Solving Unconstrained Minimization Problems with a New Hybrid Conjugate Gradient Method

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Abstract
Conjugate gradient (CG) method is an efficient method for solving unconstrained, large-scale optimization problems. Hybridization is one of the common approaches in the modification of the CG method. This paper presents a new hybrid CG and compares its efficiency with the classical CG method, which are Hestenes-Stiefel (HS), Nurul Hajar-Mustafa-Rivaie (NHMR), Fletcher-Reeves (FR) and Wei-Yao-Liu (WYL) methods. The proposed a new hybrid CG is evaluated as a convex combination of HS and NHMR method. Their performance is analyzed under the exact line search. The new method satisfies the sufficient descent condition and supports global convergence. The results show that the new hybrid CG has the best efficiency among the classical CG of HS, NHMR, FR, and WYL in terms of the number of iterations (NOI) and the central processing unit (CPU) per time.

Keywords
Conjugate gradient method, exact line search, global convergence, hybrid conjugate gradient, sufficient descent condition.

1. Introduction

Consider the following an unconstrained minimization problem in the form as follows:

$$\min_{x \in \mathbb{R}^n} f(x)$$ (1)
where $\mathbb{R}^n$ denotes an $n$-dimensional Euclidean space. $f : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function. Nonlinear conjugate gradient method is well suited to solving problems (1) of the large scale (Polak, 1997), its iterative formula is given by

$$
\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k, \quad k = 0, 1, 2, \ldots
$$

where $\mathbf{d}_k$ is a direction of $f(\mathbf{x})$ at $\mathbf{x}_k$, $\alpha_k$ is step-size obtained by one-dimensional line search and $\mathbf{g}_k$ is the gradient of the function $f$. Step size $\alpha_k$ is obtained using several forms of line search, i.e., exact or inexact line search, and the form is as follows:

$$
f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) = \min_{\alpha \geq 0} f(\mathbf{x}_k + \alpha \mathbf{d}_k) \quad (3)
$$

and

$$
f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + \delta \alpha \mathbf{g}_k^T \mathbf{d}_k, \quad g(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \mathbf{d}_k \geq \sigma \mathbf{g}_k^T \mathbf{d}_k \quad (4)
$$

with $0 < \delta < \sigma < 1$.

$$
f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + \delta \alpha \mathbf{g}_k^T \mathbf{d}_k, \quad |g(\mathbf{x}_k + \alpha_k \mathbf{d}_k)| \mathbf{d}_k \leq -\sigma \mathbf{g}_k^T \mathbf{d}_k \quad (5)
$$

with $0 < \delta < \sigma < 1$ (Nocedal and Wright, 2006).

Equation (3) in the form of exact line and inequality (4), (5) are forms of inexact line. The step size $\alpha_k$ in this paper uses the exact line (3). The search direction $\mathbf{d}_k$ on this gradient conjugate method uses the following rules:

$$
\mathbf{d}_k = \begin{cases} 
-\mathbf{g}_k, & k = 0 \\
-\mathbf{g}_k + \beta_k \mathbf{d}_{k-1}, & k > 0
\end{cases}
$$

where $\mathbf{g}_k = \nabla f(\mathbf{x}_k)$ is gradient $f$ at $\mathbf{x}_k$, and $\beta_k$ is the scalar parameter. There are many formulas that have been proposed to compute the $\beta_k$. Among them, several well-known formulas as follows

$$
\beta_k^{HS} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{d}_{k-1} \|^2}, \quad \beta_k^{FR} = \frac{\| \mathbf{g}_k \|^2}{\| \mathbf{g}_{k-1} \|^2}, \quad \beta_k^{PRP} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{g}_{k-1} \|^2}, \quad \beta_k^{DY} = \frac{\| \mathbf{g}_k \|^2}{\| \mathbf{d}_{k-1} \|^2},
$$

$$
\beta_k^{LS} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{d}_{k-1} \|^2}, \quad \beta_k^{CD} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{d}_{k-1} \|^2}, \quad \beta_k^{HNS} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{d}_{k-1} \|^2}, \quad \beta_k^{HNS} = \frac{\mathbf{g}_k^T (\mathbf{g}_k - \mathbf{g}_{k-1})}{\| \mathbf{d}_{k-1} \|^2},
$$

$$
\beta_k^{WYL} = \max \left\{ 0, \frac{\| \mathbf{g}_k \|^2 - \| \mathbf{g}_{k-1} \|^2}{\| \mathbf{d}_{k-1} \|^2} \right\}, \quad \beta_k^{SMR} = \max \left\{ 0, \frac{\| \mathbf{g}_k \|^2 - \| \mathbf{g}_{k-1} \|^2}{\| \mathbf{d}_{k-1} \|^2} \right\}, \quad \beta_k^{PMP} = \max \left\{ 0, \frac{\| \mathbf{g}_k \|^2 - \| \mathbf{g}_{k-1} \|^2}{\| \mathbf{d}_{k-1} \|^2} \right\},
$$

where $\| \cdot \|$ denotes the Euclidean norm of vector. The above methods are known as Hestenes-Stiefel (HS) (Hestenes and Stiefel, 1952), Fletcher-Reeves (FR) (Fletcher and Reeves, 1964), Polak-Ribiere-Polyak (PRP) (Polak and Ribiere, 1969), Conjugate Descent (CD) (Fletcher, 1987), Liu-Storey (LS) (Liu and Storey, 1991), and Dai-Yuan (DY) (Dai and Yuan, 1999).

Furthermore, some modifications of previous methods have been introduced such as WYL (Wei-Yao-Liu) (Wei et al., 2006), RMI (Rivaie-Mustafa-Ismail-Leong) (Rivaie et al., 2012), NHMR (Nurul Hajar-Mustafa-Rivaie) (Hajar et al., 2015), SMR (Sharafina-Mustafa-Rivaie) (Mohamed et al., 2019), SMAR (Sulaiman-Mustafa-Abdelrhaman-Rivaie) (Mohammed et al., 2015), and SM (Sulaiman-Mustafa) (Ibrahim and Mamat, 2018).
\[
\beta^S_k = \frac{g_k^T (g_k - g_{k-1} d_{k-1} - d_{k-1})}{d_{k-1}^T d_{k-1}}
\]

Conjugate gradient method can be classified into six different groups; classical, hybrid, scaled, modified, and accelerated according to the formula for \( \beta_k \) (Andrei, 2007). Methods mentioned above are called classical CG due to their simple approaches. The first hybrid conjugate algorithm was given by Touati-Ahmed and Storey (Touati and Storey, 1990); the method is a combination of different conjugate gradient algorithms. Recently, some of hybrid conjugate gradient methods

\[
\beta^HUS_k = \max\{0, \min\{\beta^P_k, \beta^F_k\}\}, \beta^HY_k = \max\{0, \min\{\beta^H_k, \beta^D_k\}\}, \beta^HLSCD_k = \max\{0, \min\{\beta^L_k, \beta^C_k\}\}, \beta^KK_k = \max\{\min\{c \beta^P_k, \beta^F_k\}, \min\{\beta^F_k, \beta^P_k\}\}, \beta^HSMR_k = \max\{0, \min\{\beta^S_k, \beta^RMIL_k\}\}, \beta^ISM_k = \max\{0, \min\{\beta^{SAR}_k, \beta^{SM}_k\}\}, \beta^{ISM1}_k = \max\{\beta^{SAR}_k, \min\{\beta^{SMAR}_k, \beta^{SM}_k\}\}. 
\]

HHUS is a combination of PRP and FR (Touati and Storey, 1990), HDY is a modification from Dain and Yuan (Dain and Yuan, 2001) combining its algorithm with Hestenes and Steifel, HLSCD is the combination of LS and CD (Zhou et al., 2011), KK is the combination PRP, FR, and PRP (Adeleke and Osinuga, 2018), HSMR is the combination SMR and RMIL (Mohamed et al., 2019), ISM is the combination SMAR and SM (Sulaiman et al., 2019), and ISM1 is the combination SMAR, SMARZ and SM (Sulaiman et al., 2019). Other references about the new conjugate gradient coefficient that can be seen in Malik et al., 2020. Based on the idea of these hybrid forms, in this paper, we propose a new Hybrid CG method, then proves the sufficient descent condition, the validity of global convergence, and compare the performance of classical with the new Hybrid CG method.

The structure of this paper is arranged as follows. The new Hybrid CG is proposed in Section 2. In Section 3, we presented the sufficient-descent condition and global convergence analysis of the new hybrid CG method. Numerical results and performance profile corresponding to the new hybrid conjugate gradient are reported in Section 4. The conclusion is presented in Section 5.

2. A New Hybrid CG Method

In this paper, we introduce a new hybrid choice for parameter \( \beta_k \), i.e., a combination of HS and NHMR as follows:

\[
\beta^{HSNHMR}_k = \max\{0, \min\{\beta^H_k, \beta^{NHMR}_k\}\}. 
\]

The new algorithm of \( \beta^{HSNHMR}_k \) is given as in Algorithm 1 as follows:

**Step 1.** Initialization. Given \( x_0 \in \mathbb{R}^n \), and stopping criteria \( \epsilon \). Set \( d_0 = -g_0 \), \( k := 0 \).

**Step 2.** If \( \|g_k\| \leq \epsilon \), then stop; otherwise, go to the next step.

**Step 3.** Compute step length \( \alpha_k \) by the exact line search (3).

**Step 4.** Let \( x_{k+1} = x_k + \alpha_k d_k \). If \( \|g_{k+1}\| \leq \epsilon \), then stop.

**Step 5.** Calculate the search direction \( d_k \) by (6).

**Step 6.** Set \( k := k + 1 \), and go to **Step 3**.

3. Convergence Analysis

In this section, the new hybrid conjugate method is proven to meet the global convergence properties and hold sufficient descent condition.

3.1 Sufficient Descent Condition

To prove sufficient descent condition of \( \beta^{HSNHMR}_k \), we need this definition:
Sufficient descent condition holds when
\[ g_k^T d_k \leq -C \| g_k \|^2, \quad \text{for } k \geq 0 \quad \text{and} \quad C > 0. \]  
\( (8) \)

**Theorem 1.** Consider a Hybrid CG with search direction \( d_k \) in (6), \( \beta_k^{HSHNMR} \) gave as equation (10), then, the condition (11) will hold for all \( k \geq 0 \) (\( d_k \) is descent direction).

**Proof.** Let \( \beta_k^{HSHNMR} = \beta^* \). If \( k = 0 \), then \( d_0 = -g_0 \), so \( g_0^T d_0 = g_0^T (-g_0) = -\left( \sqrt{g_0^T g_0} \right)^2 = -\|g_0\|^2 < 0 \).

Hence, condition (8) holds true for \( k = 0 \). Next, we will show that for \( k > 0 \), condition (8) will hold true.

Multiply (6) by \( g_k^T \), then
\[ g_k^T d_k = -\|g_k\|^2 + \beta^* g_k^T d_{k-1}. \]

For exact line search, \( g_k^T d_{k-1} = 0 \). Thus,
\[ g_k^T d_k = -\|g_k\|^2 < 0. \]

Hence, condition (8) holds true for \( k > 0 \). So, it has been proven that for every \( k \geq 0 \), search direction \( d_k \) is descent direction. The proof is complete. \( \square \)

#### 3.2 Global Convergence Properties

In the analysis of global convergence properties, the following assumption is needed.

**Assumption 1.**

(i) The level set \( \Omega = \{ x \in \mathbb{R}^n : f(x) \leq f(x_0) \} \) is bounded, where \( x_0 \) is a given starting point.

(ii) In an open convex set \( \Omega_0 \) that contains \( \Omega \), \( f \) is continuous and differentiable, and its gradient is Lipschitz continuous; that is, for any \( x, y \in \Omega_0 \), there exists a constant \( M > 0 \) such that
\[ \|g(x) - g(y)\| \leq M \|x - y\|. \]

One of the most important lemmas used to illustrate the global convergence properties is the following lemma (Zoutendijk, 1970).

**Lemma 1.** Suppose that Assumptions 1 hold, let \( x_k \) be generated by Algorithm 1, where \( d_k \) is a descent search direction, and \( \alpha_k \) is obtained by (3), then the following condition, known as the Zoutendijk condition, holds
\[ \sum_{k=0}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty. \]

Now, we can prove the following global convergence theorem for the new hybrid CG method.

**Theorem 2.** Suppose Assumption 1 hold, \( \{x_k\} \) generated by Algorithm 1, where the step size \( \alpha_k \) is determined by the exact line (3), then:
\[ \lim_{k \to \infty} \inf \|g_k\| = 0. \]  
\( (9) \)

**Proof:** Proof by contradiction. Suppose (12) is not correct, then there is a constant \( \epsilon > 0 \) such that
\[ \|g_k\| \geq \epsilon , \quad \text{for every } k \geq 0. \]  
\( (10) \)

Rewriting (6),
\[ d_{k+1} = -g_{k+1} + \beta_k^{\ast} d_k \Rightarrow d_{k+1} + g_{k+1} = \beta_k^{\ast} d_k \]
and squaring both sides, we get
\[ \|d_{k+1} + g_{k+1}\|^2 = \|\beta_{k+1}^* d_k\|^2 \]
\[ \Leftrightarrow \|d_{k+1}\|^2 + \|g_{k+1}\|^2 + 2g_{k+1}^T d_{k+1} = (\beta_{k+1}^*)^2 \|d_k\|^2 \]
\[ \Leftrightarrow \|d_{k+1}\|^2 = (\beta_{k+1}^*)^2 \|d_k\|^2 - 2g_{k+1}^T d_{k+1} - \|g_{k+1}\|^2. \]

Using \((g_{k+1}^T d_{k+1})^2\) and dividing both sides, we obtain

\[ \frac{\|d_{k+1}\|^2}{(g_{k+1}^T d_{k+1})^2} = \frac{(\beta_{k+1}^*)^2 \|d_k\|^2}{(g_{k+1}^T d_{k+1})^2} - \frac{2}{(g_{k+1}^T d_{k+1})^2} \|g_{k+1}\|^2 \leq \frac{1}{\|g_{k+1}\|^2} + \frac{1}{\|g_{k+1}\|^2} \frac{1}{\|g_{k+1}\|^2} + \frac{1}{\|g_{k+1}\|^2}. \]

Note that there are two cases of value \(\beta_{k}^*\).

**Case 1.** If \(\beta_{k}\) < 0, then \(\beta_{k}^* = 0\). While \(\beta_{k}^* = 0\), we get \(d_k = -g_k\), so \(g_k^T d_k = g_k^T (-g_k) = -\|g_k\|^2 < 0\). This statement is true.

**Case 2.** If \(\beta_{k}\) \geq 0, then \(\beta_{k}^* \neq 0\) and can either be \(\beta_{k}\) or \(\beta_{k}^H\).

We choose \(\beta_{k}^* = \beta_{k}\). It is known that (Hajar et al., 2016)

\[ \beta_{k}^NMR \leq \frac{\|g_k\|^2}{\|g_{k-1}\|^2} \]

So, the inequality above is

\[ \frac{\|d_{k+1}\|^2}{(g_{k+1}^T d_{k+1})^2} \leq \frac{\|g_{k+1}\|^4 \|d_k\|^2}{\|g_k\|^4 (g_{k+1}^T d_{k+1})^2} + \frac{1}{\|g_{k+1}\|^2} \leq \frac{\|g_{k+1}\|^4 \|d_k\|^2}{\|g_k\|^4 \|g_{k+1}\|^4} + \frac{1}{\|g_{k+1}\|^2} \leq \frac{\|d_k\|^2}{\|g_k\|^2} + \frac{1}{\|g_{k+1}\|^2}. \]

We rewrite the inequality above as

\[ \frac{\|d_k\|^2}{\|g_k\|^2} \leq \frac{\|d_{k-1}\|^2}{\|g_{k-1}\|^2} + \frac{1}{\|g_k\|^2}. \]  \(\text{(11)}\)

From (11), for \(k = 0\), \(d_0 = -g_0\), we get

\[ g_k^T d_0 = -g_k^T g_0 = -\|g_0\|^2. \]

For \(k = 1\),

\[ \frac{\|d_1\|^2}{\|g_1\|^2} \leq \frac{\|d_0\|^2}{\|g_0\|^2} + \frac{1}{\|g_1\|^2} \leq \frac{1}{\|g_0\|^2} + \frac{1}{\|g_1\|^2} = \sum_{k=0}^1 \frac{1}{\|g_k\|^2}. \]

For \(k = 2\),

\[ \frac{\|d_2\|^2}{\|g_2\|^2} \leq \frac{\|d_1\|^2}{\|g_1\|^2} + \frac{1}{\|g_2\|^2} \leq \frac{1}{\|g_0\|^2} + \frac{1}{\|g_1\|^2} + \frac{1}{\|g_2\|^2} = \sum_{k=0}^2 \frac{1}{\|g_k\|^2}. \]

\[ : \]

For \(k = n\),

\[ \frac{\|d_n\|^2}{\|g_n\|^2} \leq \frac{\|d_{n-1}\|^2}{\|g_{n-1}\|^2} + \frac{1}{\|g_n\|^2} \leq \frac{1}{\|g_0\|^2} + \frac{1}{\|g_1\|^2} + \frac{1}{\|g_2\|^2} + \cdots + \frac{1}{\|g_{n-1}\|^2} = \sum_{k=0}^n \frac{1}{\|g_k\|^2}. \]
So that,
\[
\frac{\|d_n\|^2}{\|g_n\|^4} \leq \sum_{k=0}^{n} \frac{1}{\|g_k\|^2}.
\]  
(12)

From (10), we obtain
\[
\|g_k\| \geq \epsilon \iff \frac{\|g_k\|^2}{\epsilon} \geq \frac{1}{\|g_k\|^2} \leq \frac{1}{\epsilon^2},
\]
therefore, the right side of (12) is
\[
\sum_{k=0}^{n} \frac{1}{\|g_k\|^2} \leq \frac{n+1}{\epsilon^2}.
\]
So, we have
\[
\sum_{k=0}^{n} \frac{\|g_k\|^4}{\|d_k\|^2} \geq \sum_{k=0}^{n} \frac{\epsilon^2}{\|g_k\|^2},
\]
and further, we get
\[
\sum_{k=0}^{\infty} \frac{\left(\frac{\|g_k\|^2}{\|d_k\|^2}\right)^2}{\|d_k\|^2} \geq \epsilon^2 \sum_{k=0}^{\infty} \frac{1}{k+1}.
\]  
(13)

From (13), it can be concluded that
\[
\sum_{k=0}^{\infty} \frac{\left(\frac{\|g_k\|^2}{\|d_k\|^2}\right)^2}{\|d_k\|^2} \geq \epsilon^2 \sum_{k=0}^{\infty} \frac{1}{k+1} + \infty,
\]
this statement is a contradiction with Zoutendijk condition in Lemma 1. Therefore, the proof is completed.

4. Numerical Experiments

In this section, a numerical result comparison will be made between the hybrid HSNHMR with HS, NHMR, FR, and WYL of classical conjugate gradient methods. A comparison of these methods will be carried out using some non-constrained non-linear functions in the paper (Hajar et al., 2017; Andrei, 2008). The function used is an artificial function. Artificial functions are used to see algorithmic behavior in different situations. These include the length of the narrow valleys, unimodal functions, and functions with a large number of significant local optimal (Andrei, 2008). There are ten nonlinear functions to be tested in this paper, as listed in Table 1. We are choosing the random of the initial point to test the performance profile of our method.

<table>
<thead>
<tr>
<th>Test Function</th>
<th>Dimension</th>
<th>Initial Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extended White &amp; Holst function</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(3, …, 3), (5, …, 5), (7, …, 7), (9, …, 9)</td>
</tr>
<tr>
<td>Extended Rosenbrock</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(13, …, 13), (25, …, 25), (30, …, 30), (50, …, 50)</td>
</tr>
<tr>
<td>Extended Himmelblau</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(10, …, 10), (50, …, 50), (100, …, 100), (200, …, 200)</td>
</tr>
<tr>
<td>Extended Tridiagonal 1</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(10, …, 10), (12, …, 12), (20, …, 20), (30, …, 30)</td>
</tr>
<tr>
<td>Generalized Quartic</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(10, …, 10), (50, …, 50), (100, …, 100), (200, …, 200)</td>
</tr>
<tr>
<td>Diagonal 4</td>
<td>2, 4, 10, 100, 500, 1000</td>
<td>(10, …, 10), (50, …, 50), (100, …, 100), (200, …, 200)</td>
</tr>
<tr>
<td>Three-hump Camel</td>
<td>2</td>
<td>(1, -1), (-1, 1), (2, -2), (-2, 2)</td>
</tr>
<tr>
<td>Six-hump Camel</td>
<td>2</td>
<td>(8, 8), (-8, -8), (10, 10), (-10, -10)</td>
</tr>
<tr>
<td>Trecanni</td>
<td>2</td>
<td>(5, 5), (10, 10), (20, 20), (50, 50)</td>
</tr>
<tr>
<td>Booth</td>
<td>2</td>
<td>(10, 10), (25, 25), (50, 50), (100, 100)</td>
</tr>
</tbody>
</table>

Evaluation of the tests was based on the MATLAB subroutine system on Intel Core i7, 2 GHz evaluated on the number of iterations, and CPU times. The stopping criterion is set to \(\|g_k\| \leq 10^{-6}\), where \(\epsilon = 10^{-6}\). The numerical results are combined using the profile results described in Dolan and More (Dolan and More, 2002). The profile results are illustrated in Figures 1 and 2. Figures 1 and 2, respectively, are the results of the iteration and running time profiles. The results in Figures 1 and 2 are obtained in the following way:
\[ r_{p,s} = \frac{a_{p,s}}{\min \{a_{p,s}: s \in S\}} \]

where \( r_{p,s} \) is performance ratio, \( a_{p,s} \) is the number of iterations or CPU time, \( P \) is to set test, and \( S \) is set of solvers on the test set \( P \). Overall profile results can be obtained in the following ways:

\[ \rho_s(\tau) = \frac{1}{n_p} \text{size} \{ p \in P : r_{p,s} \leq \tau \} \]

with \( \rho_s(\tau) \) is the probability for solver \( s \in S \) that a performance ratio \( r_{p,s} \) is within a factor \( \tau \in \mathbb{R} \) of the best possible ratio, and \( n_p \) is the number of functions. The function \( \rho_s(\tau) \) is the distribution function for the performance ratio. The value of \( \rho_s(1) \) is the probability that solver will win over the rest of solvers.

Figure 1. Performance Profile Based on Number of Iterations

Figure 2. Performance Profile Based on the CPU Time
The corresponding profiles are plotted in Figures 1 and 2, where the HSNHMR at the top curve and based on the numerical result shows that the HS only reaches 85%, the FR 98.75%, the WYL 94.375%, and NHMR, HSNHMR 100%. Therefore, it is also concluded that HSNHMR is the best method compared with the other methods.

5. Conclusion

The hybrid gradient conjugate method is an iterative method, and this method can be used to search for optimization problems without constraints in large-scale cases. This paper proposes a new hybrid gradient conjugate method, the hybrid HSNHMR method. The proposed new method fulfills global convergence property by using the exact line search and holds the sufficient descent condition. The numerical results show that this new method is more efficient than the HS, NHMR, FR, and WYL methods.

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References


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