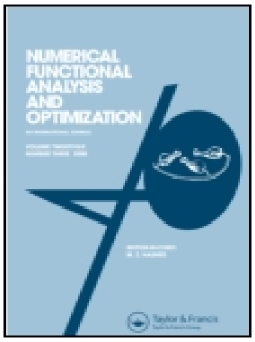

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Applying the Powell's Symmetrical Technique to Conjugate Gradient Methods with the Generalized Conjugacy Condition

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ABSTRACT

This article proposes new conjugate gradient method for unconstrained optimization by applying the Powell symmetrical technique in a defined sense. Using the Wolfe line search conditions, the global convergence property of the method is also obtained based on the spectral analysis of the conjugate gradient iteration matrix and the Zoutendijk condition for steepest descent methods. Preliminary numerical results for a set of 86 unconstrained optimization test problems verify the performance of the algorithm and show that the Generalized Descent Symmetrical Hestenes-Stiefel algorithm is competitive with the Fletcher-Reeves (FR) and Polak-Ribiére-Polyak (PRP^+) algorithms.

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1. Introduction

Nonlinear conjugate gradient methods (NCG) are well-known and practicable methods that minimize the large-scale unconstrained optimization problem:

$$\min_{x\in\mathbb{R}^n} f(x). \tag{1}$$

The classical conjugate gradient methods with line searches are as follows:

$$x_{k+1} = x_k + \alpha_k d_k, \tag{2}$$

where α_k is the step length of a line search and the directions d_k are given by

$$\begin{cases} d_0 = -g_0, \\ d_{k+1} = -g_{k+1} + \beta_k d_k, \quad \forall k > 0, \end{cases} \tag{3}$$

where $g_k = g(x_k) = \bigtriangledown f(x_k)$ and β_k is a scalar. In order to guarantee the global convergence property of the NCG methods, the descent property or the

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sufficient descent property is necessary and important [1], namely,

$$d_{k+1}^T g_{k+1} < 0 \quad \text{(the descent property)} \tag{4}$$

$$d_{k+1}^T g_{k+1} \leq -c_0 ||g_{k+1}||^2, \quad c_0 > 0 \quad \text{(the sufficient descent property).} \tag{5}$$

However, unlike the quasi-Newton methods, in general the NCG methods may not meet the descent or the sufficient descent property for inexact line searches. By applying the symmetrical technique [8] to conjugate gradient methods, a symmetrized conjugate gradient method satisfies the property (5) for any line search. It is introduced here, and this idea can also be applied to other conjugate gradient algorithms.

2. Application of the symmetrical technique to conjugate gradient methods

According to Perry's notation [9], for the HS conjugate gradient method with the CG update parameter β_k [7],

$$\beta_k = \frac{y_k^T g_{k+1}}{d_k^T y_k},$$

the line search direction, d_{k+1}, can be rewritten as follows:

$$d_{k+1} = -D_{k+1} g_{k+1}, \tag{6}$$

with

$$D_{k+1} = \left(I - \frac{d_k y_k^T}{d_k^T y_k} \right) = \left(I - \frac{s_k y_k^T}{s_k^T y_k} \right), \tag{7}$$

where $s_k = x_{k+1} - x_k = \alpha_k d_k$, $y_k = g_{k+1} - g_k$ and the matrix D_{k+1} is called a *conjugate gradient iteration matrix*. For a general NCG method, if its conjugate gradient iteration matrix is a symmetric positive definite, then it immediately satisfies the sufficient descent property (5).

Since D_{k+1} may not be a non-symmetric positive definite matrix, d_{k+1} may not satisfy the descent property (4). To guarantee the descent property, the symmetrical technique [8] is applied to D_{k+1}.

First, the sequence $\{C_k\}$ is introduced as follows:

$$\begin{cases} C_1 = I - \dfrac{dy^T}{d^T y}, \\ C_2 = \dfrac{C_1 + C_1^T}{2} \end{cases} \quad \textit{and} \quad \begin{cases} C_{2k+1} = C_{2k} - \dfrac{dy^T}{d^T y} C_{2k}, \\ C_{2k+2} = \dfrac{C_{2k+1} + C_{2k+1}^T}{2}. \end{cases}$$

Set $E_k = C_{2k}$, $u_k = E_k y$ and $u_0 = E_0 y = Iy$, thus,

$$E_{k+1} = E_k - \frac{1}{2} \frac{du_k^T + u_k d^T}{d^T y}$$

and

$$u_{k+1} = E_k y - \frac{1}{2}\frac{du_k^T y + u_k d^T y}{d^T y} = \left(\frac{dy^T}{d^T y}\right) u_k = Du_k = D^{k+1}u_0,$$

where $D = \frac{1}{2}\left(\frac{dy^T}{d^T y}\right)$. Obviously, the eigenvalues of D are 0 and $\frac{1}{2}$ (n - 1 multiplicity), so

$$\sum_{k=0}^{\infty} u_k = \sum_{k=0}^{\infty} D^k u_0 = (I-D)^{-1}u_0 = 2\left(I - \frac{1}{2}\frac{dy^T}{d^T y}\right)y = 2Iy - \frac{dy^T}{d^T y}y.$$

Thus,

$$\sum_{k=0}^{\infty}(E_{k+1} - E_k) = -\frac{1}{2}\sum_{k=0}^{\infty}\frac{du_k^T + u_k d^T}{d^T y} = -\frac{1}{d^T y}\left(yd^T + dy^T - \frac{yy^T}{d^T y}dd^T\right). \tag{8}$$

So $\lim_{x\to\infty} C_k$ exists, denoted by C. From (8), it follows that:

$$C = \lim_{x\to\infty} C_k = \lim_{x\to\infty} E_k = E_0 + \sum_{k=0}^{\infty}(E_{k+1} - E_k)$$
$$= I - \frac{yd^T + dy^T}{d^T y} + \frac{y^T y}{(d^T y)^2}dd^T = \left(I - \frac{dy^T}{d^T y}\right)\left(I - \frac{yd^T}{d^T y}\right).$$

Thus, the matrix C_1 can be symmetrized by the matrix C. Then, from the above symmetrizing procedure, we conclude that the conjugate gradient iteration matrix D_{k+1} can be symmetrized by $\bar{D}_{k+1}$ as follows:

$$\bar{D}_{k+1} = I - \frac{y_k d_k^T + d_k y_k^T}{d_k^T y_k} + \frac{y_k^T y_k}{(d_k^T y_k)^2}d_k d_k^T = \left(I - \frac{d_k y_k^T}{d_k^T y_k}\right)\left(I - \frac{y_k d_k^T}{d_k^T y_k}\right). \tag{9}$$

Thus, the conjugate gradient directions (3) are rewritten as:

$$\begin{cases} d_0 = -g_0, \\ d_{k+1} = -\bar{D}_{k+1}g_{k+1}, \quad \forall k > 0. \end{cases} \tag{10}$$

So d_{k+1} is called *the symmetrical conjugate gradient direction* and $\bar{D}_{k+1}$ is called *the symmetrical conjugate gradient iteration matrix* or *the symmetrical Hestenes-Stiefel matrix (SHS matrix)*. If the matrix $\bar{D}_{k+1}$ is updated with the rank-1 matrix as follows:

$$\hat{D}_{k+1} = \bar{D}_{k+1} + \frac{s_k \varsigma_k^T}{y_k^T \varsigma_k}, \qquad \forall \varsigma_k \in \mathbb{R}^n,$$

then $\hat{D}_{k+1}$ satisfies the quasi-Newton equation, $\hat{D}_{k+1}y_k = s_k$, and under the exact line searches $d_{k+1} = -\hat{D}_{k+1}g_{k+1}$ satisfies the condition:

$$y_k^T d_{k+1} = 0, \quad \forall k \geq 0 \text{ (conjugacy)}. \tag{11}$$

If $\varsigma_k = s_k$, then

$$d_{k+1}^{mBFGS} = -\left(\bar{D}_{k+1} + \frac{s_k s_k^T}{y_k^T s_k}\right) g_{k+1},$$

which just is the formula of the search direction of the memoryless Broyden-Fletcher-Goldfarb-Shanno (BFGS).

In this article, (11) is substituted by [4]

$$y_k^T d_{k+1} = -\sigma s_k^T g_{k+1}, \tag{12}$$

which is called the Dai and Liao conjugacy condition or *the generalized conjugacy condition*, where σ is a parameter. Now, we suppose that $\bar{D}_{k+1}$ in (10) be updated by a rank one matrix, namely

$$\overline{P}_{k+1} = \bar{D}_{k+1} + uv^T,$$

where u and v two vectors in $\mathbb{R}^n$ such that (12) holds.

Thus, it follows from (9), (12) and $d_{k+1} = -\overline{P}_{k+1} g_{k+1}$ that:

$$\begin{aligned} y_k^T d_{k+1} &= -y_k^T \left(\bar{D}_{k+1} g_{k+1} + uv^T g_{k+1}\right) \\ &= -y_k^T \left(I - \frac{d_k y_k^T}{d_k^T y_k}\right)\left(I - \frac{y_k d_k^T}{d_k^T y_k}\right) g_{k+1} - y_k^T uv^T g_{k+1} \\ &= -\left(y_k^T - y_k^T\right)\left[\left(I - \frac{y_k d_k^T}{d_k^T y_k}\right) g_{k+1}\right] - y_k^T uv^T g_{k+1} \\ &= -y_k^T uv^T g_{k+1} \\ &= -\left(y_k^T u\right) v^T g_{k+1}, \end{aligned}$$

so,

$$-\left(y_k^T u\right) v^T g_{k+1} = -\sigma s_k^T g_{k+1} \Rightarrow \left(\sigma s_k - v y_k^T u\right)^T g_{k+1} = 0.$$

Thus, we can select v such that $v = \frac{\sigma s_k}{y_k^T u}$. Hence

$$\overline{P}_{k+1} = \bar{D}_{k+1} + \sigma \frac{u s_k^T}{y_k^T u}, \tag{13}$$

where the vector u is any vector in $\mathbb{R}^n$ such that $y_k^T u \neq 0$. The matrix $\overline{P}_{k+1}$ is also called *the SHS matrix*. So, we can introduce a new line search direction as follows:

$$\begin{cases} d_0 = -g_0, \\ d_{k+1} = -\overline{P}_{k+1} g_{k+1}, \quad \forall k > 0, \end{cases} \tag{14}$$

where $\overline{P}_{k+1}$ is defined by (13) with $u = u_k$, i.e.,

$$d_{k+1} = -\bar{D}_{k+1} g_{k+1} - \sigma \frac{u_k s_k^T}{y_k^T u_k} g_{k+1}. \tag{15}$$

Thus, with different σ and u_k $\left(y_k^T u_k \neq 0\right)$, a family of methods can be obtained by (2) and (14) with d_{k+1} defined by (15), which is called *the family of Generalized Symmetrical Hestenes-Stiefel gradient method*, or **GSHS** for short. $\overline{P}_{k+1}$ is also called *the iteration matrix of the generalized symmetrical Hestenes-Stiefel gradient method*.

In this article, we take $u_k = y_k$ and $\sigma = c\frac{y_k^T y_k}{s_k^T y_k}$, $c > 0$. Thus

$$\overline{P}_{k+1} = \bar{D}_{k+1} + c\frac{y_k s_k^T}{s_k^T y_k},$$

and,

$$d_{k+1} = -\bar{D}_{k+1} g_{k+1} - c\frac{d_k^T g_{k+1}}{d_k^T y_k} y_k. \tag{16}$$

We denote the iterative scheme (2) and (14) with d_{k+1} calculated by (16) by the **GDSHS**.

3. The sufficient descent property and descent algorithm

In this section, we consider the sufficient descent property of the **GDSHS** method, that is,

$$d_{k+1}^T g_{k+1} \leq -c_0 ||g_{k+1}||^2, \quad c_0 > 0.$$

By Theorem (2.1) in [8], we have that $\bar{D}_{k+1}$ is a positive semi-definite matrix and the eigenvalues of this matrix are 0, 1(n - 2 multiplicity) and λ_{max}^{k+1} , respectively, where λ_{max}^{k+1} is the maximum eigenvalue:

$$\lambda_{max}^{k+1} = \frac{||y_k||^2 ||d_k||^2}{(d_k^T y_k)^2}.$$

By (16), we obtain:

$$d_{k+1}^T g_{k+1} = -g_{k+1}^T \bar{D}_{k+1} g_{k+1} - c\frac{y_k^T g_{k+1}}{d_k^T y_k} d_k^T g_{k+1},$$

since,

$$g_{k+1}^T \bar{D}_{k+1} g_{k+1} \geq 0,$$

so,

$$d_{k+1}^T g_{k+1} \leq -c\frac{y_k^T g_{k+1}}{d_k^T y_k} d_k^T g_{k+1} \frac{d_k^T y_k}{d_k^T y_k} \quad \Rightarrow$$

$$d_{k+1}^T g_{k+1} \leq -c\frac{((g_{k+1}^T y_k) d_k)^T ((d_k^T y_k) g_{k+1})}{(d_k^T y_k)^2}.$$

From the following inequality,

$$u^T v \leq \frac{1}{2}\left(a||u||^2 + \frac{1}{a}||v||^2\right), \quad \forall a > 0,$$

it can be derived that,

$$\begin{aligned} d_{k+1}^T g_{k+1} &\leq -\frac{c}{2(d_k^T y_k)^2}\left(a||(g_{k+1}^T y_k)d_k||^2 + \frac{1}{a}||(d_k^T y_k)g_{k+1}||^2\right) \\ &\leq -\frac{c}{2(d_k^T y_k)^2}\left(a(g_{k+1}^T y_k)^2||d_k||^2 + \frac{1}{a}(d_k^T y_k)^2||g_{k+1}||^2\right) \\ &\leq -\frac{ca||g_{k+1}||^2||y_k||^2||d_k||^2}{2(d_k^T y_k)^2} - \frac{c}{2a}||g_{k+1}||^2. \end{aligned}$$

So,

$$d_{k+1}^T g_{k+1} \leq -\left(ca\frac{||y_k||^2||d_k||^2}{2(d_k^T y_k)^2} + \frac{c}{2a}\right)||g_{k+1}||^2.$$

Thus (5) is true for

$$c_0 = ca\frac{||y_k||^2||d_k||^2}{2(d_k^T y_k)^2} + \frac{c}{2a}.$$

From the above discussion, we have

$$d_{k+1} = -\bar{D}_{k+1} g_{k+1} - c\frac{d_k^T g_{k+1}}{d_k^T y_k} y_k.$$

Thus, the conjugate gradient directions (14) are rewritten as

$$\begin{cases} d_0 = -g_0, \\ d_{k+1} = -\overline{P}_{k+1} g_{k+1} = -v_{k+1} + \beta_k d_k - c\zeta_k y_k, \end{cases} \tag{17}$$

where,

$$\begin{aligned} v_{k+1} &= t_k g_{k+1} + (1 - t_k)g_k = g_{k+1} - (1 - t_k)y_k = g_k + t_k y_k, \\ \beta_k &= \frac{v_{k+1}^T y_k}{d_k^T y_k} = t_k \frac{g_{k+1}^T y_k}{d_k^T y_k} + (1 - t_k)\frac{g_k^T y_k}{d_k^T y_k}, \\ \zeta_k &= \frac{d_k^T g_{k+1}}{d_k^T y_k}, \end{aligned}$$

and,

$$t_k = \frac{-d_k^T g_k}{d_k^T y_k}.$$

Thus, we can obtain *the Generalized Descent Symmetrical Hestenes-Stiefel algorithm*, denoted by **GDSHS**, as follows:

Algorithm 3.1.

Step 1. Give an initial point x_0 and $\varepsilon \geq 0$. Set $k = 0$.

Step 2. Calculate $g_0 = g(x_0)$. If $||g_k|| \leq \varepsilon$, then stop; otherwise let $d_0 = -g_0$ and continue with **Step 3**.

Step 3. Calculate steplength α_k with Wolfe line searches:

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta_1 \alpha_k d_k^T g_k \quad (18)$$

and,

$$d_k^T g(x_k + \alpha_k d_k) \geq \delta_2 d_k^T g_k, \quad (19)$$

where δ_1 and δ_2 are positive constants such that

$$0 < \delta_1 < \delta_2 < 1.$$

Step 4. Set $x_{k+1} = x_k + \alpha_k d_k$.

Step 5. Calculate $g_{k+1} = g(x_{k+1})$.

Step 6. If $||g_{k+1}|| \leq \varepsilon$, then stop.

Step 7. Calculate the direction d_{k+1} via (17). Set $k = k + 1$, then go to **Step 3**

For the numerical demonstration in Section 5, one concrete algorithm is as follows:

GDSHS1: the direction d_{k+1} is computed by (17) and $c = 1$.

4. The convergence of the GDSHS algorithm

In this section, to analyze the convergence of the **GDSHS** algorithm, we first introduce the following assumptions about the objective function $f(x)$.

H1. f is bounded below in $\mathbb{R}^n$ and f is continuously differentiable in a neighborhood $\aleph$ of the level set $\Gamma \stackrel{\text{def}}{=} \{x : f(x) \leq f(x_0)\}$, where x_0 is the starting point of the iteration.

H2. The gradient of f is Lipschitz continuous in $\aleph$, that is, there exists a constant $L > 0$ such that

$$||\nabla f(\bar{x}) - \nabla f(x)|| \leq L||\bar{x} - x||, \quad \forall \bar{x}, x \in \aleph.$$

Next, we introduce the spectral condition theorem of the global convergence for an objective function satisfying **H1** and **H2**, which generates Theorem 4.1 in [8].

Theorem 4.1. *Assume that the line search direction of a NCG method satisfies*

$$\begin{cases} d_0 = -g_0, \\ d_k = -\overline{P}_k g_k, \quad \forall k > 0. \end{cases} \tag{20}$$

Let the objective function $f(x)$ satisfy **H1** *and* **H2**. *For a NCG method ((2) and (20)), which satisfies the sufficient descent condition (5), if its line search satisfies the Wolfe conditions (18) and (19), and [3]*

$$\sum_{k=0}^{\infty} \Lambda_k = +\infty, \qquad (\text{the spectral condition}) \tag{21}$$

where Λ_k is the maximum eigenvalue of $\overline{P}_k^T \overline{P}_k$, then:

$$\lim_{x\to\infty} inf ||g_k|| = 0. \tag{22}$$

Moreover, if $\Lambda_k \leq \tilde{\Lambda}$, where $\tilde{\Lambda}$ is a positive constant, then

$$\lim_{x\to\infty} ||g_k|| = 0. \tag{23}$$

Proof. Assume that

$$g_k \neq 0, \quad \forall k \geq 0$$

and

$$\lim_{x\to\infty} inf ||g_k|| \neq 0,$$

then there exists $\gamma > 0$ such that

$$||g_k|| > \gamma, \quad \forall k \geq 0,$$

and the sufficient descent condition (5) implies that

$$d_k \neq 0, \quad \forall k \geq 0.$$

From (20) and the fact that $\overline{P}_k^T \overline{P}_k$ is symmetric and positive semi-definite, it follows that

$$||d_k||^2 = g_k^T \overline{P}_k^T \overline{P} g_k = ||\overline{P}_k^T \overline{P}|| ||g_k||^2 \leq \Lambda_k ||g_k||^2.$$

Thus, from (5) and the above inequality, it can be deduced that

$$\begin{aligned} \cos^2 \theta_k &= \frac{(-d_k^T g_k)^2}{||d_k||^2 ||g_k||^2} \\ &\geq c_0^2 \frac{||g_k||^2}{||d_k||^2} \\ &\geq \frac{c_0^2}{\Lambda_k}, \end{aligned}$$

where θ_k is the angle between d_k and $-g_k$. Thus,

$$\sum_{k\geq 0} ||g_k||^2 \cos^2\theta_k \geq \gamma^2 \sum_{k\geq 0} \frac{c_0^2}{\Lambda_k} = \infty,$$

which contradicts to the Zoutendijk's condition in [11],

$$\sum_{k\geq 0} ||g_k||^2 \cos^2\theta_k = \sum_{k\geq 0} \frac{(g_k^T d_k)^2}{||d_k||^2} < \infty \quad \text{(the Zoutendijk's condition).} \tag{24}$$

Therefore, (21) implies that either $g_k = 0$ for some $k > 0$, or (22) holds.

If $\Lambda_k \leq \tilde{\Lambda}$ for large enough k, then $\cos^2\theta_k \geq \frac{c_0^2}{\tilde{\Lambda}_k} > 0$, which together with (24), implies (23). □

5. Numerical experiment

In this section, we compare the performance of the new conjugate gradient method GDSHS with the parameter $c = 1$, denoted GDSHS1, to the standard FR method and PRP^+ version of the conjugate gradient method developed by Gilbert and Nocedal [6], where the β_k associated with the Polak-Ribiere-Polyak conjugate gradient method [10] is kept nonnegative. When comparing between the three algorithms we have used the backtracking line search written by M. Al-Baali (SQU, April 2015). The test problems are the 86 unconstrained problems found in this work, and each test function is made as an experiment with the number of variables being 2, 10, 100, 1000, 2000,…, 3500, respectively. The starting points used are those given in An Unconstrained Optimization Test Functions Collection [2].

The termination criterion of all algorithms is that $||g_k|| < 10^{-7}$. The tests are performed on a PC using a Pentium Dual-core CPU T4400@2.20GHz, 2.0GB RAM, Mobil Intel 4 Series Express Chipset Family, using MATLAB codes.

We have adopted the performance profiles of [5] to compare the performance among the tested methods.

Figures 1, 2 and 3 display the performance profiles measured by CPU time (or process time), the number of iterations and the 2-norm of the gradient of the objective function at approximate minimal point, respectively.

In Figure 1, GDSHS1 performed well from the viewpoint of CPU time.

But, the numerical performance should be compared by measures different from CPU time. For this reason we provide Figures 2 and 3.

In Figures 2 and 3, we see that GDSHS1 algorithm is better and more competitive than the FR and PRP^+ algorithms, especially in performance regarding the number of iterations.

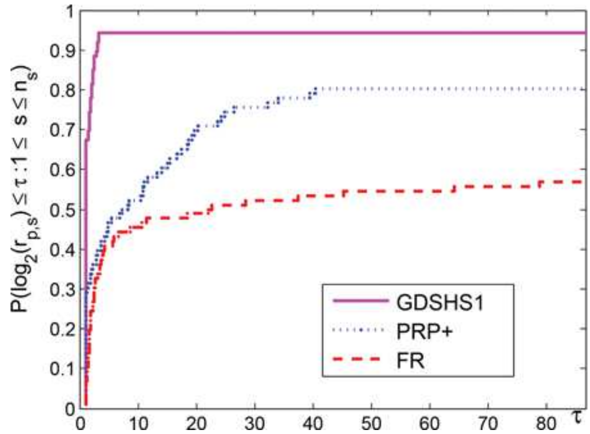

Figure 1. Performance profile by CPU time.

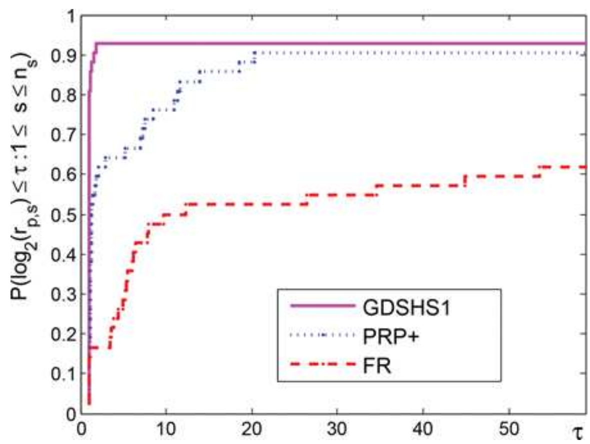

Figure 2. Performance profile by number of iterations.

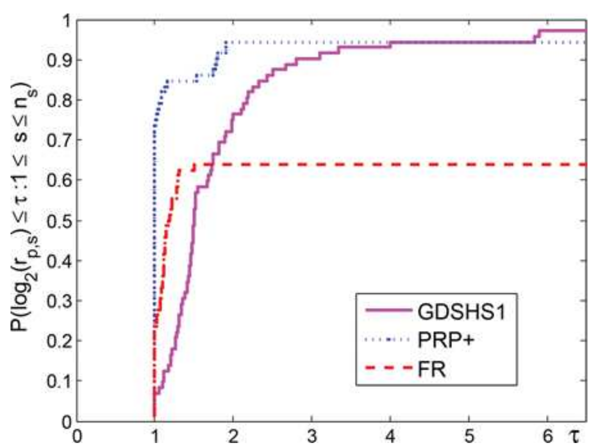

Figure 3. Performance profile by 2-norm of the gradient of the objective function.

6. Concluding remarks

In this article, we have proposed a new conjugate gradient method (Algorithm 3.1) which always produces a descent search direction. In Section 4, we have proved the global convergence property of our method by using the spectral analysis of the conjugate gradient iteration matrix and Zoutendijk's condition. Some numerical results have been reported. These results showed the effectiveness of our method if we choose a good parameter c. As a perspective, we propose an optimal value for it. The theoretical choice for this parameter is currently under study. The performance profile for our conjugate gradient algorithm ((2) and (20)), implemented with our new line search algorithm, was higher than those of the FR and PRP^{+} methods for a test set consisting of 86 problems from [2].

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