

Two New Preconditioned Conjugate Gradient Methods for Minimization Problems

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Abstract In application to general function, each of the conjugate gradient and Quasi-Newton methods has particular advantages and disadvantages. Conjugate gradient (CG) techniques are a class of unconstrained optimization algorithms with strong local and global convergence qualities and minimal memory needs. Quasi-Newton methods are reliable and efficient on a wide range of problems and they converge faster than the conjugate gradient method and require fewer function evaluations but they have the disadvantage of requiring substantially more storage and if the problem is ill-conditioned, they may take several iterations. A new class has been developed, termed preconditioned conjugate gradient (PCG) method. It is a method that combines two methods, conjugate gradient and Quasi-Newton. In this work, two new preconditioned conjugate gradient algorithms are proposed namely New PCG1 and New PCG2 to solve nonlinear unconstrained optimization problems. A new PCG1 combines conjugate gradient method Hestenes-Stiefel (HS) with new self-scaling symmetric Rank one (SR1), and a new PCG2 combines conjugate gradient method Hestenes-Stiefel (HS) with new self-scaling Davidon, Fletcher and Powell (DFP). The algorithm uses the strong Wolfe line search condition. Numerical comparisons with standard preconditioned conjugate gradient algorithms show that for these new algorithms, computational scheme outperforms the preconditioned conjugate gradient.

Keywords Unconstrained Optimization, Quasi-Newton Method, Self-Scaling Quasi-Newton Method, Preconditioned Conjugate Gradient Method

1. Introduction

We are interested to consider the following nonlinear unconstrained minimization problem

$$\text{Min}f(x), x \in R^n \quad (1)$$

where $f: R^n \rightarrow R$ is a twice continuously differentiable. Nonlinear unconstrained conjugate gradient algorithms to solve (1) are iterative technique and have the form

$$x_{m+1} = x_m + \alpha_m d_m \quad (2)$$

which is starting from an initial guess $x_0 \in R^n$, the positive step length α_m is calculated by one dimensional line search and d_m is the search direction. The preconditioned conjugate gradient techniques have two search directions, the first one has the form:

$$d_0 = -H_0 g_0, H_0 = I \text{ and } g_0 = \nabla f(x_0). \quad (3)$$

and the other search direction has the form:

$$d_{m+1} = -H_{m+1}g_{m+1} + \beta_m d_m \quad (4)$$

where $g_{m+1} = \nabla f(x_{m+1})$, β_m is a conjugate coefficient. The most well-know formulas of β_m are called Hestenes Stiefel (HS) [1], Polak Ribiere Polyak (PRP) [3], Dai Yuan (DY)[4] and Fletcher Reeves(FR)[5].

H_{m+1} is the inverse Hessian approximation and H_{m+1} is chosen to satisfy the following quasi-Newton equation

$$H_{m+1}y_m = v_m \quad (5)$$

where $y_m = g_{m+1} - g_m$ and $v_m = x_{m+1} - x_m$. The Quasi-Newton is very similar to method of Newton, but avoids the requirement to compute Hessian matrices by repeating from iteration to iteration.

We obtain the corresponding update formula for the inverse Hessian approximation[2]

$$H_{m+1} = H_m + \frac{(v_m - H_m y_m)(v_m - H_m y_m)^T}{y_m^T (v_m - H_m y_m)} \quad (6)$$

And also there are other methods to find the inverse Hessian approximation like Davidon, Fletcher and Powell (DFP)

$$H_{m+1} = H_m + \frac{v_m v_m^T}{v_m^T y_m} - \frac{(H_m y_m)(H_m y_m)^T}{y_m^T H_m y_m} \quad (7)$$

and Broyden, Fletcher, Goldfarb and Shanno Method (BFGS)

$$H_{m+1} = H_m + (1 + \frac{y_m^T H_m y_m}{y_m^T v_m}) \frac{v_m v_m^T}{v_m^T y_m} - \frac{(H_m y_m v_m^T) + (H_m y_m v_m)^T}{y_m^T y_m} \quad (8)$$

Self-scaling is one of the common approaches in the modification of the Quasi-Newton method. The general strategy of self-scaling Quasi-Newton method (SS) is to scale the Hessian approximation matrix before it is updated at each iteration. This is to avoid large differences in the eigenvalues of the approximated Hessian of the function. There are many self-scalings suggested, for example Oren [6] proposed some good characteristics, with a self-scaling parameter ρ_m , this class of updates can be written as

$$H_{m+1} = (H_m - \frac{H_m y_m y_m^T H_m}{y_m^T H_m y_m} + \Phi_m (y_m^T H_m y_m) \bar{v}_m \bar{v}_m^T) \rho_m + \frac{v_m v_m^T}{v_m^T y_m}, \quad (9)$$

with $\bar{v}_m = \frac{v_m}{v_m^T y_m} + \frac{H_m y_m}{y_m^T H_m y_m}$

(Oren and Luenberger)[7] suggest to use the self - adaptable values for the parameter

$$\rho_m = t \frac{g_m^T v_m}{g_m^T H_m y_m} + (1 - t) \frac{v_m^T y_m}{y_m^T H_m y_m}$$

and usually the value $t = 0$ is recommended for the updates in the convex class.

To improve the performance of Quasi-Newton update, Biggs [8] proposed to choose H_{m+1} to satisfy the following modified equation

$H_{m+1}y_m = \gamma_m v_m$. where $\gamma_m > 0$ is a scaling parameter. Biggs showed that a modified BFGS could be derived as follows

$$H_{m+1} = H_m + \frac{H_m y_m v_m^T + v_m y_m^T H_m}{v_m^T y_m} + (\frac{1}{\tau_m} + \frac{y_m^T H_m y_m}{v_m^T y_m}) \frac{v_m v_m^T}{v_m^T y_m} \quad (10)$$

where $\tau_m = \frac{1}{\gamma_m} = \frac{6}{v_m^T y_m} (f(x_m) - f(x_{m+1}) + v_m^T g_{m+1}) - 2$

also, Yang, Xu and Gao[9] made a little modification for self-scaling symmetric rank one update with Davidon's optimal condition [10] as follows

$$H_{m+1} = r_m H_m + \frac{(v_m - \gamma_m H_m \hat{y}_m)(v_m - \gamma_m H_m \hat{y}_m)^T}{\hat{y}_m^T (v_m - \gamma_m H_m \hat{y}_m)} \quad (11)$$

where r_m is the scaling factor,

$$\hat{y}_m = \left(\frac{1 + \theta_m}{v_m^T y_m} \right) y_m, \theta_m = 6(f_m - f_{m+1}) + 3(g_m - g_{m+1})^T v_m \text{ and } f_m = f(x_m).$$

The structure of the paper is as follows. In section 2, we introduce two new self-scaling Quasi-Newton methods (new self-scaling symmetric rank one and new self-scaling Davidon, Flecher and Powell). In section 3, we present the outlines of the New PCG1 and New PCG2. In section 4, we will prove the Quasi-Newton condition and positive definite condition for the new self-scaling symmetric rank one and new self-scaling Davidon, Flecher and Powell. We give some numerical results to show the efficiency of these new algorithms in section 5.

2. Two New Self-Scaling Quasi-Newton Methods

In this section, we will derive two new self-scaling variable metrics for unconstrained minimization problems, the first one is new self-scaling symmetric rank one and the second one is new self-scaling DFP. Consider the equation

$$y_m^* = y_m + \mu_m v_m \tag{12}$$

Suppose that $\mu_m = \tau * \frac{N_m}{1+N_m}$,

$$N_m = \frac{y_m^T v_m}{\|v_m\|} \text{ and } \tau \in (0,1)$$

The updating H_{m+1} matrix is chosen to satisfy the following Quasi-Newton equation

$$H_{m+1} y_m^* = \delta_1 v_m \tag{13}$$

where $\delta_1 = \sqrt{\frac{|y_m^T H_{m+1} y_m^*|}{y_m^T v_m}}$

Let

$$H_{m+1} = H_m + \theta_m w_m w_m^T \tag{14}$$

Where the correction term $\theta_m w_m w_m^T$ is symmetric, α_m is a scalar belong to R and w_m is a vector belong to R^n .

Give H_m , y_k^* and v_m so that the required relationship $H_{m+1} y_m^* = \delta_1 v_m$ is satisfied.

To find θ_m and w_m , multiply both sides of equation(14) by y_m^* and by using (13), we have

$$H_{m+1} y_m^* = (H_m + \theta_m w_m w_m^T) y_m^* = \delta_1 v_m \tag{15}$$

first note that $w_m^T y_m^*$ is a scalar. Thus

$$\delta_1 v_m - H_m y_m^* = (\theta_m w_m^T y_m^*) w_m \tag{16}$$

Here,

$$w_m = \frac{\delta_1 v_m - H_m y_m^*}{\theta_m (w_m^T y_m^*)}$$

Hence,

$$\theta_m w_m w_m^T = \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{\theta_m (w_m^T y_m^*)^2} \tag{17}$$

So,

$$H_{m+1} = H_m + \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{\theta_m (w_m^T y_m^*)^2} \tag{18}$$

Now multiply (16) by y_m^{*T} to obtain

$$\delta_1 y_m^{*T} v_m - y_m^{*T} H_m y_m^* = y_m^{*T} (\theta_m w_m^T y_m^*) w_m \tag{19}$$

Observe that θ_m is scalar and

$y_m^{*T} w_m = w_m^T y_m^*$, then the above equation becomes

$$\delta_1 y_m^{*T} v_m - y_m^{*T} H_m y_m^* = \theta_m (w_m^T y_m^*)^2 \tag{20}$$

By substituting equation (20) in equation (18) we have a new self-scaling symmetric rank one as follows,

$$H_{m+1} = H_m + \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{y_m^{*T} (\delta_1 v_m - H_m y_m^*)} \tag{21}$$

Also we suggest new self-scaling DFP formula to find the inverse of Hessian matrix as follows:

$$H_{m+1} = H_m + \frac{v_m v_m^T}{\delta_1 v_m^T y_m^*} - \frac{(H_m y_m^*)(H_m y_m^*)^T}{y_m^{*T} H_m y_m^*} \tag{22}$$

where $y_m^* = y_m + \mu_m v_m$

$$\mu_m = \tau * \frac{N_m}{1+N_m}, \quad N_k = \frac{y_m^T v_m}{\|v_m\|} \text{ and } \tau \in (0,1) \text{ and } \delta_1 = \sqrt{\frac{|y_m^T H_{m+1} y_m^*|}{y_m^T v_m}}$$

Now, in the algorithm below we will combine the new self-scaling symmetric rank one with parameter of HS to become New PCG1, and we will combine the new self-scaling DFP with parameter of HS to become New PCG2.

3. The Outlines of the New PCG1 and New PCG2

Step1: Set $m = 0$, chose x_0 , a real symmetric positive definite $H_0 = I$ and ε is a small positive integer.

Step2: Calculate $g_m = \nabla f(x_m) = \frac{\partial f}{\partial x_m}$.

Step3: Evaluate $d_m = -H_m g_m$.

Step4: Find $\alpha_m > 0$, satisfying the strong Wolfe condition

$$f(x_m + \alpha_m d_m) - f(x_m) < k_1 \alpha_m g_m^T d_m \text{ and } |g_{m+1}^T d_m| < k_2 |g_m^T d_m|$$

where, $0 < k_1 < k_2 < 1$.

Step5: Set $v_m = \alpha_m d_m$,

$$x_{m+1} = x_m + v_m \text{ and } y_m = g_{m+1} - g_m.$$

Step6: Compute $g_{m+1} = \nabla f(x_{m+1})$,

if $\|g_{m+1}\| < \varepsilon$, then stop.

Step7: Calculate H_{m+1} using (21) or H_{m+1} using (22)

step8: Evaluate d_{m+1} by

$$d_{m+1} = -H_{m+1} g_{k+1} + \frac{g_{m+1}^T H_{m+1} y_m}{d_m^T y_m} d_m \text{ or } d_{m+1} = -H_{m+1} g_{k+1} + \frac{g_{m+1}^T H_{m+1} y_m}{d_m^T y_m} d_m$$

Step9: If $|g_m^T g_{m+1}| \geq 0.2 \|g_{m+1}\|^2$ then go to step (4), else continue.

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

4. Quasi-Newton Condition and Positive Definite

In this section, we will study the Quasi-Newton condition and positive definite condition of our two new self-scaling Quasi-Newton methods.

Theorem 1: If the new self-scaling symmetric rank one is applied to the quadratic functions with Hessian $Q = Q^T$, we have

$$H_{m+1} y_i^* = \delta_1 v_i, 0 \leq i \leq m.$$

Proof:

Multiply both sides of (21) by y_i^* , so, we get

$$H_{m+1} y_i^* = H_m y_i^* + \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{y_m^{*T} (\delta_1 v_m - H_m y_m^*)} y_i^* \quad (23)$$

for $m = 0$

$$H_1 y_0^* = H_0 y_0^* + \frac{(\delta_1 v_0 - H_0 y_0^*)(\delta_1 v_0 - H_0 y_0^*)^T}{y_0^{*T} (\delta_1 v_0 - H_0 y_0^*)} y_0^*$$

Since $(\delta_1 v_0 - H_0 y_0^*)^T y_0^* = y_0^{*T} (\delta_1 v_0 - H_0 y_0^*)$ because they are scalars

Here we get,

$$H_1 y_0^* = H_0 y_0^* + \delta_1 v_0 - H_0 y_0^* = \delta_1 v_m \quad (24)$$

Suppose that it is true for case $m - 1$, that is, $H_m y_i^* = \delta_1 v_i$.

Now, for $m + 1$, if $m = i$

$$H_{m+1} y_m^* = H_m y_m^* + \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{y_m^{*T} (\delta_1 v_m - H_m y_m^*)} y_m^* = \delta_1 v_m$$

Consider if $i < m$

$$H_{m+1} y_i^* = H_m y_i^* + \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{y_m^{*T} (\delta_1 v_m - H_m y_m^*)} y_i^*$$

To complete the proof it is enough to show the second term on the right hand side of the above equation is equal to zero. Consider

$$\begin{aligned} (\delta_1 v_m - H_m y_m^*)^T y_i^* &= \delta_1 v_m^T y_i^* - y_m^{*T} H_m y_i^* \\ &= \delta_1 v_m^T y_i^* - \delta_1 y_m^{*T} v_i \end{aligned}$$

$$\begin{aligned} &= \delta_1 v_m^T y_i^* - \delta_1 v_m^T Q v_i \\ &= \delta_1 v_m^T y_i^* - \delta_1 v_m^T y_i^* = 0 \end{aligned}$$

So, we have $H_{m+1} y_i^* = H_m y_i^*$

Then, $H_{m+1} y_m^* = \delta_1 v_m$

Theorem 2: Suppose that $g_m \neq 0$. In equation (21), if H_m is positive definite. It turns that if $y_m^{*T} (\delta_1 v_m - H_m y_m^*) > 0$, then H_{m+1} is positive definite.

Proof: Let X be any non-zero vector, multiply both sides of equation (21) by X^T from left and by X from right, so, we get

$$X^T H_{m+1} X = X^T H_m X + X^T \frac{(\delta_1 v_m - H_m y_m^*)(\delta_1 v_m - H_m y_m^*)^T}{y_m^{*T} (\delta_1 v_m - H_m y_m^*)} X \tag{25}$$

since

$$X^T (\delta_1 v_m - H_m y_m^*) = (\delta_1 v_m - H_m y_m^*)^T X$$

then, the equation (25) gives

$$X^T H_{m+1} X = X^T H_m X + \frac{(X^T (\delta_1 v_m - H_m y_m^*))^2}{(\delta_1 y_m^{*T} v_m - y_m^{*T} H_m y_m^*)} \tag{26}$$

a sufficient condition for H_{m+1} to be positive definite is $(\delta_1 y_m^{*T} v_m - y_m^{*T} H_m y_m^*) > 0$

if the denominator of the correction formula becomes zero or negative, H_{m+1} can be discarded and H_m can be used for the subsequent iteration. However, if this problem occurs frequently, the possibility exists that H_{m+1} may not converge to H^{-1} . Then the expected rapid convergence may not materialize.

Since H_m is positive definite and

$$\delta_1 y_m^{*T} v_m = \delta_1 (y_m + \mu_m v_m)^T v_m = \delta_1 \mu_m \|v_m\|^2 + \delta_1 y_m^T v_m > 0$$

then, the above equation becomes

$$X^T H_{m+1} X > X^T H_m X + \frac{(X^T (\delta_1 v_m - H_m y_m^*))^2}{\delta_1 y_m^{*T} v_m} \tag{27}$$

Here we observe that the right hand side of the (27) is positive, then H_{m+1} is positive definite.

Theorem 3: If the new self-scaling DFP is applied to the quadratic function with Hessian $Q = Q^T$, we have $H_{m+1} y_i^* = \delta_1 v_i, 0 \leq i \leq m$.

Proof:

Multiplying the equation (22) by y_i^* , so, we get

$$H_{m+1} y_i^* = H_m y_i^* + \frac{\delta_1 v_m v_m^T}{v_m^T y_m^*} y_i^* - \frac{(H_m y_m^*)(H_m y_m^*)^T}{y_m^{*T} H_m y_m^*} y_i^* \tag{28}$$

for $m = 0$, we have

$$H_1 y_0^* = H_0 y_0^* + \frac{\delta_1 v_0 v_0^T}{v_0^T y_0^*} y_0^* - \frac{(H_0 y_0^*)(H_0 y_0^*)^T}{y_0^{*T} H_0 y_0^*} y_0^*$$

Since $(H_0 y_0^*)^T y_0^*$ and $y_0^{*T} H_0 y_0^*$ are scalars, then $(H_0 y_0^*)^T y_0^* = y_0^{*T} H_0 y_0^*$

Therefore,

$$H_1 y_0^* = H_0 y_0^* + \delta_1 v_0 - H_0 y_0^* = \delta_1 v_0 \tag{29}$$

Assume it is true for $m - 1$, that is $H_m y_i^* = \delta_1 v_i$.

Now, we show that $H_{m+1} y_i^* = \delta_1 v_i$, if $i = m$

$$H_{m+1} y_m^* = H_m y_m^* + \frac{\delta_1 v_m v_m^T}{v_m^T y_m^*} y_m^* - \frac{(H_m y_m^*)(H_m y_m^*)^T}{y_m^{*T} H_m y_m^*} y_m^* = \delta_1 v_m$$

Now, consider the case $i < m$

$$\begin{aligned} H_{m+1} y_i^* &= H_m y_i^* + \frac{\delta_1 v_m v_m^T}{v_m^T y_m^*} y_i^* - \frac{(H_m y_m^*)(y_m^{*T} H_m)}{y_m^{*T} H_m y_m^*} y_i^* \\ &= \delta_1 v_i + \frac{\delta_1 v_m}{v_m^T y_m^*} v_m^T y_i^* - \frac{(H_m y_m^*)}{y_m^{*T} H_m y_m^*} \delta_1 y_m^{*T} v_i \end{aligned}$$

$$v_m^T y_i^* = v_m^T Q v_i^* = \alpha_m \alpha_i d_m^T Q d_i^* = 0 \text{ and also } y_m^{*T} v_i = 0 \text{ then,}$$

$$H_{m+1}y_i^* = \delta_1 v_i$$

Theorem 4: Suppose that $g_m \neq 0$. In equation (22), if H_m is positive definite, then so is H_{m+1} .

Proof: Let X be any non-zero vector, multiplying the equation(22) by X^T from the left and by X from the right, so, we have

$$X^T H_{m+1} X = X^T H_m X + \frac{\delta_1 X^T v_m v_m^T X}{v_m^T y_m^*} - \frac{X^T (H_m y_m^*) (H_m y_m^*)^T X}{y_m^{*T} H_m y_m^*} \quad (30)$$

implies that

$$X^T H_{m+1} X = X^T H_m X + \frac{\delta_1 (v_m^T X)^2}{v_m^T y_m^*} - \frac{(X^T H_m y_m^*)^2}{y_m^{*T} H_m y_m^*} \quad (31)$$

Define

$$a_1 = H_m^{\frac{1}{2}} X \text{ and } a_2 = H_m^{\frac{1}{2}} y_m^*$$

where

$$H_m = H_m^{\frac{1}{2}} H_m^{\frac{1}{2}}$$

Using the definitions of a_1 and a_2 , we obtain

$$X^T H_{m+1} X = X^T H_m^{\frac{1}{2}} H_m^{\frac{1}{2}} X = a_1^T a_1$$

$$X^T H_{m+1} y_m^* = X^T H_m^{\frac{1}{2}} H_m^{\frac{1}{2}} y_m^* = a_1^T a_2$$

and

$$y_m^{*T} H_{m+1} y_m^* = y_m^{*T} H_m^{\frac{1}{2}} H_m^{\frac{1}{2}} y_m^* = a_2^T a_2$$

hence,

$$X^T H_{m+1} X = a_1^T a_1 + \frac{\delta_1 (v_m^T X)^2}{v_m^T y_m^*} - \frac{(a_1^T a_2)^2}{a_2^T a_2}$$

or

$$X^T H_{m+1} X = \frac{\|a_1\|^2 \|a_2\|^2 - \langle a_1, a_2 \rangle^2}{\|a_2\|^2} + \frac{\delta_1 (v_m^T X)^2}{v_m^T y_m^*} \quad (32)$$

We also have

$$\begin{aligned} v_m^T y_m^* &= v_m^T (y_m + \mu_m v_m) = v_m^T y_m + \mu_m \|v_m\|^2 = v_m^T (g_{m+1} - g_m) + \mu_m \|v_m\|^2 \\ &= -v_m^T g_m + \mu_m \|v_m\|^2 \end{aligned}$$

Since $v_m^T g_{m+1} = \alpha_m d_m^T g_{m+1} = 0$ by (in the conjugate direction algorithm $d_i^T g_{m+1} = 0$ for all m , $0 \leq m \leq n-1$ and $0 \leq i \leq m$)

Because $v_m = \alpha_m d_m = -\alpha_m H_m g_m$

Then, we have

$$v_m^T y_m^* = \alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2$$

So, equation (32) gives

$$X^T H_{m+1} X = \frac{\|a_1\|^2 \|a_2\|^2 - \langle a_1, a_2 \rangle^2}{\|a_2\|^2} + \frac{(v_m^T X)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2} \quad (33)$$

By Cauchy-Schwarz the first term in the right side of the equation (33) is nonnegative and the second term is nonnegative also, because H_m is positive definite.

To complete the proof, we need to show that at least one of the terms is not equal to zero.

Only when if a_1 and a_2 are proportional does the first term disappear, that is if $a_1 = \beta_1 a_2$ for some scalars β_1 . Therefore, to complete the proof, it is only to prove that if $a_1 = \beta_1 a_2$, then,

$$\frac{(v_m^T X)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2} > 0.$$

observe that

$$H_m^{\frac{1}{2}}X = a_1 = \beta_1 a_2 = \beta_1 H_m^{\frac{1}{2}}y_m^* = H_m^{\frac{1}{2}}(\beta_1 y_m^*)$$

Hence, $X_m = \beta_1 y_m^*$

Here, we obtain

$$\frac{(v_m^T X)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2} = \frac{\beta_1^2 (v_m^T y_m^*)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2}$$

Implies that

$$\frac{(v_m^T X)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2} = \frac{\beta_1^2 (\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2)^2}{\alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2} = \beta_1^2 \alpha_m g_m^T H_m g_m + \mu_m \|v_m\|^2 > 0.$$

Thus, for all for $X_m \neq 0$

$$X^T H_{m+1} X > 0$$

5. Numerical Results of the New PCG1 and New PCG2

Testing the new methods implementation is the focus of this section. We compare New PCG1 with standard PCG(SR1/HS) and New PCG2 with standard PCG(DFP/HS). Tables 1 and 2 of the findings provide specific references to the number of iterations NOI and the number of functions NOF. The results in the two tables below confirm that the New PCG1 and the New PCG2 algorithms are superior to standard PCG methods with respect to NOI and NOF.

Table 1. Comparing the Performance of the Two Algorithms

Standard PCG (SR1 with HS) and New PCG1 (New self-scaling SR1 with HS)

Test Function	N.	Standard PCG (SR1 with /HS)		New PCG1 (New self-scaling SR1 with HS)	
		NOI	NOF	NOI	NOF
Cubic	4	14	42	14	41
	50	15	48	16	49
	100	16	53	16	49
	500	16	67	16	48
	1000	16	54	16	48
	2000	16	50	16	48
	3000	16	50	16	48
Dixon	4	14	31	14	32
	50	420	2119	290	955
	100	444	4447	305	1012
	500	301	2202	221	727
	1000	439	2033	296	1030
	2000	414	1865	333	1348
	3000	425	9277	228	762
G-Central	4	36	253	18	109
	50	43	331	22	140
	100	43	331	25	176
	500	60	496	27	200
	1000	66	554	36	314
	2000	66	554	43	405
	3000	72	616	40	351

Table 1 Continued

Miele	4	34	329	38	346
	50	41	182831	40	580
	100	47	182999	45	414
	500	53	183098	46	33657
	1000	53	183098	47	4274
	2000	59	183164	62	776
	3000	59	183164	40	1515
Non-Diagonal	4	28	75	25	72
	50	49	120	31	87
	100	51	123	31	85
	500	44	108	31	87
	1000	*	*	31	89
	2000	49	118	33	97
	3000	48	116	32	92
Powell	4	30	80	48	329
	50	31	93	27	75
	100	32	95	27	74
	500	33	97	30	87
	1000	33	97	30	88
	2000	33	97	30	90
	3000	33	97	30	87
Rosen	4	30	89	33	91
	50	31	89	33	92
	100	31	89	33	92
	500	36	102	34	95
	1000	36	102	34	94
	2000	34	98	34	94
	3000	37	100	34	94
Shallow	4	8	21	8	21
	50	8	21	8	21
	100	9	24	8	21
	500	9	24	8	21
	1000	9	24	8	21
	2000	9	24	9	24
	3000	9	24	9	24
Sum	4	3	11	3	11
	50	12	76	12	76
	100	14	83	14	83
	500	21	119	21	114
	1000	23	123	22	112
	2000	29	142	29	141
	3000	34	180	32	169
Total		4286	1127254	3224	52518

Table 2. Comparing the Performance of the Two Algorithms

Standard PCG (DFP with HS) and New PCG2 (New self-scaling DFP with HS)

Test Function	N.	Standard PCG (DFP with HS)		New PCG2 (New self-scaling DFP with HS)	
		NOI	NOF	NOI	NOF
Cubic	4	14	40	13	37
	50	17	49	14	39
	100	17	49	14	39
	500	16	46	14	39
	1000	17	49	14	39
	2000	16	47	14	39
	3000	16	46	14	39

Table 2 Continued

Dixon	4	14	31	14	30
	50	455	1809	377	1461
	100	487	1913	410	1586
	500	464	1823	403	1577
	1000	465	1829	421	1632
	2000	499	1971	395	1552
	3000	448	1759	391	1498
Fred	4	8	24	8	23
	50	8	24	8	23
	100	8	24	8	23
	500	8	24	8	23
	1000	8	24	8	23
	2000	8	24	8	23
	3000	8	24	8	23
G-Central	4	34	237	27	198
	50	39	295	33	271
	100	39	295	32	249
	500	49	423	48	411
	1000	54	479	46	364
	2000	59	542	22	145
	3000	65	610	51	489
Miele	4	66	300	76	340
	50	80	374	78	355
	100	86	411	85	398
	500	94	454	37	145
	1000	100	496	50	233
	2000	105	525	75	390
	3000	107	543	73	364
Non-Diagonal	4	27	74	26	68
	50	44	107	31	82
	100	53	128	32	84
	500	49	118	31	82
	1000	49	119	31	85
	2000	48	116	31	82
	3000	48	116	31	82
OSP	4	8	45	8	45
	50	43	198	34	143
	100	56	227	49	189
	500	104	334	98	313
	1000	125	388	135	434
	2000	198	645	190	642
	3000	239	830	225	734
Rosen	4	34	95	30	82
	50	34	94	30	82
	100	34	94	30	82
	500	34	94	30	82
	1000	35	97	30	82
	2000	35	98	31	84
	3000	37	102	31	84
Wolf	4	11	24	8	18
	50	42	85	40	81
	100	44	89	44	89
	500	47	95	47	95
	1000	50	101	49	99
	2000	56	113	54	109
	3000	99	201	71	143
Wood	4	20	50	22	52
	50	23	57	20	49
	100	23	57	22	53
	500	23	57	20	48
	1000	23	57	20	48
	2000	23	57	20	48
	3000	23	57	20	48
Total		5819	22832	4918	18743

6. Conclusions

We proposed two new preconditioned conjugate gradient algorithms, New PCG1 that combines conjugate gradient method Hestenes-Stiefel (HS) with new self-scaling symmetric Rank one (SR1), and New PCG2 that combines conjugate gradient method Hestenes-Stiefel (HS) with new self-scaling Davidon, Fletcher and Powell (DFP) to find the minimum of the nonlinear problems, and new self-scaling SR1 and new self-scaling DFP satisfy the Quasi-Newton condition and the positive definite condition. The numerical tests were conducted on problems with low and high dimensionality, with comparisons made between different test functions. The effectiveness of the New PCG1 algorithm and New PCG2 algorithm is seen in Tables 1 and 2.

Appendix. The Test Functions for Unconstrained Optimization

1. Generalized Central Function:

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

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

2. Generalized Cubic Function:

$$f(x) = \sum_{i=1}^{n/2} (100(x_{2i} - x_{2i-1}^3)^2 + (1 - x_{2i})^2), x_0 = (-1.2, 1, \dots, -1.2, 1)^T.$$

3. Generalized Non-Diagonal Function:

$$f(x) = \sum_{i=2}^n (100(x_1 - x_i^2)^2 + (1 - x_i)^2), x_0 = (-1, \dots, -1)^T.$$

4. Generalized Rosen Brock Banana Function:

$$f(x) = \sum_{i=1}^{n/2} (100(x_{2i} - x_{2i-1}^2)^2 + (1 - x_{2i-1})^2), x_0 = (-1.2, 1, \dots, -1.2, 1)^T.$$

5. Generalized Shallow Function:

$$f(x) = \sum_{i=1}^{n/2} ([x_{2i-1}^2 - x_{2i}]^2 + (1 - x_{2i-1})^2), x_0 = (-2, -2, \dots, -2, -2)^T.$$

6. Miele Function:

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

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

7. Sum of Quadratics (SUM) Function:

$$f(x) = \sum_{i=1}^n (x_i - i)^4, x_0 = (1, 1, \dots, 1)^T.$$

8. Powell Function:

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

9. Oren and Spedicato OSP Function:

$$f(x) = \left(\sum_{i=1}^n i(x_i)^2 \right)^2, x_0 = (1, \dots, 1)^T.$$

10. Wolfe Function:

$$f(x) = \left(-x_1 \left(3 - \frac{x_1}{2} \right) + 2x_2 - 1 \right)^2 + \sum_{i=1}^{n-1} \left(x_{i-1} - x_i \left(3 - \frac{x_i}{2} + 2x_{i+1} - 1 \right) \right)^2 + \left(x_{n-1} - x_n \left(3 - \frac{x_n}{2} \right) - 1 \right)^2, x_0 = (-1, \dots, -1)^T.$$

11. Extended Wood Function:

$$f(x) = \sum_{i=1}^{n/4} (100(x_{4i-3}^2 - x_{4i-2})^2 + (x_{4i-3} - 1)^2 + 90(x_{4i-1}^2 - x_{4i})^2 + (1 - x_{4i-1})^2 + 10.1(x_{4i-2} - 1)^2 + (x_{4i} - 1)^2 + 19.8(x_{4i-2} - 1)(x_{4i} - 1)), x_0 = (-3, -1, \dots, -3, -1)^T.$$

12. Fred Function:

$$f(x) = \sum_{i=1}^{n/2} \left((-13 + x_{2i-1} + ((5 - x_{2i})x_{2i} - 2)x_{2i})^2 + (-29 + x_{2i-1} + ((1 + x_{2i})x_{2i} - 14)x_{2i})^2 \right), x_0 = (30, 3, \dots, 30, 3)^T.$$

13. Generalized Dixon Function:

$$f(x) = \sum_{i=1}^{n-1} (x_i^2 - x_{i+1})^2, x_0 = (-1, \dots, -1)^T.$$

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