ALGORITHMS FOR FINDING ZEROS AND EXTREMA OF FUNCTIONS WITHOUT CALCULATING DERIVATIVES

BY

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Preface

The problem of finding numerical approximations to the zeros and extrema of functions, using hand computation, has a long history. In the last few years, considerable progress has been made in the development of algorithms suitable for use on a digital computer. The aim of this work is to suggest improvements to some of these algorithms, extend the mathematical theory behind them, and describe some new algorithms for approximating local and global minima. The unifying thread is that all the algorithms considered depend entirely on sequential function evaluations: no evaluations of derivatives are required. Such algorithms are very useful if derivatives are difficult to evaluate, and this is often true in practical problems.

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This work is dedicated to Oscar and Nancy, sine quis non.

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13. ABSTRACT

Theorems are given concerning the order (i.e., rate) of convergence of a successive interpolation process for finding simple zeros of a function or its derivatives, using only function evaluations. Special cases include the successive linear interpolation process for finding zeros, and a parabolic interpolation process for finding turning points. Results on interpolation and finite differences include weakening the hypotheses of a theorem of Ralston on the derivative of the error in Lagrangian interpolation.

The theoretical results are applied to given algorithms for finding zeros or local minima of functions of one variable, in the presence of rounding errors. The algorithms are guaranteed to converge nearly as fast as would bisection or Fibonacci search, and in most practical cases convergence is superlinear, and much faster than for bisection or Fibonacci search.

The problem of finding a global minimum of a function f, of one variable, is investigated. We give a nearly optimal algorithm which is applicable if an upper bound on f'' is known. A generalization, useful in practice if $n \leq 3$, is given for functions of n variables. The effect of rounding errors in these algorithms can be accounted for.

Finally, we present a modification of Powell's algorithm for finding a local minimum of a function of several variables without calculating derivatives. The modification ensures that the search directions can not become linearly dependent, and numerical examples suggest that the algorithm compares favorably with other methods which do not require derivatives.

A bibliography on unconstrained minimization is given, and ALGOL implementations of all the above algorithms are included.

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