TECHNICAL NOTE

A Generalized Conjugate Gradient Algorithm

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Abstract. We present modifications of the generalized conjugate gradient algorithm of Liu and Storey for unconstrained optimization problems (Ref. 1), extending its applicability to situations where the search directions are not defined. The use of new search directions is proposed and one additional condition is imposed on the inexact line search. The convergence of the resulting algorithm can be established under standard conditions for a twice continuously differentiable function with a bounded level set. Algorithms based on these modifications have been tested on a number of problems, showing considerable improvements. Comparisons with the BFGS and other quasi-Newton methods are also given.

Key Words. Nonlinear programming, unconstrained optimization, conjugate gradient methods, inexact line searches.

1. Introduction

One of the leading approaches for solving the unconstrained optimization problem \( \min_{x \in \mathbb{R}^n} f(x) \) is the use of conjugate gradient (c.g.) methods. These techniques aim to solve the problem by a sequence of line searches,

\[ x_{k+1} = x_k + \lambda_k d_k, \]

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along directions
\[ d_k = -g_k + \beta_k d_{k-1}, \]
where \( g_k = \nabla f(x_k) \),
and only need vector storage. There are many formulas for \( \beta_k \) [see, for instance, Fletcher (Ref. 2)] which are equivalent for quadratic functions and give descent directions if the line searches are exact. When \( f \) is twice continuously differentiable with a bounded level set, Powell (Ref. 3) has shown that the Fletcher-Reeves method with exact line searches achieves the limit
\[ \lim_{k \to \infty} \inf \| g_k \| = 0 \]  
(1)
and that other c.g. methods are not globally convergent unless one additional condition is imposed. Furthermore, Al-Baali (Ref. 4) extends the convergence of the Fletcher-Reeves method for an inexact line search when \( \lambda_k \) satisfies the condition
\[ |\nabla f(x_k + 1)^T d_k| \leq -\sigma g_k^T d_k, \]  
(2)
suggested by Fletcher (Ref. 2), and the Goldstein requirement (Ref. 5)
\[ f(x_k + 1) \leq f(x_k) + \lambda_k \rho g_k^T d_k, \]  
(3)
where \( d_k \) is a descent direction at the current point \( x_k \) and \( 0 < \rho < \sigma < 1/2 \).

It is accepted that using an inexact line search to evaluate the steplength \( \lambda_k \) can save computational effort. In order to take into account the effects of inexact line searches, Refs. 1 and 6 propose modifications that generalize several formulas of c.g. methods. Liu and Storey (Ref. 1) modify the search directions in the following way:
\[ d_k = -bg_k + md_{k-1}, \]  
(4)
where the values of \( b \) and \( m \) are suitably chosen. They prove convergence under technical restrictions on \( f \); in comparison with other c.g. methods, the Liu and Storey (LS) method needs fewer iterations to converge (Ref. 7). In our opinion, the key to its good performance is that the combined analysis of the parameters \( b \) and \( m \) results in a more flexible and efficient definition of the search directions. Thus, we have extended the applicability of (4) to more general situations, without losing those advantages.

2. Modifications of the Search Direction

Let us assume that \( f \) is twice continuously differentiable and has a bounded level set. The LS method chooses \( b \neq 0 \) and \( m \neq 0 \) so that the search