An Efficient Line Search for Nonlinear Least Squares

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Abstract. The line search subproblem in unconstrained optimization is concerned with finding an acceptable steplength which satisfies certain standard conditions. Prototype algorithms are described which guarantee finding such a step in a finite number of operations. This is achieved by first bracketing an interval of acceptable values and then reducing this bracket uniformly by the repeated use of sectioning in a systematic way. Some new theorems about convergence and termination of the line search are presented.

Use of these algorithms to solve the line search subproblem in methods for nonlinear least squares is considered. We show that substantial gains in efficiency can be made by making polynomial interpolations to the individual residual functions rather than the overall objective function. We also study modified schemes in which the Jacobian matrix is evaluated as infrequently as possible, and show that further worthwhile savings can be made. Numerical results are presented.

Key Words. Unconstrained optimization, line search, sectioning, nonlinear least squares.

1. Introduction

This paper studies the line search subproblem for descent methods in unconstrained optimization. In general, a local minimizer $x^*$ of a function $f(x), x \in \mathbb{R}^n$ is sought and the gradient vector $g(x) = \nabla f(x)$ is available for any $x$. We examine line search methods in which an iterative sequence \( \{x^{(k)}\}, k = 1, 2, \ldots \), is derived, hopefully converging to $x^*$. On each iteration a search direction $s^{(k)}$ is determined (which depends on the particular

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method in use) and a steplength $\alpha^{(k)}$ is obtained (ideally) by solving the line search subproblem

$$\alpha^{(k)} = \arg \min_{\alpha} f(x^{(k)} + \alpha s^{(k)}).$$

The next iterate is then defined by

$$x^{(k+1)} = x^{(k)} + \alpha^{(k)} s^{(k)}.$$

The iteration is terminated when

$$f^{(k-1)} - f^{(k)} \leq \epsilon,$$

where $\epsilon$ is some user supplied tolerance on $f$ [and $f^{(k)}$ refers to $f(x^{(k)})$]. We shall be interested in descent methods in which the vector $s^{(k)}$ has the property that

$$s^{(k)} g^{(k)} < 0.$$

For convenience, we shall denote

$$f(\alpha) = f(x^{(k)} + \alpha s^{(k)}),$$

to refer to the restriction of $f(x)$ along the line

$$x = x^{(k)} + \alpha s^{(k)},$$

and it follows from the chain rule that the slope is given by

$$f'(\alpha) = s^{(k)T} g(x^{(k)} + \alpha s^{(k)}).$$

Thus, (4) is equivalent to $f'(0) < 0$, showing that $f$ is decreasing at $\alpha = 0$, and we can expect a local solution of (1) for some $\alpha^{(k)} > 0$. In fact, (1) is a nonlinear problem and cannot generally be solved in a finite number of iterations. Thus, we seek an approximate solution which satisfies certain conditions. Since it is not efficient to look for high accuracy when $x^{(k+1)}$ is remote from $x^*$, these conditions are chosen so as to be readily satisfied. The actual conditions to be used are inter-related with the requirement that the descent method is required to converge. A convergence theorem consequent on the work of Goldstein (Ref. 1), Wolfe (Ref. 2), and Powell (Ref. 3) (see Fletcher, Ref. 4) can be stated when $\alpha^{(k)}$ is chosen on each iteration to satisfy both

$$f(\alpha) \leq f(0) + \alpha \rho f'(0)$$

and

$$f'(\alpha) \geq \sigma f''(0),$$

where $\rho \in (0, \frac{1}{2})$ and $\sigma \in (0, 1)$ are preset parameters.