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INTERVAL BOUNDS FOR STATIONARY VALUES OF FUNCTIONALS.(U)
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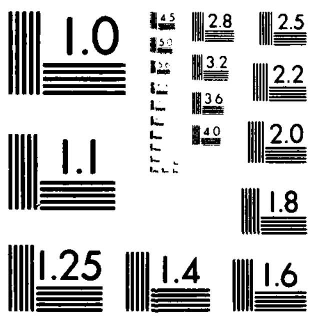

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INTERVAL BOUNDS FOR STATIONARY VALUES OF FUNCTIONALS

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ABSTRACT

A number of important problems in applied mathematics can be reduced to finding stationary values of functionals (maxima, minima, and critical values). For functionals defined in terms of integrals, the method of interval integration provides a way to obtain interval (two-sided) bounds for these stationary values. As a special case of this method, upper and lower bounds for eigenvalues of linear operators can be obtained. The inclusion of stationary values in intervals is based on the use of interval functions which include the function for which the functional is stationary, and its derivatives. A simple way to construct such interval functions is given, and examples are presented of a minimum and an eigenvalue problem. The improvement of initial results by iteration is indicated.

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SIGNIFICANCE AND EXPLANATION

Solutions to many problems in physical mathematics and applied analysis can be found as maxima, minima, or other critical points of certain functionals defined in terms of integrals. Such points are called stationary points of the functional, and include, for example, eigenvalues of linear operators. The solution of these so-called variational problems by scientific computation can be improved, in many cases, by the use of interval integration, which yields two-sided bound (that is, lower and upper bounds, or simply interval bounds) for stationary values. In order to apply this method, one needs a set of interval functions which enclose a function for which the functional is stationary. A way to construct such interval functions, using the boundary conditions and reasonable assumptions on the highest derivatives is given, and the possibility of obtaining improved bounds by iteration is indicated. The use of interval methods has the additional advantage that interval values can be assigned to the boundary conditions, so that problems in which the boundary conditions are not known precisely can be studied, or the response of a system to a range of conditions can be estimated.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

INTERVAL BOUNDS FOR STATIONARY VALUES OF FUNCTIONALS

L. B. Rall

1. Variational problems. A number of important problems in physical mathematics and applied analysis, particularly the calculus of variations and control theory, reduce to finding maxima and minima of functionals

(1.1) $$f = f[y], \quad y \in A,$$

where A is the class of *admissible functions* for the problem. In addition to the *extremal values*

(1.2) $$\underline{f} = \min_{y \in A}\{f[y]\}, \quad \overline{f} = \max_{y \in A}\{f[y]\},$$

of f, one may seek its *critical values*

(1.3) $$f^* = f[y^*],$$

where the *critical point* $y^* \in A$ of f satisfies the *Euler equation*

(1.4) $$f'[y] = 0,$$

it being assumed in this case that the Gâteaux derivative f' of f exists on A [5]. Under this assumption, *extremal points* $\underline{y}, \overline{y} \in \mathrm{int}A$ such that $\underline{f} = f[\underline{y}]$, $\overline{f} = f[\overline{y}]$ will be critical points of f [2]. For simplicity, extremal and critical points and values of a functional will be called its *stationary* points and values, respectively. A *variational problem* for f on A is to find one or more of the pairs $(\underline{f}, \underline{y})$,

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$(\bar{f},\bar{y})$, (f^*,y^*), if such exist.

An *interval bound* for a stationary value f^* of a functional f is simply an interval $[a,b]$ such that $f^* \in [a,b]$, that is,

$$a \le f^* \le b. \tag{1.5}$$

For functionals defined in terms of integrals, such as

$$f[y] = \int_{x_0}^{x_1} f(x,y,y',y'',\ldots,y^{(n)})dx, \quad y \in A, \tag{1.6}$$

it will be shown that the method of interval integration [1], [4], provides a way to obtain interval bounds for stationary values of f. In the variational problem for f defined by (1.6), the class A of admissible functions is usually characterized by continuity, differentiability, and boundary conditions on y.

It should be noted that *one-sided* bounds for extremal values are easy to obtain: For arbitrary $\hat{y} \in A$, one has

$$\underline{f} \le f[\hat{y}] \le \bar{f}. \tag{1.7}$$

Lower bounds for minima and upper bounds for maxima, however, are often not easy to obtain, and in the case of nonextremal stationary values (such as intermediate eigenvalues of a linear operator), one is often completely in the dark. The two-sided bounds (1.5) furnished by interval integration are easy to compute, by contrast, as will be seen below. The methodology will be developed for functionals of the form (1.6) for clarity, and its immediate extension to several independent variables will be presented in the final section.

2. Interval integration. Interval analysis [3] is the branch of mathematics which takes real bounded intervals $[a,b]$ as its basic units, and studies transformations of them. Its relationship to real analysis is somewhat analogous to that of complex analysis, since the reals can be identified with the subset of intervals which have equal endpoints, the so-called *degenerate* intervals $x = [x,x]$ for real x. An *interval function* Y of a real variable x assigns the interval

$[\underline{y}(x), \overline{y}(x)]$ to each x in its interval of definition $X = [x_0, x_1]$. The *interval integral* of Y over X is the interval

$$(2.1) \qquad \int_X Y(x)dx = [(LD)\int_{x_0}^{x_1} \underline{y}(x)dx \ , \ (UD)\int_{x_0}^{x_1} \overline{y}(x)dx],$$

where (LD) and (UD) denote lower and upper Darboux integrals, respectively [1]. Since these Darboux integrals exist for all real functions, it follows that all interval functions are integrable, and hence integration is a universal operation in interval analysis [1].

In the study of interval transformations, the transformation T of X into T(X) is said to be *monotone* if $X \subset Z \Rightarrow T(X) \subset T(Z)$, and a transformation U *includes* T on X if $T(X) \subset U(X)$, in particular, if y is a real function, then the interval function Y includes y on X if

$$(2.2) \qquad y(X) = \{y(x) \mid x \in X\} \subset Y(X)$$

[3]. In this sense, the interval function Y is the set of *all* real functions y such that $\underline{y}(x) \le y(x) \le \overline{y}(x)$ for $x \in X$, and one writes $y \in Y$ in this case. The interval integral (2.1) is a monotone function of its integrand [1], so that

$$(2.3) \qquad \int_{x_0}^{x_1} y(x)dx \subset \int_{x_0}^{x_1} Y(x)dx \quad \text{for} \quad y \in Y,$$

whether or not y has a real (Riemann or Lebesgue) integral. The real interval of a real function, if it exists, is of course contained in its interval integral, which always exists [1], [4]. The calculation of the interval integral of Y is simplified if the *endpoint functions* $\underline{y}, \overline{y}$ of Y are Riemann (R) integrable. Then,

$$(2.4) \qquad \int_X Y(x)dx = [(R)\int_X \underline{y}(x)dx \ , \ (R)\int_X \overline{y}(x)],$$

so that inclusions of interval integrals can be computed for integrands $Z \supset Y$ with Riemann integrable endpoint functions [1].

3. Interval bounds. Considering the integrand of (1.6) to be a fu...ion $f(x,u_0,u_1,\dots,u_n)$ of n + 2 variables, an interval inclusion $F(X,U_0,U_1,\dots,U_n)$ of it can be constructed by interval arithmetic [3] or otherwise. Then, interval integration provides the following result.

Theorem 3.1. Suppose that $\hat{y} \in A$ is a stationary point of the functional f defined by (1.6), $\lambda = f[\hat{y}]$ is the corresponding stationary value of f, and the interval functions $Y_0, Y_1, \dots, Y_n$ on $X = [x_0,x_1]$ are such that $\hat{y}^{(i)} \in Y_i$, $i = 0,1,\dots,n$. Then,

$$\lambda \in [a,b] = \int_{x_0}^{x_1} F(x,Y_0(x),Y_1(x),\dots,Y_n(x))dx. \tag{3.1}$$

This result provides the two-sided bounds (1.5) for λ immediately. It appears, however, that one must assume a lot about $\hat{y}$ and its derivatives to use (3.1). In many cases, one only has to assume something about $\hat{y}^{(n)}$ (for example, that it is bounded), and then the interval functions $Y_{n-1}, \dots, Y_1, Y_0$ can be constructed by use of interval integration and the boundary conditions. For example, suppose that

$$y^{(n)} \in Y_n, \quad y^{(n-1)}(x_0) \in [\alpha_0,\beta_0], \quad y^{(n-1)}(x_1) \in [\alpha_1,\beta_1]. \tag{3.2}$$

Note that *interval* boundary conditions can be prescribed. Thus, interval techniques can be useful in practical problems in which boundary conditions are not known precisely, or in which it is desired to study the behavior of a system over a range of boundary conditions.

Indefinite interval integration of (3.2) gives the functions

$$Y_L(x) = [\alpha_0,\beta_0] + \int_{x_0}^{x} Y_n(t)dt, \quad Y_R(x) = [\alpha_1,\beta_1] + \int_{x_1}^{x} Y_n(t)dt. \tag{3.3}$$

Definition 3.1. The interval function Y_n is said to be *admissible* for the boundary conditions (3.2) if $[\alpha_1,\beta_1] \in Y_L(x_1)$, $[\alpha_0,\beta_0] \in Y_R(x_0)$, and the intersection $Y_L(x) \cap Y_R(x)$ is nonempty for $x \in X$.

Theorem 3.2. If the interval function Y_n is admissible for the boundary conditions (3.2) and $\hat{y}^{(n)} \in Y_n$, then

$$\hat{y}^{(n-1)} \in Y_{n-1} = Y_L \cap Y_R. \tag{3.4}$$

Proof. By construction, the interval function Y_{n-1} defined by (3.4) contains all real functions g such that $g' \in Y_n$, $g(x_0) \in [\alpha_0,\beta_0]$ and $g(x_1) \in [\alpha_1,\beta_1]$, as a consequence of the definition of the indefinite interval integral [1]. QED.

It should be noted that Y_{n-1} constructed in this way also contains other real functions which satisfy the boundary conditions, but may have no continuity or differentiability properties at all. An example of the actual construction of an interval function of this type is given in the next section.

4. <u>The simplest problem of the calculus of variations</u>. This is the case $n = 1$ of (1.6) [2], and to simplify matters further, the boundary conditions

$$y(x_0) = y_0, \quad y(x_1) = y_1 \tag{4.1}$$

will be imposed. The class A of admissible functions will be restricted to those for which y' is *bounded*, that is, $y' \in [\underline{m},\overline{m}]$, where $\underline{m},\overline{m}$ denote constant interval functions with the corresponding real value. Interval integration gives

$$Y_L(x) = y_0 + [\underline{m},\overline{m}](x - x_0), \quad Y_R(x) = y_1 - [\underline{m},\overline{m}](x - x_1), \tag{4.2}$$

and thus $Y_1 = [\underline{m},\overline{m}]$ is admissible for (4.1) if

$$\underline{m} \le m \le \overline{m}, \quad m = \frac{y_1 - y_0}{x_1 - x_0}. \tag{4.3}$$

The graph of the corresponding interval function Y_0 is thus a parallelogram with vertices (x_0,y_0) and (x_1,y_1), bounded above by the intersecting lines

$$\overline{y}_L(x) = y_0 + \overline{m}(x - x_0), \quad \overline{y}_R(x) = y_1 - \underline{m}(x - x_1), \tag{4.4}$$

and below by

(4.5) $$\underline{y}_L(x) = y_0 + \underline{m}(x - x_0), \quad \underline{y}_R(x) = y_1 - \bar{m}(x - x_1).$$

Using this interval function Y_0, one has immediately that

(4.6) $$f[y] \in \int_{x_0}^{x_1} F(x, Y_0(x), [\underline{m}, \bar{m}])\,dx$$

on the class A of functions satisfying (4.1) for which $y' \in [\underline{m}, \bar{m}]$. For example, suppose that

(4.7) $$f[y] = \int_{x_0}^{x_1} \sqrt{1 + (y')^2}\,dx,$$

and one seeks $\lambda = \min f[y]$ on A. Since

(4.8) $$(y')^2 \in [0, \max\{\underline{m}^2, \bar{m}^2\}],$$

which gives

(4.9) $$\lambda \in [x_1 - x_0, d], \quad d = \int_{x_0}^{x_1} \sqrt{1 + m^2}\,dx = \sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2},$$

since each admissible Y_1 contains $y' = m$, and thus each Y_0 contains the degenerate interval (real) function

(4.10) $$y_m(x) = y_0 + m(x - x_0),$$

for which the value $F[y_m] = d$ is attained, so that $\lambda \le d$. The lower bound in (4.9), $\lambda = x_1 - x_0$, can be attained by a step function $s \in Y_0$ if $0 \in Y_1$. In variational problems, additional restrictions are often imposed on the elements of Y_0 (continuity, boundedness of derivatives) to eliminate solutions such as this, and one works with the functions in $Y_0 \cap A$ [2]; in this class, however, two-sided bounds may not be available as they are in interval analysis.

5. Eigenvalue problems. For selfadjoint linear operators A in a Hilbert space H, its *eigenvalues* are critical values of the *Rayleigh quotient*

(5.1) $$R(y) = (Ay, y)/(y, y), \quad y \ne 0.$$

An eigenvalue λ satisfies the Euler equation

$$(5.2) \qquad Ay - \lambda y = 0, \quad y \neq 0,$$

and the corresponding critical points y in a function space H are called *eigenfunctions* of A belonging to λ [2]. If the inner product (,) in H is defined in terms of integrals, then interval integration can be applied as above to find lower and upper bounds for eigenvalues of A. If Y_0, Y_1 are interval functions such that $\hat{y} \in Y_0$, $0 \notin Y_0$, and $A\hat{y} \in Y_1$ for some eigenfunction $\hat{y}$ of A, then

$$(5.3) \qquad \lambda \in (Y_1, Y_0)/(Y_0, Y_0) = [a,b]$$

for the corresponding eigenvalue λ, thus giving an interval bound. Once again, the interval functions Y_0, Y_1 are to be determined in some way, perhaps on the basis of an approximate solution of (5.2). If A is an integral operator, then one may use interval integration to get $Y_1 = AY_0$. On the other hand, if A is a differential operator, it may be possible to obtain Y_0 from Y_1 by use of interval integration and the boundary conditions, as before. For example, suppose that

$$(5.4) \qquad Ay = -y'', \quad y(0) = y(\pi) = 0.$$

Since eigenfunctions are determined by (5.1) and (5.2) only up to a multiplicative constant, it is useful to introduce a normalization condition which excludes y = 0 in particular. In this case, suppose that $-y''(\pi/2) = 1$, and take Y_1 defined by

$$(5.5) \qquad \overline{y}_1(0) = [0,1], \quad \overline{y}_1(x) = 1, \ 0 < x < \pi, \quad \overline{y}(\pi) = [0,1],$$

($\overline{y}_1(x)$ is an interval step function [1]), and

$$(5.6) \qquad \underline{y}_1(x) = (2/\pi)x, \ 0 \le x \le \pi/2, \quad \underline{y}_1 = (2/\pi)(\pi - x), \ \pi/2 \le x \le \pi.$$

By integrating $Y_1(x)$ twice and using the boundary conditions in (5.4), one gets Y_0 defined by

$$(5.7) \qquad \overline{y}_0(x) = \frac{x}{2}(\pi - x), \quad 0 \le x \le \pi,$$

and

$$(5.8)\qquad Y_0(x) = \begin{cases} x\left(\frac{\pi}{4} - \frac{x^2}{3\pi}\right), & 0 \le x \le \pi/2, \\ (\pi - x)\left(\frac{\pi}{4} - \frac{(\pi - x)^2}{3\pi}\right), & \pi/2 \le x \le \pi. \end{cases}$$

Computation with these interval functions gives

$$(5.9)\qquad (Y_1,Y_0) = \frac{\pi^3}{6}\left[\frac{1}{5}, \frac{1}{2}\right], \quad (Y_0,Y_0) = \frac{\pi^5}{120}\left[\frac{17}{42}, 1\right],$$

and thus eigenvalues λ belonging to eigenfunctions $\hat{y} \in Y_0$ will be elements of the *interval Rayleigh quotient* $(Y_1,Y_0)/(Y_0,Y_0)$, that is,

$$(5.10)\qquad \lambda \in \Lambda_0 = \frac{20}{\pi^2}\left[\frac{1}{5}, \frac{21}{17}\right] \subset [0.4052\ , 2.5033].$$

In this case, $\hat{y}(x) = \sin x$ is the only eigenfunction of A contained in Y_0, and (5.10) provides lower and upper bounds for the corresponding eigenvalue $\lambda = 1$.

The endpoint functions (5.5) are crude approximations to $\sin x$, and it can be noted that (5.7) and (5.8) define an interval function which, when normalized, is smaller than Y_1 and bounded by *better approximations to the eigenfunction*. This suggests an iteration process, the next step being to take $(2/\pi)^2 Y_0 = Y_1$ as a new interval function containing $-y''$, which leads to an improved Y_0 and a corresponding value Λ_1 for the interval Rayleigh quotient. Indeed, if $\Lambda_1 \subset \Lambda_0$, then the existence of an eigenvalue $\lambda \in \Lambda_1$ of A is guaranteed by the Schauder fixed point theorem [5].

6. Variational problems in several dimensions. The extension of Theorem 3.1 to problems in several independent variables follows immediately from the corresponding extension of the interval integral. In R^ν, let $x = (\xi_1,\xi_2,\ldots,\xi_\nu)$, and the region of integration be denoted by Ω. Following the prescription given in [1], partition Ω by elements $\Omega_1, \Omega_2,\ldots, \Omega_m$ with measures (areas or volumes) $d\Omega_i$, $i = 1,2,\ldots,m$, and let

$$(6.1)\qquad \nabla Y_i = \left[\inf_{x\in\Omega_i}\{Y(x)\}\ , \sup_{x\in\Omega_i}\{Y(x)\}\right],$$

where Y is an interval-valued function defined on Ω. If $\mathcal{D}_m$ denotes the set of of all partitions of Ω into m subregions, then

(6.2) $$\Sigma_m = \bigcap_{\mathcal{D}_m} \sum_{i=1}^{m} Y_i \cdot d\Omega_i, \quad m = 1,2,3,\ldots,$$

form a nested sequence of closed intervals, and thus the interval integral of Y over Ω,

(6.3) $$\int_\Omega Y(x)\,d\Omega = \bigcap_{m=1}^{\infty} \Sigma_m$$

exists for arbitrary Y. It is not difficult to show that this interval integral is an inclusion monotone function of its integrand, using the same arguments as in [1].

Now, one can let D_i denote the vector of partial differential operators of order i in R^ν, for example, $D_1 = (\partial/\partial\xi_1, \partial/\partial\xi_2, \ldots, \partial/\partial\xi_\nu)$ and consider the functional

(6.4) $$f[y] = \int_\Omega f(x,y,D_1y,D_2y,\ldots,D_ny)\,d\Omega,$$

which is the analogue of (1.6) in R^ν. If F is an interval inclusion of the integrand of (6.4), and $\lambda = f[\hat{y}]$ is a stationary value of f, then interval integration provides the following result.

Theorem 6.1. If $\hat{y}$ is a stationary point of f and interval vector functions $Y_0, Y_1, \ldots, Y_n$ exist such that $D_i\hat{y} \in Y_i$, $i = 0,1,\ldots,n$ on Ω, then

(6.5) $$\lambda = f[\hat{y}] \in \int_\Omega F(x,Y_0(x),Y_1(x),\ldots,Y_n(x))\,d\Omega.$$

As an application of this theorem, suppose that in R^3 the values of y are prescribed on the boundary $\partial\Omega$ of a region Ω, and one wishes interval bounds for

(6.6) $$\lambda = \min \int_\Omega (\partial^2y/\partial\xi^2 + \partial^2y/\partial\eta^2 + \partial^2y/\partial\zeta^2)\,d\Omega$$

over some class A of admissible functions. A construction similar to the one in §3 can be used, or Y_0 can be constructed on the basis of an approximate solution of the Euler equation for (6.6), which in this case is simply the Laplace equation

$$\Delta y = 0, \quad y = y_0 \text{ on } \partial\Omega. \tag{6.7}$$

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A number of important problems in applied mathematics can be reduced to finding stationary values of functionals (maxima, minima, and critical values). For functionals defined in terms of integrals, the method of interval integration provides a way to obtain interval (two-sided) bounds for these stationary values. As a special case of this method, upper and lower bounds for eigenvalues of linear operators can be obtained. The inclusion of stationary values in intervals is based on the use of interval functions which include —

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