E-12	0.752E-06	4
11	500	1001	0.105143334E-03	0.167E-02	12
12	283	567	1.92460901	0.839E-06	4
13	38	76	-8.05139211	0.937E-06	4
14	69	138	-0.385263183E-01	0.871E-06	4
15	86	173	-0.251419625E-01	0.968E-06	4
Total	3041	7296			

TIME= 0:00:00.06

Table (4-11)

Algorithm	New t-BFGS algorithm with $\eta = 0.8$ and N=100				
Problem	NOI	NOF	F	g	ITERM
1	229	1001	374.048162	0.217E+01	12
2	500	1000	0.903159788E-04	0.175E-01	12
3	480	1001	25.2062513	0.462E-02	12
4	43	73	0.484891937E-11	0.730E-06	4
5	91	178	0.308638605E-10	0.755E-06	4
6	48	102	33.3754297	0.843E-06	4
7	154	382	1057.85018	0.257E-04	2
8	52	54	-98.8560279	0.598E-06	4
9	337	1002	16.3828346	0.257E+01	12
10	7	14	0.920423803E-13	0.892E-07	4
11	500	1001	0.110666145E-05	0.118E-04	12
12	334	1002	2.39784602	0.109E+00	12
13	360	743	-49.9997833	0.783E-05	2
14	500	1000	-0.217226015E-02	0.204E-01	12
15	515	1000	0.100577269E-01	0.103E+00	12
Total	4150	9553			

TIME= 0:00:00.53

Table (4-12)

Algorithm	New t-BFGS algorithm with $\eta = 0.8$ and N=500				
Problem	NOI	NOF	F	g	ITERM
1	2	21	320193.528	0.197E+06	-6
2	500	1000	0.170900860E-03	0.220E-01	12
3	421	1000	133.781155	0.599E-02	12
4	42	75	0.491093324E-10	0.900E-06	4
5	93	177	0.238605480E-10	0.803E-06	4
6	54	117	168.291764	0.241E-05	2
7	44	134	163899.853	0.613E-03	2
8	21	43	90.9672145	0.752E-06	4
9	330	1000	77.7916010	0.325E+01	12
10	6	12	0.499546372E-13	0.316E-06	4
11	132	265	0.101551041E-07	0.100E-05	4
12	334	1002	2.66906251	0.436E-01	12
13	352	1002	-218.905261	0.149E+00	12
14	334	1001	0.310280282	0.209E-01	12
15	334	1002	0.120585472	0.261E-01	12
Total	2999	7851			

TIME= 0:00:01.92

Table (4-13)

Algorithm	New t-BFGS algorithm with $\eta = 0.8$ and N=1000				
Problem	NOI	NOF	F	g	ITERM
1	2	21	450850.163	0.256E+06	-6
2	500	1000	0.182658186E-03	0.269E-01	12
3	411	1000	269.499613	0.311E-02	12
4	47	83	0.471625462E-10	0.886E-06	4
5	90	173	0.243391123E-10	0.809E-06	4
6	57	123	336.937181	0.947E-06	4
7	53	170	761774.954	0.252E-02	2
8	25	48	316.436141	0.290E-05	2
9	286	1000	148.400432	0.163E+02	12
10	5	10	0.110653719E-10	0.299E-06	4
11	10	21	0.129032045E-08	0.992E-06	4
12	334	1002	2.68842398	0.300E-01	12
13	358	1001	-427.404476	0.118E-02	12
14	334	1001	0.335617639	0.154E-01	12
15	334	1002	0.128686577	0.194E-01	12
Total	2846	7655			

TIME= 0:00:03.94

5. Conclusions and Discussions :

In this paper, we have proposed a new Transformation updating formula to the standard BFGS update, call it t-BFGS update for solving unconstrained minimization problems. The computational test shows that the Transformed BFGS approach, given in this paper, is successful. We claim that the new formulae (15) is better than the standard BFGS formula. Namely, for the formula (15) with $\eta = 0.5$ and $\eta = 0.8$ there are about (23–24)% improvements in NOI , (6)% improvements in NOF and there are about (15)% improvements in time overall the calculations and for all different dimensions ($10 \leq N \leq 1000$).

Table (5-1)

Relative efficiency of standard BFGS, New t-BFGS.

Methods	NOI	NOF	TIME
standard BFGS	100	100	100
New t-BFGS with $\eta = 0.5$	76.85	94.49	85.09
New t-BFGS with $\eta = 0.8$	77.23	94.48	85.09

6. Test problems for general sparse & partially separable unconstrained optimization

We seek a minimum of either a general objective function $f(x)$ or a partially separable objective function

$$f(x) = \sum_{k=1}^{n_A} f_k(x) \quad , \quad x \in R^n$$

From the starting point $\bar{x}$. For positive integers k & l , we use the notation $\text{div}(k, l)$ for integer division, i.e., maximum integer not greater than k/l , and $\text{mod}(k, l)$ for the remainder after integer division, i.e., $\text{mod}(k, l) = l(k/l - \text{div}(k, l))$. The description of individual problems follows.

problem 1: Chained Wood function.

$$f(x) = \sum_{j=1}^k [100(x_{i-1}^2 - x_i)^2 + (x_{i-1} - 1)^2 + 90(x_{i+1}^2 - x_{i+2})^2 + (x_{i+1} - 1)^2 + 10(x_i + x_{i+2} - 2)^2 + (x_i - x_{i+2})^2 / 10]$$

$$i = 2j, \quad k = (n-2)/2$$

$$\bar{x}_i = -3, \quad \text{mod}(i,2) = 1, \quad i \leq 4, \quad \bar{x}_i = -2, \quad \text{mod}(i,2) = 1, \quad i > 4$$

$$\bar{x}_i = -1, \quad \text{mod}(i,2) = 0, \quad i \leq 4, \quad \bar{x}_i = 0, \quad \text{mod}(i,2) = 0, \quad i > 4$$

problem 2: Chained Powell singular function.

$$f(x) = \sum_{j=1}^k [(x_{i-1} + x_i)^2 + 5(x_{i+1} - x_{i+2})^2 + (x_i - 2x_{i+1})^4 + 10(x_{i-1} - x_{i+2})^4]$$

$$i = 2j, \quad k = (n-2)/2$$

$$\bar{x}_i = 3, \quad \text{mod}(i,4) = 1, \quad \bar{x}_i = -1, \quad \text{mod}(i,4) = 2$$

$$\bar{x}_i = 0, \quad \text{mod}(i,2) = 3, \quad \bar{x}_i = 1, \quad \text{mod}(i,4) = 0$$

problem 3: Chained Cragg and Levy function.

$$f(x) = \sum_{j=1}^k [(e^{x_{i-1}} - x_i)^4 + 100(x_i - x_{i+1})^6 + \tan^4(x_{i+1} - x_{i+2}) + x_{i-1}^8 + (x_{i+2} - 1)^2]$$

$$i = 2j, \quad k = (n-2)/2$$

$$\bar{x}_i = 1, \quad i = 1, \quad \bar{x}_i = 2, \quad i > 1$$

problem 4: Chained Cragg and Levy function.

$$f(x) = \sum_{i=1}^n \|(3 - 2x_i)x_i - x_{i-1} - x_{i+1} + 1\|^p$$

$$p = 7/3, \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = -1, \quad i \geq 1$$

problem 5: generalized Broyden banded function.

$$f(x) = \sum_{i=1}^n \left\| (2 + 5x_i^2)x_i + 1 + \sum_{j \in J_j} x_j(1 + x_j) \right\|^p$$

$$p = 7/3, \quad J_j = \{j: \max(1, i-5) \leq \min(n, i+1)\}$$

$$\bar{x}_i = -1, \quad i \geq 1$$

problem 6: Seven-diagonal generalization of the Broyden tridiagonal function.

$$f(x) = \sum_{i=1}^n \|(3 - 2x_i)x_i - x_{i-1} - x_{i+1} + 1\|^p + \sum_{i=1}^{n/2} \|x_i + x_{i+n/2}\|$$

$$p = 7/3, \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = -1, \quad i \geq 1$$

problem 7 : Sparse modification of the Nazareth trigonometric function.

$$f(x) = \frac{1}{n} \sum_{i=1}^n \left(n + i - \sum_{j \in J_i} (a_{ij} \sin x_j + b_{ij} \cos x_j) \right)^2$$

$$a_{ij} = 5[1 + \text{mod}(i, 5) + \text{mod}(j, 5)], \quad b_{ij} = (i + j)/10$$

$$J_i = \{j : \max(1, i - 2) \leq \min(n, i + 2)\} \cup \{j : \|j - i\| = n/2\}$$

$$\bar{x}_i = 1/n, \quad i \geq 1$$

problem 8 : Another trigonometric function.

$$f(x) = \frac{1}{n} \sum_{i=1}^n \left(i(1 - \cos x_i) - \sum_{j \in J_i} (a_{ij} \sin x_j + b_{ij} \cos x_j) \right)$$

$$a_{ij} = 5[1 + \text{mod}(i, 5) + \text{mod}(j, 5)], \quad b_{ij} = (i + j)/10$$

$$J_i = \{j : \max(1, i - 2) \leq \min(n, i + 2)\} \cup \{j : \|j - i\| = n/2\}$$

$$\bar{x}_i = 1/n, \quad i \geq 1$$

problem 9 : Chained Wood function.

$$f(x) = \sum_{j \in J} \left\{ \exp P \left(\prod_{j=1}^5 x_{i+1-j} \right) + 10 \left(\sum_{j=1}^5 x_{i+1-j}^2 - 10 - \lambda_1 \right)^2 \right. \\ \left. + 10(x_{i-3}x_{i-2} - 5x_{i-1}x_i - \lambda_2)^2 + 10(x_{i-4}^3 + x_{i-3}^3 + 1 - \lambda_3)^2 \right\}$$

$$\lambda_1 = -0.002008, \quad \lambda_2 = -0.001900, \quad \lambda_3 = -0.000261$$

$$j = \{i, \text{mod}(i, 5) = 0\}$$

$$\bar{x}_i = -2, \quad \text{mod}(i, 5) = 1, \quad i \leq 2, \quad \bar{x}_i = -1, \quad \text{mod}(i, 5) = 1, \quad i > 2$$

$$\bar{x}_i = 2, \quad \text{mod}(i, 5) = 2, \quad i \leq 2, \quad \bar{x}_i = -1, \quad \text{mod}(i, 5) = 2, \quad i > 2$$

$$\bar{x}_i = 2, \quad \text{mod}(i, 5) = 3, \quad \bar{x}_i = -1, \quad \text{mod}(i, 5) = 4$$

$$\bar{x}_i = -1, \quad \text{mod}(i, 5) = 0$$

problem 10 : Generalization of the Brown 2 function.

$$f(x) = \sum_{i=2}^n [(x_{i-1}^2)^{(x_i^2+1)} + (x_i^2)^{(x_{i-1}^2+1)}]$$

$$\bar{x}_i = -1.0, \quad \text{mod}(i, 2) = 1, \quad \bar{x}_i = 1.0, \quad \text{mod}(i, 2) = 0$$

problem 11 : Discrete boundary value problem.

$$f(x) = \sum_{i=1}^n [2x_i - x_{i-1} - x_{i+1} + h^2(x_i + ih + 1)^3 / 2]$$

$$h = 1 / (n + 1), \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = ih(1 - ih), \quad i \geq 1$$

problem 12 : Discretization of a variational problem.

$$f(x) = 2 \sum_{i=1}^n \left[x_i (x_i - x_{i+1}) / h + 2h \sum_{i=0}^n \left[(e^{x_{i+1}} - e^{x_i}) / (x_{i+1} - x_i) \right] \right]$$

$$h = 1 / (n+1) \quad , \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = ih (1 - ih) \quad , \quad i \geq 1$$

problem 13 : Banded trigonometric problem.

$$f(x) = \sum_{i=1}^n i [(1 - \cos x_i) + \sin x_{i-1} - \sin x_{i+1}]$$

$$x_0 = x_{n+1} = 0$$

$$\bar{x}_i = 1 / n \quad , \quad i \geq 1$$

problem 14 : Variational problem 1.

This problem is a finite difference analogue of a variational problem defined as a minimization of the functional :

$$f(x) = \int_0^1 \left[\frac{1}{2} x^2(t) + e^{x(t)} - 1 \right] dt$$

where $x(0) = 0$ & $x(1) = 0$. We use the trapezoidal rule together with 3 - point finite differences on a uniform grid having $n+1$ internal nodes. The starting point is given by the formula

$$\bar{x}_i = x(t_i) = ih (1 - ih) \quad , \quad \text{where } h = 1 / (n+1) \quad .$$

problem 15 : Variational problem 2.

This problem is a finite difference analogue of a variational problem defined as a minimization of the functional :

$$f(x) = \int_0^1 [x^2(t) - x^2(t) - 2t x(t)] dt$$

where $x(0) = 0$ & $x(1) = 0$. We use the trapezoidal rule together with 3 - point finite differences on a uniform grid having $n+1$ internal nodes. The starting point is given by the formula

$$\bar{x}_i = x(t_i) = ih (1 - ih) \quad , \quad \text{where } h = 1 / (n+1) \quad .$$

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