



General Letters in Mathematics (GLM)

Journal Homepage: <http://www.refaad.com/views/GLM/home.aspx>

ISSN: 2519-9277 (Online) 2519-9269 (Print)



A new self-scaling variable metric (DFP) method for unconstrained optimization problems

Salah Gazi Shareef^a, Alaa Luqman Ibrahim^{b*}, Zinah Talal Yaseen^c

^{a,b} Department of Mathematics, Faculty of Science, University of Zakho, Zakho, Kurdistan Region, Iraq.

^c Department of Mathematics, College of Computer Science and Mathematics, University of Mosul, Mosul, Iraq.

E- mails: ^a salah.shareef@uoz.edu.krd, ^b alaa.ibrahim@uoz.edu.krd, ^c Zena-talal@uomosul.edu.iq

Abstract: In this study, a new self-scaling variable metric (VM)-updating method for solving nonlinear unconstrained optimization problems is presented. The general strategy of (New VM-updating) is to propose a new quasi-newton condition used for update the usual DFP Hessian to a number of times in a way to be specified in some iteration with PCG method to improve the performance of the Hessian approximation. We show that it produces a positive definite matrix. Experimental results indicate that the new suggested method was more efficient than the standard DFP method, with respect to the number of functions evaluations (NOF) and number of iterations (NOI).

Keywords: Unconstrained optimization; self-scaling; Variable metric; Hessian approximation; DFP update.
2010 MSC No: 49J15, 74Pxx, 78M50.

1. Introduction

In 1970 Broyden [1] introduce the Quasi-Newton family of variable metric formula that is the most efficient technique for minimizing a non-linear function $h(x)$.

$$\min h(x) \quad \forall x \in R^n \quad (1)$$

Often needed to update the iterate matrix. Traditionally, satisfies the following quasi-Newton equation:

$$B_{j+1} s_j = y_j \quad (2)$$

If H_j is to be viewed as an approximation to B_j^{-1} , it is natural to require that:

$$H_{j+1} y_j = s_j \quad (3)$$

Where $s_j = x_{j+1} - x_j = \alpha_j d_j$ and $y_j = g_{j+1} - g_j$ [1,2,10]. The search direction is computed by

$$d_j = -B_j^{-1} g_j, \quad j = 0,1,2, \dots \quad (4)$$

where g_j is the gradient of h evaluated at the current iteration x_j . One then computes the next iteration by

$$x_{j+1} = x_j + \alpha_j d_j, \quad j = 0,1,2, \dots \quad (5)$$

where $\alpha_j > 0$ is the step length satisfies the Wolfe's conditions [8]:

*Corresponding author

Email address: alaa.ibrahim@uoz.edu.krd (Alaa Luqman Ibrahim)

doi: [10.31559/glm2020.9.1.6](https://doi.org/10.31559/glm2020.9.1.6)

Received: 21 Dec 2019; Accepted 18 Jun 2020

$$h(x_j + \alpha_j d_j) - h(x_j) \leq \rho \alpha_j g_j^T d_j \tag{6}$$

$$g(x_j + \alpha_j d_j)^T d_j \geq \sigma g_j^T d_j \tag{7}$$

Where $\rho \in (0, \frac{1}{2})$ and $\sigma \in (0, 1)$.

Now, after determined the point x_{j+1} we obtain the improved inverse Hessian matrix H_{j+1} by merge the information generated in the last iteration. The matrix H_{j+1} is given by for the parameter

$$H_{j+1} = H_j + \frac{s_j^T s_j}{s_j^T y_j} - \frac{H_j y_j y_j^T H_j}{y_j^T H_j y_j} + \vartheta R_j R_j^T \tag{8}$$

where $R_j = \frac{s_j}{s_j^T y_j} - \frac{H_j^T y_j}{y_j^T H_j y_j} H_0 = I$ and $\vartheta \in [0, 1]$

Different values of the scalar ϑ correspond to different member of Broyden's Quasi-Newton -family, noted that if $\vartheta = 0$ then equation (8) corresponds to the standard DFP algorithm introduced by Davidon [13] and Fletcher and Powell [9]. In studying the theoretical behavior of this technique it was shown by Fletcher and Powell that, on quadratic function with the exact line search, the standard DFP formula generates conjugate directions and hence minimizes a quadratic function in at most the iterations. Many modulations have been applied on QN-methods in bid to improve its performance. In 1974 Oren [11] develops the self-scaling VM-algorithms, Oren's formula can be written as:

$$H_{j+1} = [H_j - \frac{H_j y_j y_j^T H_j}{y_j^T H_j y_j} + \vartheta R_j R_j^T] \gamma_j + \frac{s_j^T s_j}{s_j^T y_j} \tag{9}$$

Where $\gamma_j = \frac{s_j^T y_j}{y_j^T H_j y_j}$ and $\vartheta = 1$

Clearly when $\gamma_j = 1$, formula (9) reduces to Broyden's class update defined in (7). Also, to improve the performance of VM updates Biggs [6] proposed to choose H_{j+1} to satisfy the following modified equation $H_{j+1} y_j = \epsilon_j s_j$, where $\epsilon_j > 0$ is a scaling parameter. The modified BFGS may be written as:

$$H_{j+1} = H_j + \frac{H_j y_j s_j^T + s_j y_j^T H_j}{s_j^T y_j} + (\frac{1}{\tau_j} + \frac{y_j^T H_j y_j}{s_j^T y_j}) \frac{s_j^T s_j}{s_j^T y_j} \tag{10}$$

where $\tau_j = \frac{1}{\epsilon_j} = \frac{6}{s_j^T y_j} (h(x_j) - h(x_{j+1}) + s_j^T g_{j+1}) - 2$

also S. Shareef, and A. Ibrahim [12] made a modification for self-scaling symmetric rank one update with QN condition $H_{j+1} \bar{y}_j = \tau s_j$ as follow

$$H_{j+1} = H_j + \frac{(\tau s_j - H_j \bar{y}_j)(\tau s_j - H_j \bar{y}_j)^T}{(\tau s_j - H_j \bar{y}_j)^T \bar{y}_j} \tag{11}$$

where $\tau = t(1 + (1 - \vartheta)\rho_j)$, $t \geq 0$, $\vartheta \in (0, 1)$ and $\rho_i = \frac{s_i^T y_i}{\|s_i\|^2}$.

We end this general introduction by content of this paper which is organized as follows: In section two, we present the new method. In section three, Numerical results, percentages and discussion are reported. In the final section, we present a conclusion. Throughout this paper, $\| \cdot \|$ denotes the Euclidean norm of a vector or matrix.

2. Derivation of New Self-scaling VM methods

In this section a new formula for a self-scaling VM-method with preconditioned conjugate gradient (PCG) method is presented. Further, Zhang et al. [4] and Zhang and Xu [5] expanded this condition and derived a class of modified secant condition with a vector parameter, in the form

$$H_{j+1} \hat{y}_j = s_j, \hat{y}_j = y_j + \frac{\theta_j}{s_j^T u} u \tag{12}$$

where u is any vector satisfying $s_j^T u > 0$, and θ_j is defined by:

$$\theta_j = 6 (f_j - f_{j+1}) + 3(g_j + g_{j+1})^T s_j$$

For the new method we have investigated a new expression for the QN-condition as follows:

$$H_{j+1} \bar{y}_j = s_j, \bar{y}_j = y_j + \mu \frac{\theta_j}{s_j^T y_j} y_j \tag{13}$$

Where $\mu \in (0,1)$ and $\theta_j = \alpha^{BB} = \frac{s_j^T s_j}{s_j^T y_j}$ for more details see [3]

Then, the new self-scaling VM method becomes as follows

$$H_{j+1} = H_j - \frac{H_j \bar{y}_j \bar{y}_j^T H_k}{\bar{y}_j^T H_j \bar{y}_j} + \left(\frac{s_j^T s_j}{s_j^T y_j} \right) \tag{14}$$

2.1 The Outlines of the New Self-Scaling VM Method with PCG Method

Step (1): Set $j = 0$, select x_0 and a real symmetric positive definite $H_0 = I$, $\varepsilon = 10^{-5}$.

Step (2): If $g_j = 0$, stop; else $d_j = -H_j g_j$, where $g_i = \nabla h(x_j)$.

Step (3): Find $\alpha_j = \arg \min h(x_{j+1} + s_i)$.

Step (4): Set $x_{j+1} = x_j + s_j$ and $y_j = g_{j+1} - g_j$.

Step (5): Compute g_{j+1} if $\|g_{j+1}\| < \varepsilon$, then stop.

Step (6): Calculate H_{j+1} from equation (14).

Step (7): Evaluate $d_{j+1} = -H_{j+1} g_{j+1} + \frac{\bar{y}_j^T H_{j+1} g_{j+1}}{d_j^T \bar{y}_j} d_j$,

Step (8): If $|g_j^T g_{j+1}| \geq 0.2 \|g_{j+1}\|^2$ go to step (2) else continue.

Set $j = j + 1$ and repeat from Step (3).

Theorem 1: If the new self-scaling VM method is applied to the quadratic with Hessian $B = B^T$, then $H_{j+1} \bar{y}_j = s_j$, $j \geq 0$.

Proof: By multiplying equation (14) by \bar{y}_j from the right, we obtained:

$$H_{j+1} \bar{y}_j = H_j \bar{y}_j - \frac{H_j \bar{y}_j \bar{y}_j^T H_k}{\bar{y}_j^T H_j \bar{y}_j} \bar{y}_j + \left(\frac{s_j^T s_j}{s_j^T y_j} \right) \bar{y}_j \tag{15}$$

Since $\bar{y}_j^T H_j \bar{y}_j$ and also $s_j^T \bar{y}_j$ are scalars. Then

$$H_{j+1} \bar{y}_j = H_j \bar{y}_j - H_j \bar{y}_j + s_j \tag{16}$$

Then, $H_{j+1} \bar{y}_j = s_j$

The proof is complete. ■

Theorem 2: In the new self-scaling VM method, if H_j is positive definite, then so is the matrix H_{j+1} .

Proof: we can write the equation (14) in quadratic form:

$$X^T H_{j+1} X = X^T H_j X - \frac{X^T H_j \bar{y}_j \bar{y}_j^T H_j X}{\bar{y}_j^T H_j \bar{y}_j} + X^T \left(\frac{v_j v_j^T}{v_j^T \bar{y}_j} \right) X, \tag{17}$$

$$X^T H_{j+1} X = X^T H_j X - \frac{(X^T H_j \bar{y}_j)^2}{\bar{y}_j^T H_j \bar{y}_j} + \frac{(X^T v_j)^2}{v_j^T \bar{y}_j}. \tag{18}$$

Now, define $a = H_j^{\frac{1}{2}} X$, $b = H_j^{\frac{1}{2}} \bar{y}_j$ where $H_j = H_j^{\frac{1}{2}} H_j^{\frac{1}{2}}$

And by using the definitions of a and b , we obtain

$$X^T H_j X = X H_j^{\frac{1}{2}} H_j^{\frac{1}{2}} X = a^T a,$$

$$X^T H_j \bar{y}_j = X H_j^{\frac{1}{2}} H_j^{\frac{1}{2}} \bar{y}_j = a^T b$$

and

$$\bar{y}_j^T H_j \bar{y}_j = \bar{y}_j^T H_j^{\frac{1}{2}} H_j^{\frac{1}{2}} \bar{y}_j = b^T b.$$

$$\text{Hence, } X^T H_{j+1} X = a^T a - \frac{(a^T b)^2}{b^T b} + \frac{(X^T v_j)^2}{v_j^T \bar{y}_j},$$

$$X^T H_{j+1} X = \frac{\|a\|^2 \|b\|^2 - (a^T b)^2}{\|b\|^2} + \frac{(X^T v_j)^2}{v_j^T \bar{y}_j}. \tag{19}$$

We know that $s_j^T y_j$ and $s_j^T s_j$ are positive and $\mu \in (0,1)$, so we have

$s_j^T \bar{y}_j = s_j^T y_j + \mu \frac{s_j^T s_j}{(s_j^T y_j)^2} y_j^T y_j$ is positive. The fractional terms on the right-hand side of (18) are nonnegative. Therefore, to show that $X^T H_{j+1} X > 0$, for $X \neq 0$, we need only to demonstrate that these terms do not both vanish simultaneously. The first term vanishes only if a and b are proportional, that is, if $a = \beta b$ for some scalar β . To complete the proof it is enough to show that if $a = \beta b$ then

$$\frac{(x^T v_j)^2}{v_j^T \bar{y}_j} > 0. \text{ First observe that}$$

$$H_j^{\frac{1}{2}} X = a = \beta b = \beta H_j^{\frac{1}{2}} \bar{y}_j = H_j^{\frac{1}{2}} (\beta \bar{y}_j).$$

Hence $X = \beta \bar{y}_j$,

By using the above expression for X and $v_j^T \bar{y}_j$,

$$\frac{(x^T v_j)^2}{v_j^T \bar{y}_j} = \frac{(v_j^T \beta \bar{y}_j)^2}{v_j^T \bar{y}_j} = \frac{\beta^2 (v_j^T \bar{y}_j)^2}{v_j^T \bar{y}_j} = \beta^2 \left(s_j^T y_j + \mu \frac{s_j^T s_j}{(s_j^T y_j)^2} y_j^T y_j \right) > 0.$$

Thus for all $X \neq 0$,

$$X^T H_{j+1} X > 0.$$

Then the proof is completed. ■

3. Numerical Results

This section is devoted to test the implementation of the new VM method. The comparative test involve well-known nonlinear problems (standard test function) [7] given in the Appendix with different dimensions, are tested in the range ($4 \leq n \leq 5000$), all programs are written in FORTRAN95 language. The numerical results in Table (1) illustrate that, the VM method is more efficient than standard DFP method with respect to NOI and NOF. Table (2) confirms that the new VM method is superior to standard DFP VM method. Namely there are an improvement of the new suggested about 25.77801 % in NOI and 33.66278 % in NOF by using the new suggested VM algorithm. Generally, the New VM method was improved by 29.72039 % compared with DFP method.

Table (1): Comparison between the performance of the (new VM and DFP) methods

Test Function	n	DFP		New- VM	
		NOI	NOF	NOI	NOF
Powell	4	35	96	32	87
	10	36	107	33	96
	50	37	110	37	119
	100	38	112	35	105
	500	38	111	35	105
	1000	38	111	35	105
	5000	39	113	36	105
Mile	4	66	300	32	153
	10	67	302	32	145
	50	80	374	36	160
	100	86	411	31	127
	500	94	454	38	177
	1000	100	496	47	231
	5000	112	575	104	533
Central	4	34	237	19	91
	10	49	423	22	132
	50	39	295	21	122
	100	39	295	34	269
	500	49	423	31	221
	1000	54	479	30	216
	5000	71	682	55	546
Rosen	4	34	94	33	92
	10	34	94	34	95
	50	34	94	34	92
	100	35	97	34	92
	500	35	97	34	95
	1000	34	95	34	93
	5000	38	104	36	98
Cubic	4	14	40	14	40
	10	14	40	14	40
	50	16	47	15	43
	100	17	49	16	46
	500	16	46	16	46
	1000	17	49	16	46
	5000	16	46	16	46
Non-Diagonal	4	27	74	27	73
	10	36	92	35	90

	50	47	114	47	113
	100	55	132	54	131
	500	112	255	49	117
	1000	49	119	49	119
	5000	47	114	49	119
Total		1928	8398	1431	5571

Table (2): Percentage performance of the (new VM and DFP) methods

Tools	DFP	New-VM
NOI	100%	74.22199%
NOF	100%	66.33722%

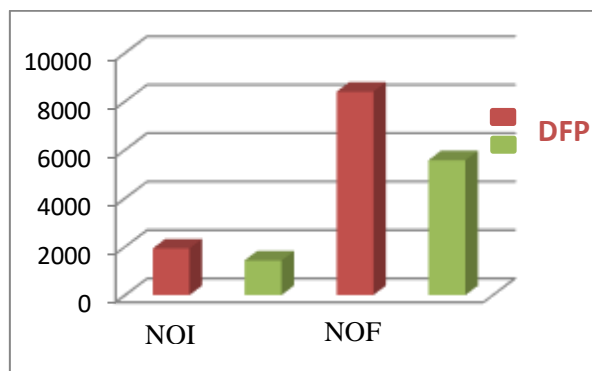


Figure (1): Shows the comparison between New-VM method and the standard algorithm (DFP) according to the total number of iterations (NOI) and the total number of functions (NOF).

4. Conclusion

In this paper, we have offered a VM-type for unconstrained optimization problems based on a modified quasi-Newton condition. We showed that the new method satisfy the modified quasi-newton condition and positive definite property. It is clear that from the numerical results the new modified VM-updating formula has an improvement on the standard DFP method in about 29% in both NOI and NOF.

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Appendix

Standard Test Functions for Nonlinear Unconstrained Optimization Problems

1. Generalized Central Function:

$$h(x) = \sum_{j=1}^{n/4} \left(\exp(x_{4j-3} + x_{4j-2})^4 + 100((x_{4j-2} - x_{4j-1})^6 + \arctan((x_{4j-1} - x_{4j})^4 + x_{4j-3})) \right),$$

$$x_0 = (1, 2, 2, 2, \dots, 1, 2, 2, 2)^T.$$

2. Generalized Cubic Function:

$$h(x) = \sum_{j=1}^{n/2} \left(100(x_{2j} - x_{2j-1}^3)^2 + (1 - x_{2j})^2 \right), \quad x_0 = (-1.2, 1, \dots, -1.2, 1)^T.$$

3. Generalized Non-Diagonal Function:

$$h(x) = \sum_{j=2}^n \left(100(x_1 - x_j^2)^2 + (1 - x_j)^2 \right), \quad x_0 = (-1, \dots, -1)^T.$$

4. Generalized Rosen Brock Banana Function:

$$h(x) = \sum_{j=1}^{n/2} \left(100(x_{2j} - x_{2j-1}^2)^2 + (1 - x_{2j-1})^2 \right), \quad x_0 = (-1.2, 1, \dots, -1.2, 1)^T.$$

5. Mile Function:

$$h(x) = \sum_{j=1}^{n/4} \left((e^{x_{4j-3}} + 10x_{4j-2})^2 + 100(x_{4j-2} + x_{4j-1})^6 + (\tan(x_{4j-1} - x_{4j}))^4 + (x_{4j-3})^8 + (x_{4j} - 1)^2 \right),$$

$$x_0 = (1, 2, 2, \dots, 1, 2, 2)^T.$$

6. Powell Function:

$$h(x) = \sum_{j=1}^{n/4} \left((x_{4j-3} - 10x_{4j-2})^2 + 5(x_{4j-1} - x_{4j})^2 + (x_{4j-2} - 2x_{4j-1})^4 + 10(x_{4j-3} - x_{4j})^4 \right), x_0 = (3, -1, 0, 1, \dots, 3, -1, 0, 1)^T.$$