Parallel Implementation of a Generalized Conjugate Gradient Algorithm

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Abstract. This paper presents a parallel version of a Generalized Conjugate Gradient algorithm proposed by Liu and Story in which the search direction considers the effect of the inexact line search. We describe the implementation of this algorithm on a parallel architecture and analyze the related speedup ratios. Numerical results are given for a shared memory computer (Cray C92).

Key words: parallel algorithms, unconstrained high-dimensional optimization, conjugate gradient methods, parallelism, shared memory computer.

1. Introduction

Conjugate gradient methods have been used successfully for the solution of unconstrained high-dimensional minimization problems. When exact line searches are used, conjugate gradient methods give finite termination for quadratic problems. Since the exact line search can cause excessive computational effort, conjugate gradient algorithms are generally used with an inexact line search, Fletcher and Reeves (1964), Polak and Ribière (1969), Shanno (1985), Touati–Ahmed and Storey (1990).

Liu and Storey (1991) proposed a new conjugate gradient algorithm in which the search direction considers the effect of the inexact line search. They proved that the method is globally convergent when the function to be minimized is twice continuously differentiable with a bounded level set.

In this paper we describe parallel versions of two conjugate gradient algorithms, LSA and LSH, proposed by Liu and Story. Whereas algorithm LSH is based on the computation of the Hessian matrix at each iteration, algorithm LSA uses some form of finite difference approximation in order to avoid the computation and the storage of the Hessian matrix. Numerical results for an implementation on a shared memory computer (Cray C92) are given. Then, we evaluate the advantages of parallel versions by computing the related speedup ratios.
2. Generalized Conjugate Gradient

We are concerned with unconstrained minimization problem

\[
\min_{x \in \mathbb{R}^n} f(x)
\]

for a twice continuously differentiable function \( f \) with a bounded level set.

Several algorithms for solving \((P)\) use the concept of conjugacy. The classical conjugate gradient algorithms aim is to solve \((P)\) by a sequence of line searches

\[
x_{k+1} = x_k + t_k d_k, \quad k = 1, 2, \ldots,
\]

where \( t_k \) is the step length and \( d_k \), the search direction, is of the form

\[
d_k = -g_k + \beta_k d_{k-1},
\]

with \( g_k = \nabla f(x_k) \). There are various formulas for computing the coefficient \( \beta_k \); see, e.g., Fletcher and Reeves (1964), Polak and Ribiére (1969) or Gilbert and Nocedal (1992).

Liu and Storey (1991) proposed a new conjugate gradient algorithm in which the search direction \( d_k \) takes into account the effect of the inexact line search. The search direction of the conjugate gradient algorithm of Liu and Storey is of the form

\[
d_k = -\alpha_k g_k + \beta_k d_{k-1}, \quad \alpha_k > 0.
\]

Coefficients \( \alpha_k \) and \( \beta_k \) are given by

\[
\alpha_k = \left[ v_k (g_k^T g_k) - w_k (g_k^T d_{k-1}) \right] / D_k, \quad (1)
\]

\[
\beta_k = \left[ w_k (g_k^T g_k) - u_k (g_k^T d_{k-1}) \right] / D_k, \quad (2)
\]

\[
D_k = u_k v_k - (w_k)^2, \quad (3)
\]

where

\[
u_k = g_k^T H_k g_k, \quad v_k = d_{k-1}^T H_k d_{k-1}, \quad w_k = g_k^T H_k d_{k-1}. \quad (4)
\]

The formal description of the conjugate gradient algorithm LSH of Liu and Storey (1991) which uses the computation of the Hessian matrix is as follows.

**Algorithm LSH**

**Step 1.** \( k \gets 0, \quad d_0 = \nabla f(x_0). \)

**Step 2.** Line search

Compute the steplength \( t_k \) and set \( x_{k+1} = x_k + t_k d_k, \quad k \gets k + 1. \)
Step 3. If \( \|g_k\| < \varepsilon \) then STOP.

Step 4. Compute \( u_k, v_k \) and \( w_k \) with (4).

Step 5. If \( u_k > 0, v_k > 0, 1 - w_k^2/(u_kv_k) \geq 1/(4R) \) and
\[
(u_k/\|g_k\|^2)/(v_k/\|d_{k-1}\|^2) \leq R, \ R > 0,
\]
then Compute \( \alpha_k, \beta_k \) with (1)–(3).
\[
d_k = -\alpha_k g_k + \beta_k d_{k-1}. \quad \text{Go to Step 2}
\]
else \( x_0 \leftarrow x_k \). Go to Step 1.

In order to avoid the computation of matrices, Liu and Storey (1991) proposed computing \( u_k, v_k \) and \( w_k \) in Step 4 of algorithm LSH using finite–difference approximation. We call this version algorithm LSA. It is only different from LSH in Step 4 which is changed as follows.

\[
\begin{align*}
    u_k &= g_k^T (\nabla f(x_k + \gamma_k g_k) - g_k)/\gamma_k, \quad (5) \\
    v_k &= d_{k-1}^T (\nabla f(x_k + \delta_k d_{k-1}) - g_k)/\delta_k, \quad (6) \\
    w_k &= g_k^T (\nabla f(x_k + \delta_k d_{k-1}) - g_k)/\delta_k, \quad (7)
\end{align*}
\]

where \( \delta_k \) and \( \gamma_k \) are suitable small positive numbers. This requires the storage of 5 vectors of length \( n \).

Let \( \phi \) be the real–valued function given by

\[
\phi(t) = f(x_k + td_k), \quad t > 0.
\]

Then the first order derivative of \( \phi \) is given by

\[
\phi'(t) = \nabla f(x_k + td_k)^T d_k.
\]

The conjugate gradient algorithm of Liu and Storey converges under the line search conditions

\[
\begin{align*}
    \phi(t_k) - \phi(0) &\leq \sigma_1 t_k \nabla f(x_k)^T d_k, \quad 0 < \sigma_1 < 1/2, \quad (8) \\
    \left| \phi'(t_k) \right| &\leq -\sigma_2 \nabla f(x_k)^T d_k, \quad 0 < \sigma_1 < \sigma_2 < 1. \quad (9)
\end{align*}
\]

The step length \( t_k \) is determined by a line search algorithm. The formal description of a line search algorithm is as follows, Lemarechal (1981).

1. Initialization: \( t_l \leftarrow 0, t_r \leftarrow +\infty \).
   Choose \( t > 0 \).

2. Compute \( \phi(t) \) and \( \phi'(t) \)
   \[
   \begin{align*}
   \text{If } \phi(t) - \phi(0) &\leq \sigma_1 t \phi'(0) \text{ then} \\
   \text{If } \left| \phi'(t) \right| &\leq -\sigma_2 \phi'(0) \text{ then } t_k \leftarrow t, \text{ STOP.} \\
   \text{Else } \quad t \text{ is too small, } t_l \leftarrow t.
   \end{align*}
   \]
Compute a new $t$ by interpolation over $(t_l, 10t_l)$.

Else $t$ is too large, $t_r \leftarrow t$.

Compute a new $t$ by interpolation over $(t_l, t_r)$.

3. Go to 2.

3. Parallel Implementations

Many studies have been devoted to the construction of unconstrained optimization algorithms for minimizing differentiable nonlinear functions on computers with parallel processors. The main idea in these algorithms is to evaluate simultaneously the function and its gradient at different points. This strategy is well suited for a SIMD (single instruction-multiple data stream) multiprocessor. In the well known Newton or quasi-Newton algorithms, the search direction $d_k$ at the $k$th iteration is constructed through the following relation

$$d_k = -H_k \cdot g_k,$$

where $H_k$ is computed using

(i) parallel finite-difference approximation in the case of Newton algorithms Lootsma and Ragsdell (1988), Conforti and Musmanno (1993);


In both cases, matrix $H_k$ must be stored. Consequently, the use of these methods is limited to middle-size problems, due to storage requirements. In this section, we propose parallel versions of Liu and Storey algorithms LSH and LSA.

3.1. Algorithm PLSH

The parallelization of algorithm LSH is based on the parallel finite-difference approximation of Hessian $H_k$ in order to compute $u_k$, $v_k$ and $w_k$ defined in (4), without storage of matrices. In algorithm LSH, we need matrix $H_k$ only for the computation of $u_k$, $v_k$ and $w_k$ through the calculation of some vector $y_k$ in the form

$$y_k = H_k \cdot b_k,$$

where $b_k$ is $g_k$ or $d_{k-1}$. The best opportunity for parallelism of algorithm LSH is the evaluation of components of matrix $H_k$ in parallel, and then the computation of components of vector $H_k b_k$ in parallel too. The number of available processors, denoted by $p$, is limited. So a suitable decomposition of the algorithm into tasks must be done. The algorithm LSH can be viewed as composed of $p$ tasks $T_1, ..., T_p$. Each task $T_i$ corresponds to the processing of about $n/p$ rows, denoted by $\text{Rows}(T_i)$. To each processor $\pi_l$, we assign a task $T_l$. In order to avoid the computation of $H_k$ two times, $H_k \cdot g_k$ and $H_k \cdot d_{k-1}$ are
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done simultaneously. Note that for balancing the processing load between processors, if a processor treats a row \( i \), it also treats row \( n - i \) since generally \( n \gg p \). In addition, with the scheme described below, we do not need the storage of the Hessian matrix for the computation of the symmetric part.

The component \( H_k[i, j] \) is computed by using the following central finite–difference formulas. If \( i \neq j \), then

\[
H_k[i, j] = \left( f(x_k + \delta_i e^i + \delta_j e^j) - f(x_k + \delta_i e^i) - f(x_k + \delta_j e^j) \right) / (\delta_i \delta_j),
\]

and,

\[
H_k[i, i] = \left( f(x_k + \delta_i e^i) - 2f(x_k) + f(x_k - \delta_i e^i) \right) / \delta_i^2,
\]

where \( e^i \) is the \( i \)th unit vector and \( \delta_i \) a suitable, small positive number.

Since the different tasks could update concurrently vector \( y_k \), each processor \( \pi_l \) stocks the part of \( y_k \) it computes in a local vector \( y_k^l \). At the end, the different local vectors are summed to obtain \( y_k = H_k \cdot b_k \).

**Task T_l**: For each row \( i \) of matrix \( H_k \) in Rows(\( T_l \)) do

For each \( j \) in \( 1, \ldots, i - 1 \) do

Let \( h \) be the component \( H_k[i, j] \) computed as in (10)

\[
y_k^l[j] = y_k^l[j] + h \cdot b_k[i]
\]

\[
y_k^l[i] = y_k^l[i] + h \cdot b_k[j]
\]

Let \( h \) be the component \( H_k[i, i] \) computed as in (11)

\[
y_k^l[i] = y_k^l[i] + h \cdot b_k[i]
\]

### 3.2. Algorithm PLSA

For LSA, we propose a parallel version which is similar to PLSH. The central problem is the computation of some inner products

\[
s = x^T y
\]

at each iteration \( k \) to obtain \( u_k \), \( v_k \) or \( w_k \). An inner product \( s \) can be decomposed as follows

\[
s = \sum_{l=0}^{p-1} s_l,
\]

where

\[
s_l = \sum_{i=1}^{(l+1)\frac{p}{2}} x[i] \cdot y[i].
\]
So, each processor \( p_i \) computes a partial inner product \( s_l \). At the completion of the computation of these different \( s_l \), \( l \in 0, \ldots, p-1 \), they are summed to obtain \( s \). The instantiation of vector \( y \) during the computation of \( u_k, v_k \) or \( w_k \) suppose the computation of some gradient \( \nabla f(x) \) which we determine by using the central finite-difference approximation:
\[
\nabla f(x)[i] = \frac{f(x + \delta_i e_i) - f(x - \delta_i e_i))}{2\delta_i}.
\]

### 3.3. Parallel Line Search

For the line search algorithm, only the computation of \( \phi'(t) \), in Step 2, is parallelized. The interpolation routine used for computing the step length \( t_k \) reduces to one scalar operation. The parallelization of the computation of \( \phi'(t) \) is the same as the one used in §3.2 for computing \( u_k, v_k \) and \( w_k \) given by (5)–(7).

### 4. Experimental Results

Computational experiments have been carried out on a shared memory parallel computer Cray C90. The test problems are given in the appendix.

The number of variables varies according to the following values: 128, 256, 800, 1000.

We have used the line search algorithm given by Gilbert and Lemaréchal (1989), with the initial step length taken to be

\[
t_0 = 2 \min \{1, \frac{(f(x_k) - \bar{f})}{g_k^T d_k}\},
\]

where \( \bar{f} \) is the estimate of the optimal function value. For all test problems, we set \( \bar{f} = 0 \). The line search parameters, in (8)–(9), are \( \sigma_1 = 0.0001 \) and \( \sigma_2 = 0.1 \). In all cases, the stopping condition is

\[
\| g_k \| < 10^{-5} \max \{1, \| x_k \| \}.
\]

The global convergence is ensured by setting \( R = 10^{10} \).

In order to compare the performances of the two versions PLSH and PLSA, we use the speedup \( \Gamma_p \) defined as \( \Gamma_p = C_1/C_p \) where \( p \) is the number of processors and \( C_i \) the execution time required on \( i \) processors. For both algorithms PLSH and PLSA, we present in Table 1 the number of iterations \( NI \), the number of restarts \( NR \) and central processor unit CPU with 16 processors.

Numerical experiments of parallel algorithms are satisfactory from the convergence point of view. Both algorithms PLSH and PLSA always find a minimum. As can be seen from Table 1, in terms of CPU time PLSA is very good compared with PLSH even for cases where number of iterations in PLSA is greater than number of iterations in PLSH (problems 5, 8–10). The given approximations in (5), (6) and (7) are suitable to all test problems.
Due to round-off errors on finite differences approximation, the CPU time for an iteration for a dimension $n$ can be lower than the one required for a dimension $\tilde{n} > n$.

Generally the CPU time is an increasing function of the dimension $n$. However for certain problems, this is not the case as in problems 1 and 7 (for PLSH algorithm). This due to round-off errors introduced by the finite difference approximation of the Hessian matrix. Note that this is never the case for PLSA algorithm (among the 10 test problems).

In Figures 1 and 2, we present the average speedup for PLSH and PLSA related to test problems. The behavior of algorithms PLSH and PLSA is the same for all test problems. The speedup increases in terms of the processors number and vector length. It is noticeable that when the dimension $n$ is small, it is useless to consider many processors. For example, problems with dimension $n = 128$ reach the maximal speedup with $p = 8$ in PLSH as in PLSA. This is was expected since task $T_i$ has been constructed such that it sequentially treats $2 \times 7 = 14$ rows in order to reduce the number of memory locks. Although, problems in which the dimension $n$ is sufficiently large, the behavior of the speedup is almost linear in terms of the processor number.
Fig. 1. Average speedup in terms of $n$ for algorithm PLSA.

Fig. 2. Average speedup in terms of $n$ for algorithm PLSH.
5. Conclusion

Liu and Storey have proposed a new Conjugate Gradient algorithm in which the search direction considers the effect of inexact line search. We have proposed a parallel version which is based on the parallel finite–difference approximation of some gradient and Hessian matrix without storage. Computational experiments have been carried out on a shared memory parallel computer Cray C92. We have noticed that problems in which the dimension is sufficiently large, the behavior of the speedup is almost linear in numerical experiments have also shown that PLSA algorithm is less sensitive to round-off errors that PSLH algorithm.

Appendix: Test Problems

Problem 1: Extended Beale function

\[ f(x) = \sum_{i=1}^{n/2} \left[ (1.5 - x_{2i-1} (1 - x_{2i}^2))^2 + (2.25 - x_{2i-1} (1 - x_{2i}^2))^2 
+ (2.625 - x_{2i-1} (1 - x_{2i}^3))^2 \right], \quad n = 2, 4, 6, \ldots \]

with \( x^0 = (1, 1, \ldots, 1)^T \).

Problem 2: Brown function.

\[ f(x) = \left( \sum_{i=1}^{n/2} (x_{2i-1} - 3) \right)^2 + 0.0001 \sum_{i=1}^{n/2} (x_{2i-1} - 3)^2 - (x_{2i-1} - x_{2i}) 
+ \exp(20(x_{2i-1} - x_{2i})) \right), \quad n = 2, 4, 6, \ldots \]

with \( x^0 = (0, -1, 0, -1, \ldots, 0, -1)^T \).

Problem 3: Cragg and Levy function

\[ f(x) = \sum_{i \in J} \left[ (e^{x_i} - x_{i+1})^4 + 100(x_{i+1} - x_{i+2})^6 + \tan^4(x_{i+2} - x_{i+3}) 
+ x_i^8 + (x_{i+3} - 1)^2 \right], \]

where \( n \) is a multiple of 4 and \( J = \{1, 5, 9, \ldots, n - 3\} \), \( x^0 = (1, 2, 2, \ldots, 2) \).

Problem 4: Generalized tridiagonal function

\[ f(x) = 1 + \sum_{i=1}^{n} \left| (3 - 2x_i)x_i - x_{i-1} - x_{i+1} + 1 \right|^{7/3}, \]
with \( x_0 = x_{n+1} = 0 \) and \( x^0 = (-1, -1, \ldots, -1) \).

**Problem 5:** Penalty 1 function

\[
f(x) = 10^{-5} \sum_{i=1}^{n} (x_i - 1)^2 + \left( \sum_{i=1}^{n} x_i^2 - 0.25 \right)^2, \quad n = 1, 2, \ldots
\]

with \( x^0_i = i, \quad i = 1, 2, \ldots, n \).

**Problem 6:** Penalty 2 function

\[
f(x) = \sum_{i=1}^{n} (x_i - 1)^2 + 10^{-3} \left( \sum_{i=1}^{n} x_i^2 - 0.25 \right)^2, \quad n = 1, 2, \ldots
\]

with \( x^0_i = i, \quad i = 1, 2, \ldots, n \).

**Problem 7:** Extended Powell function

\[
f(x) = \sum_{i=1}^{n/4} \left[ (x_{4i-3} + 10x_{4i-2})^2 + 5(x_{4i-1} - x_{4i})^2 \\
+ (x_{4i-2} - 2x_{4i-1})^4 + 10(x_{4i-3} - x_{4i})^4 \right], \quad n = 4, 8, \ldots
\]

with \( x^0 = (3, -1, 0, 3, 3, -1, 0, 3, \ldots, 3, -1, 0, 3)^T \).

**Problem 8:** Extended Rosenbrock function

\[
f(x) = \sum_{i=1}^{n/2} \left[ 100(x_{2i} - x_{2i-1}^2)^2 + (1 - x_{2i-1})^2 \right], \quad n = 2, 4, 6, \ldots
\]

with

\[
\begin{align*}
x^0_{2i} & = 1.0 \\
x^0_{2i-1} & = -1.2 + 0.4i/n \quad i = 1, 2, \ldots, n/2.
\end{align*}
\]

**Problem 9:** Tridiagonal function

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

with \( x^0 = (1, 1, \ldots, 1)^T \).
Problem 10: Extended Wood function

\[ f(x) = \sum_{i=1}^{n/4} \left[ 100(x_{4i-2} - x_{4i-3})^2 + (1 - x_{4i-3})^2 + 90(x_{4i} - x_{4i-1})^2 ight. \\
+ \left. (1 - x_{4i-1})^2 + 10(x_{4i-2} + x_{4i} - 2)^2 + 0.1(x_{4i-2} - x_{4i})^2 \right], \quad n = 4, 8, \ldots \]

with \( x^0 = (-3\;\!\!\!\!\!\!\; -1\;\!\!\!\!\!\!\; -3\;\!\!\!\!\!\!\; -1\;\!\!\!\!\!\!\; \ldots \;\!\!\!\!\!\!\; -3\;\!\!\!\!\!\!\; -1)^T \).

References


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Lygiagreti apibendrinto jungtinių gradientų algoritmo realizacija

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