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BOUNDING GLOBAL MINIMA WITH INTERVAL ARITHMETIC.(U)

JAN 77 L J MANCINI, G P MCCORMICK

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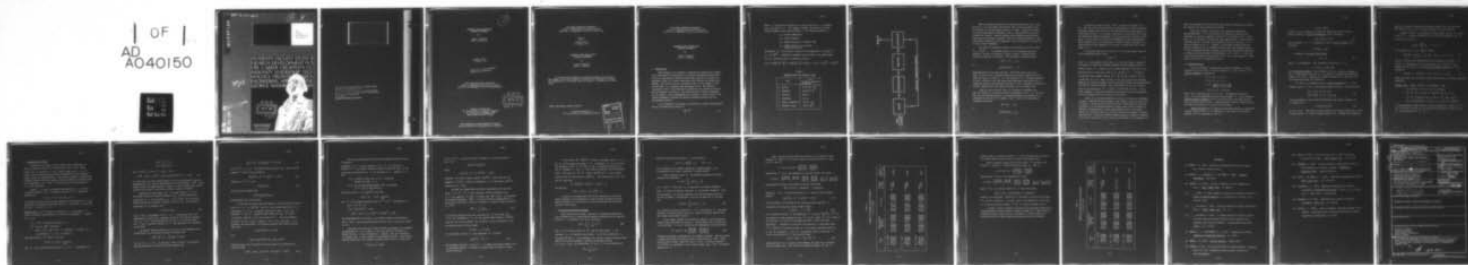
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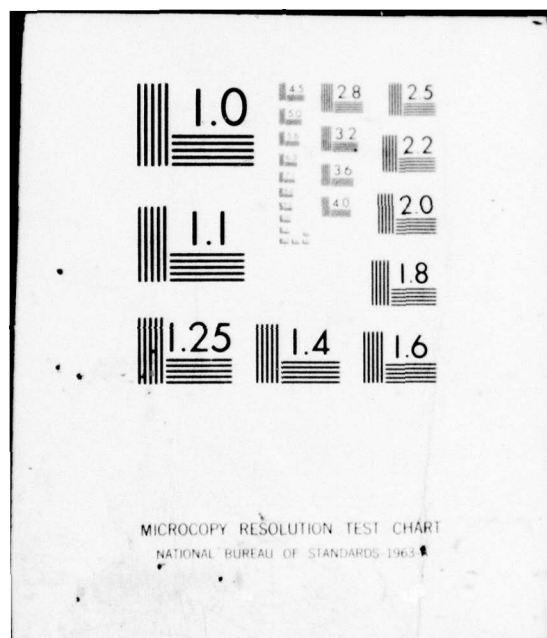
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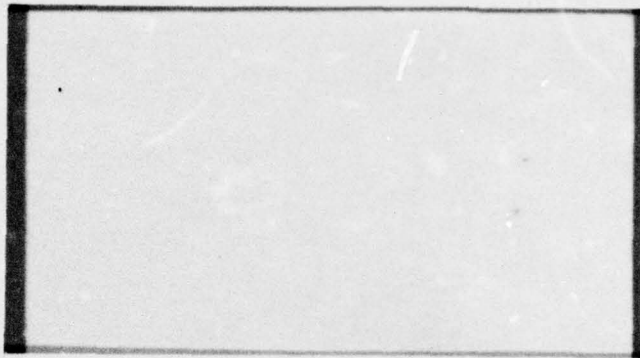


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BOUNDING GLOBAL MINIMA WITH
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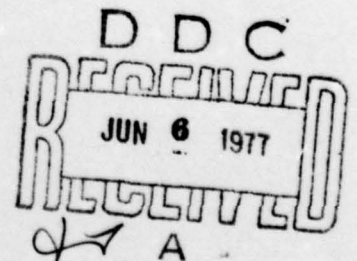
by

Louis J. Mancini
Garth P. McCormick

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31 January 1977

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Abstract
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BOUNDING GLOBAL MINIMA WITH
INTERVAL ARITHMETIC

by

Louis J. Mancini*
Garth P. McCormick

It is shown how techniques of interval arithmetic can be used to give bounds on the global minima of unconstrained optimization problems. The techniques are illustrated using the design of a hypothetical chemical plant.

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BOUNDING GLOBAL MINIMA WITH
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by

Louis J. Mancini
Garth P. McCormick

1. Introduction

Many problems in all branches of engineering, business and economics can be mathematically formulated as a nonlinear programming problem (NLP). A NLP is an optimization problem in which some objective is minimized (or maximized) subject to certain constraints which describe the system being modeled. The objective may be to minimize costs, as the example in this section shows, or to maximize some performance level. The adjective "nonlinear" refers to the fact that the objective and constraint functions may be nonlinear in contrast to the functions used in linear programming. In this respect, linear programming can be viewed as a special case of nonlinear programming; although the solution procedures used in each are considerably different.

If no constraints are present, then the NLP is termed "unconstrained"; and can be symbolically written as

$$\min_x f(x) \quad (1)$$

where f , the objective function, is a scalar function of n variables (i.e., the vector x). For example, consider the design of the hypothetical chemical plant shown in Figure 1. The design variables are

x_1 = reactor temperature

x_2 = reactor pressure

x_3 = weight fraction of a catalyst used

x_4 = weight fraction of the product leaving the reactor.

The product x_4 is an explicit function of the temperature x_1 given as $x_4 = 0.1 x_1^{0.25}$. Summing the component costs in Table 1 and substituting for x_4 yields the cost, or objective, function

$$f(x) = 0.0318 x_1^{1.1} x_2^{0.6} + 11430 x_2^{-1} x_3^{-1} + 228 x_3 + 1.5 x_2 - 25 x_1^{0.25} - 495 x_1^{0.2}.$$

Table 1

COMPONENT COSTS FOR CHEMICAL PLANT

Item	Cost (\$/100 lb. material processed)
1. Reactor	$0.0318 x_1^{1.1} x_2^{0.6}$
2. Separator	$11430 x_2^{-1} x_3^{-1}$
3. Catalyst	$228 x_3$
4. Compressor	$1.5 x_2$
5. Recycle compressor	$250 (1 - x_4)$
6. Byproduct sales	$-3123.2 x_4^{0.8}$

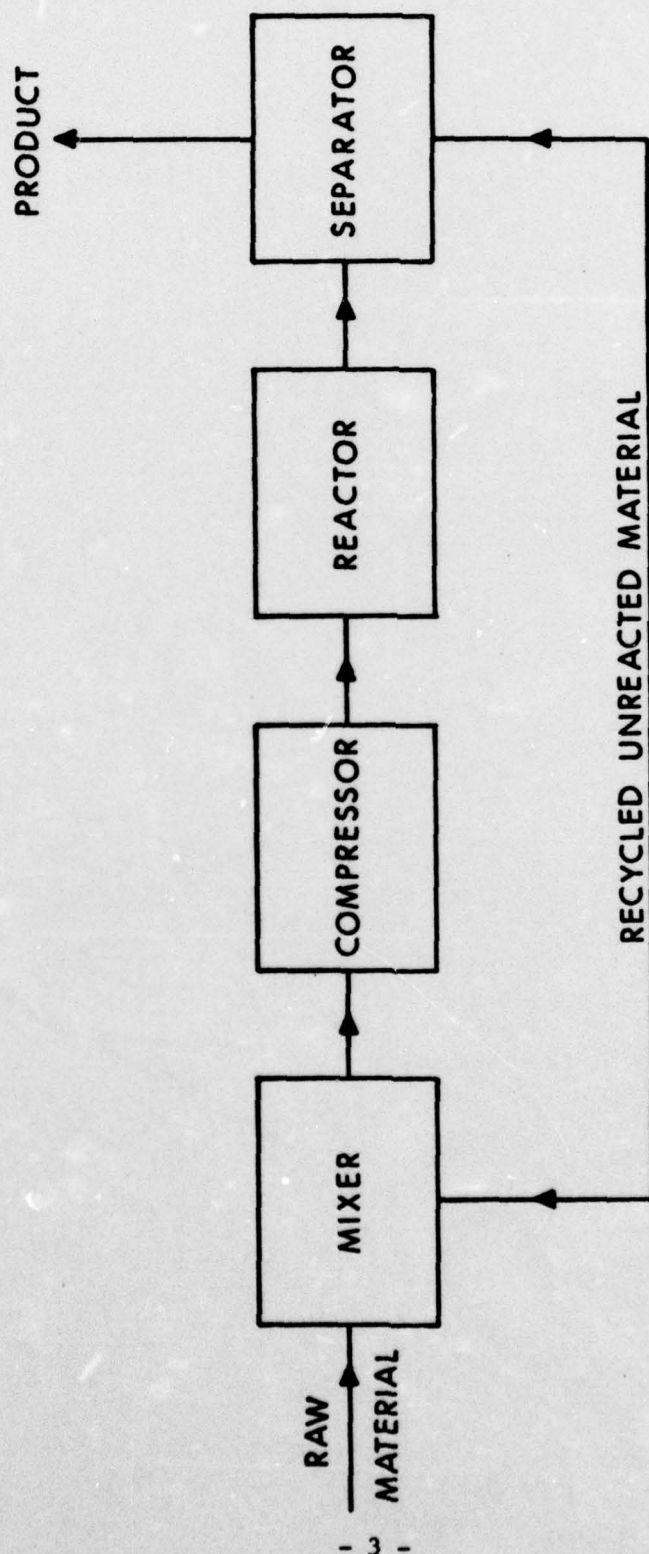


Figure 1

NLPs are usually solved with an algorithm which starts with a given point (i.e., the best guess) and performs some iterative procedure until the solution, or an approximate solution, is found. A difficult problem in any such algorithm is termination, that is, when should the iterative procedure be stopped? Computer programs which implement algorithms must contain some "convergence criterion" which is testable and which if satisfied causes termination of the algorithm. When this happens the algorithm is said to have "converged."

One class of convergence criteria are those which use the iterates $x^0, \dots, x^k, x^{k+1}, \dots$ to determine whether or not convergence has been achieved. The user is required to supply a value ϵ (presumed small) before the algorithm is initiated. The algorithm is terminated when

$$|x^{k+1} - x^k| \leq \epsilon$$

or

$$|f(x^{k+1}) - f(x^k)| \leq \epsilon$$

depending upon the criterion selected. The obvious flaw in the use of these criteria is that closeness between the successive iterates does not imply the iterate is close to x^* , the solution to (1). The main advantage of these criteria is that they prevent bad algorithms (ones which fail to change the iterates very much each iteration or fail to decrease the objective function significantly each time) from using a lot of computer time.

From the user's point of view, it is desired to terminate only when the iterate or its function value is acceptably close to x^* (or $f(x^*)$). That is, from considerations of the physical meaning of the problem it is reasonable to ask the user to supply a value ϵ and for the algorithm to terminate when either

$$|x^k - x^*| \leq \epsilon$$

or

$$|f(x^k) - f(x^*)| \leq \epsilon.$$

In some rare cases the value $f(x^*)$ is known even though x^* is not. Thus the fourth criterion would be implementable in this circumstance. In general though, this is not the case and these natural convergence criteria cannot be used. It is a major contribution of this paper that using the theoretical material developed in [7] with the tools of interval arithmetic [5], that these criteria can be implemented for unconstrained NLPs. Before showing this it is instructive to consider another convergence criterion which has been suggested in an attempt to bypass the lack of knowledge of x^* .

A necessary condition for a vector x^* to be the optimal solution to an unconstrained NLP is that

$$f'(x^*) = 0 \quad (2)$$

where f' is the gradient vector and 0 is the zero vector. Suppose we are solving (1) with some iterative procedure and the algorithm has generated a vector x^k . Based on (2), we could terminate if the norm of the gradient vector is near zero, that is, if $|f'(x^k)| \leq \epsilon$. In terms of the chemical plant example suppose $x^k = (x_1^k, x_2^k, x_3^k) = (698.33, 35.738, 1.1929)$ and $\epsilon = 0.05$. Then $|f'(x^k)| = 3.25$ and we would not terminate. However, now suppose we measure costs in dollars/lb rather than dollars/100 lb (see Table 1), and thus define $c(x) = f(x)/100$ as the new cost function. Then for the same vector x^k , $|c'(x^k)| = |f'(x^k)|/100 = 0.0325$, and we would terminate. Thus this criterion fails since the norm of the gradient vector is dependent upon the scaling of the problem.

There are two further objections to the use of this last convergence criterion. Whereas the user may have a good reason to accept a point which is within ϵ in norm from the solution vector or whose objective function is within ϵ of the optimal objective function value, there is usually no physical interpretation of a point whose gradient norm is less than ϵ . Second, as a practical matter no one ever tries this convergence criterion more than once. Except for simple problems, because of numerical considerations, there seems to be a value above zero below which it is impossible to

reduce the gradient norm even with the most powerful minimization techniques. The computer just keeps running and running.

This paper presents a solution to the termination problem for unconstrained NLPs. In [7] the authors have shown that, under certain conditions, an analytic expression exists for the difference $f(x) - f(x^*)$; where x^* is the global solution over some compact region. This difference represents how far, in terms of the objective function, the vector x is from the optimal vector x^* . However, the necessary conditions and the analytic expression for the difference usually cannot be computed exactly. It will be shown how interval analysis can be used, under certain conditions, to compute an interval bound on the difference $f(x) - f(x^*)$. In the process an interval bound on the solution vector x^* is also generated. These bounds can be used as termination criteria.

2. Interval Analysis

Interval arithmetic [8] generalizes ordinary arithmetic to closed intervals of the real line. Give two intervals $\bar{u} = [a, b]$ and $\bar{w} = [c, d]$, interval arithmetic is defined by

$$\bar{u} + \bar{w} \equiv [a + c, b + d]$$

$$\bar{u} - \bar{w} \equiv [a - d, b - c]$$

$$\bar{u} \cdot \bar{w} \equiv [\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)]$$

$$\bar{u}/\bar{w} \equiv [a, b] \cdot [1/d, 1/c]$$

where $\bar{u}/\bar{w}$ is defined only if $0 \notin [c, d]$. The degenerate interval, $[u, u]$, is not distinguished from the ordinary number u . On the computer, rounded interval arithmetic [6,15] is used in place of the exact version above to bound round off error. Rounded intervals might be slightly larger, but they are guaranteed to contain the exact result.

Interval matrices are rectangular arrays with intervals as components. A square interval matrix $\bar{A}$ is nonsingular if and only if all ordinary matrices $A \in \bar{A}$ are nonsingular, that is,

$$0 \notin \{\det A | A \in \bar{A}\}.$$

Usually it is not possible to compute the right-hand side of the above exactly, however, an interval determinant, $\det \bar{A}$, satisfying

$$\{\det A | A \in \bar{A}\} \subseteq \overline{\det \bar{A}} \quad (3)$$

can be computed. If $\bar{A}$ is nonsingular, then an interval inverse, $(\bar{A})^{-1}$, satisfies

$$\{A^{-1} | A \in \bar{A}\} \subseteq (\bar{A})^{-1}.$$

Consider the interval linear system

$$\bar{A} y = \bar{b} \quad (4)$$

where $\bar{A}$ is nonsingular. The theoretical solution set, Ω , is

$$\Omega = \{y | Ay = b, A \in \bar{A}, b \in \bar{b}\}$$

and an interval solution $\bar{y}$ must satisfy $\bar{b} \subseteq \bar{A} \bar{y}$; and hence contains Ω . The $\bar{y}$ with smallest width [8, p. 7] is desired to minimize the difference between $\bar{A} \bar{y}$ and $\bar{b}$. Hansen [3,4], Hansen and Smith [5,6], and Oettli [10] have developed methods for solving (4).

If $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is continuous, then an interval extension of f , on an interval vector $\bar{x} \subset \mathbb{R}^n$, is an interval-valued function $\bar{f}$ which satisfies

$$\begin{aligned} \bar{f}(x) &= f(x) \quad \text{for all } x \in \bar{x} \\ \bar{f}(u) &\subseteq \bar{f}(w) \quad \text{for all } u \subseteq w \subseteq \bar{x}. \end{aligned} \quad (5)$$

Interval extensions, like interval determinants and interval inverses, are not unique; and

$$\{f(u) | u \in \bar{u}\} \subseteq \bar{f}(\bar{u}) \quad (6)$$

for all $\bar{u} \subseteq \bar{x}$. The "best" interval extension, or united extension [8, p. 18], is that function $\bar{f}$ in which equality holds in (6). Finding good computable

interval extensions, limiting the difference between the left- and right-hand sides of (6), is one of the key problems in interval analysis.

Suppose $h: \mathbb{R}^n \rightarrow \mathbb{R}^n$ is continuously differentiable, and let x^* denote a zero of h . Assume continuous [8, p. 18] interval extensions, $\bar{h}'_{ij}$, of the partial derivatives

$$h'_{ij}(x) = \frac{\partial h_i}{\partial x_j}(x), \quad i, j = 1, \dots, n$$

are available on $\bar{x}$. For $\bar{u}, \bar{w} \subseteq \bar{x}$ define

$$\bar{h}'_{ij}(\bar{u}, \bar{w}) = \bar{h}'_{ij}(\bar{u}_1, \dots, \bar{u}_{j-1}, \bar{w}_j, \dots, \bar{w}_n), \quad i, j = 1, \dots, n \quad (7)$$

and let $\bar{h}'(\bar{u}, \bar{w})$ be the interval matrix with components $\bar{h}'_{ij}(\bar{u}, \bar{w})$. If $\bar{h}'(\bar{x}, \bar{x})$ is nonsingular in the interval sense, then $\bar{h}'(\bar{u}, \bar{w})$ is nonsingular for all $\bar{u}, \bar{w} \subseteq \bar{x}$; and an interval Newton operator, $\bar{N}_1$, can be defined as

$$\bar{N}_1(\bar{w}, \bar{w}) = \bar{w} - \bar{h}'(\bar{w}, \bar{w})^{-1} \cdot h(\bar{w}) \quad \text{for all } \bar{w} \in \bar{w} \subseteq \bar{x}. \quad (8)$$

Nickel has proven that the above interval Newton operator has some interesting properties.

Theorem 1 [9]: Suppose $\bar{h}'(\bar{x}, \bar{x})$ is nonsingular. Then

- (a) Any zero x^* of h in $\bar{x}$ is unique.
- (b) If $x^* \in \bar{x}$, then $x^* \in \bar{N}_1(x, \bar{x})$ for all $x \in \bar{x}$.
- (c) If $\bar{x} \cap \bar{N}_1(x, \bar{x}) = \emptyset$ for any $x \in \bar{x}$, then $x^* \notin \bar{x}$.
- (d) If $\bar{N}_1(x, \bar{x}) \subseteq \bar{x}$ for any $x \in \bar{x}$, then $x^* \in \bar{N}_1(x, \bar{x})$.

If the hypotheses in Part (d) hold, then the existence of a zero x^* of h in $\bar{x}$ has been verified, x^* is contained in the interval $\bar{N}_1(x, \bar{x})$, and x^* is the unique zero of h in $\bar{x}$.

3. Bounding Global Minima

The authors have shown [7] that, under certain conditions, an analytic expression exists for the difference $f(x) - f(x^*)$; where $f: \mathbb{R}^n \rightarrow \mathbb{R}$ and x^* minimizes f over a convex compact set, S , in $\mathbb{R}^n$. However, the necessary conditions and the expression for the difference usually cannot be computed exactly. This section presents a computational procedure, based on interval analysis, which can produce an interval bound on the difference $f(x) - f(x^*)$. In the process an interval bound on x^* is also generated.

Assume f is twice continuously differentiable on S , and that the Hessian matrix, $f''(x)$, is positive definite on S . Define the gradient set

$$U = \{u \mid u = f'(x) \text{ for some } x \in S\}.$$

It follows from the inverse function theorem and the convexity of S that there exists a unique differentiable function g defined on U such that $g[f'(x)] = x$ for all $x \in S$.

Theorem 2 [7]: Let S^I denote the interior of S , and assume f is twice continuously differentiable on an open set containing S . Suppose $x^0 \in S$ and

(i) $f''(x)$ is positive definite on S ,

(ii) the set $N(x^0)$ defined as

$$N(x^0) = \{x^0 - (\int_0^1 f''[x^0 + (x - x^0)s]ds)^{-1} \cdot f'(x^0) \mid x \in S\}$$

is contained in S , that is, $N(x^0) \subseteq S$.

Then there exists a $x^* \in N(x^0)$ such that

$$f'(x^*) = 0, \quad f(x^*) = \inf_{x \in S} f(x),$$

and x^* is the unique stationary point of f in S . Furthermore, if

$$(iii) \quad x^0 \in S^I, \text{ or}$$

$$(iv) \quad N(x^0) \subseteq S^I;$$

then $tf'(x^0) \in U$ for all $t \in [0,1]$, and

$$f(x^0) - f(x^*) = f'(x^0)^T \cdot \int_0^1 tf''[g\{tf'(x^0)\}]^{-1} dt \cdot f'(x^0). \quad (9)$$

At first glance the above theorem seems to be of only theoretical interest. Hypotheses (i), (ii) and the expression (9) for the difference $f(x^0) - f(x^*)$ usually cannot be computed exactly. However, it will be shown that interval analysis can be used to calculate an interval version of Theorem 2.

Suppose the convex compact set S is some interval $\bar{x}$ in R^n , and assume continuous interval extensions, $\bar{f}_{ij}'$, of the second partial derivatives of f are available on $\bar{x}$. Let $\bar{f}''(\bar{x}, \bar{x})$ be the interval Hessian matrix with components $\bar{f}_{ij}''(\bar{x}, \bar{x})$ given by (7). If an interval determinant (3) is computed, and

$$0 \notin \overline{\det \bar{f}''(\bar{x}, \bar{x})}, \quad (10)$$

then $f''(x)$ is nonsingular for all $x \in \bar{x}$. Furthermore, since the eigenvalues of a matrix are continuous functions of the matrix components [11]; if $f''(x)$ is positive definite for any $x \in \bar{x}$ and (10) holds, then $f''(x)$ is positive definite on $\bar{x}$, and hypothesis (i) of Theorem 2 is satisfied.

An interval Newton operator can be used to verify hypothesis (ii). The definition of an interval extension (5) implies that

$$\int_0^1 f''[x^0 + (x - x^0)s] ds \in \bar{f}''(\bar{x}, \bar{x})$$

for all x^0, x in $\bar{x}$. If (10) holds, then $\bar{f}''(\bar{x}, \bar{x})$ is invertible; and the definition of an interval inverse implies that

$$\left(\int_0^1 f''[x^0 + (x-x^0)s]ds\right)^{-1} \in \bar{f}''(\bar{x}, \bar{x})^{-1} \quad (11)$$

for all x^0, x in $\bar{x}$. An interval Newton operator, $\bar{N}_2$, which uses the symmetric $\bar{f}''(\bar{x}, \bar{x})$ can be defined as

$$\bar{N}_2(x^0, \bar{x}) = x^0 - \bar{f}''(\bar{x}, \bar{x})^{-1} \cdot f'(x^0). \quad (12)$$

Therefore, if $x^0 \in \bar{x}$ and

$$\bar{N}_2(x^0, \bar{x}) \subseteq \bar{x} \quad (13)$$

then (11) and (12) imply that

$$N(x^0) \subseteq \bar{N}_2(x^0, \bar{x}) \subseteq \bar{x},$$

and hypothesis (ii) is satisfied.

If (10) and (13) hold, then from Theorem 2, there exists a stationary point x^* of f in $\bar{N}_2(x^0, \bar{x})$, and x^* is the unique such point in $\bar{x}$.

Furthermore, if $f''(x)$ is positive definite for some $x \in \bar{x}$, then x^* minimizes f over $\bar{x}$. Assume now that either the point x^0 and/or the interval $\bar{N}_2(x^0, \bar{x})$ lie in the interior of $\bar{x}$. Then from Theorem 2, $tf'(x^0) \in U$ for all $t \in [0, 1]$, where $U = \{u | u = f'(x) \text{ for some } x \in \bar{x}\}$. Therefore, the definitions of an interval extension and interval inverse imply that

$$f''[g\{tf'(x^0)\}] \in \bar{f}''(\bar{x}, \bar{x})$$

and

$$\int_0^1 tf''[g\{tf'(x^0)\}]^{-1} dt \in \frac{1}{2} \bar{f}''(\bar{x}, \bar{x})^{-1}.$$

Using the above with (9) yields an interval bound on the difference in function values

$$f(x^0) - f(x^*) \in \frac{1}{2} f'(x^0)^T \cdot \bar{f}''(\bar{x}, \bar{x})^{-1} \cdot f'(x^0). \quad (14)$$

The previous discussion has proven the following interval version of Theorem 2.

Corollary: Let $\bar{x}$ be some interval in R^n , let $\bar{x}^{-1}$ denote the interior of $\bar{x}$, and assume continuous interval extensions, $\bar{f}_{ij}'$, of the second partial derivatives of f are available on $\bar{x}$. Suppose $x^0 \in \bar{x}$ and

(i') $0 \notin \det \bar{f}''(\bar{x}, \bar{x})$ and $f''(x)$ is positive definite for some $x \in \bar{x}$,

(ii') the interval Newton operator (12) is contained in $\bar{x}$, that is, $\bar{N}_2(x^0, \bar{x}) \subseteq \bar{x}$.

Then there exists a $x^* \in \bar{N}_2(x^0, \bar{x})$ such that

$$f'(x^*) = 0, \quad f(x^*) = \inf_{x \in \bar{x}} f(x),$$

and x^* is the unique stationary point of f in $\bar{x}$. Furthermore, if

(iii') $x^0 \in \bar{x}^{-1}$, or

(iv') $\bar{N}_2(x^0, \bar{x}) \subseteq \bar{x}^{-1}$; then

$$f(x^0) - f(x^*) \in 1/2 f'(x^0)^T \cdot \bar{f}''(\bar{x}, \bar{x})^{-1} \cdot f'(x^0).$$

The right-hand side of the above is an interval bound on the difference $f(x^0) - f(x^*)$, and the interval Newton operator (12) is an interval bound on x^* .

Note that the first part of the corollary pertaining to the existence and uniqueness of x^* is similar to Parts (a) and (d) of Theorem 1 by Nickel (let $h(x) = f'(x)$ in Theorem 1). Actually, Part (d) of Theorem 1 is stronger since it uses a tighter interval Newton operator. This follows from the definition of an interval extension since (5) and (7) imply that

$$\bar{f}''(x^0, \bar{x}) \subseteq \bar{f}''(\bar{x}, \bar{x})$$

for all $x^0 \in \bar{x}$, and since interval arithmetic is inclusion monotonic [8, p. 10]

$$\bar{N}_1(x^0, \bar{x}) \subseteq \bar{N}_2(x^0, \bar{x})$$

where

$$\bar{N}_1(x^0, \bar{x}) = x^0 - \bar{f}''(x^0, \bar{x})^{-1} \cdot f'(x^0).$$

Therefore, the interval Newton operator $\bar{N}_1(x^0, \bar{x})$, which uses the non-symmetric $\bar{f}''(x^0, \bar{x})$, might be contained in $\bar{x}$ in cases where $\bar{N}_2(x^0, \bar{x})$ defined by (12) is not.

Consider the computations involved in implementing the corollary. Given $\bar{x}$ in R^n , $x^0 \in \bar{x}$, and continuous interval extensions, $\bar{f}_{ij}'$, on $\bar{x}$; the symmetric $\bar{f}''(\bar{x}, \bar{x})$ is formed, and $\overline{\det f''(\bar{x}, \bar{x})}$ is calculated. An interval determinant, $\overline{\det A}$, can be calculated by diagonalizing $\bar{A}$, using partial pivoting in interval arithmetic, to obtain an upper triangular $\bar{A}_u$; then

$$\overline{\det A} = \prod_{i=1}^n (\bar{A}_u)_{ii}. \quad (15)$$

It is easy to show that the above satisfies (3). If (10) holds, then $f''(x)$ is nonsingular on $\bar{x}$, and the interval Newton operator $\bar{N}_2(x^0, \bar{x})$ given by (12) is well defined. Now $\bar{N}_2(x^0, \bar{x})$ can be calculated by first solving the interval linear system

$$\bar{f}''(\bar{x}, \bar{x}) \cdot y = -f'(x^0)$$

for an interval solution $\bar{y}$, and augmenting x^0 to obtain

$$\bar{N}_2(x^0, \bar{x}) = x^0 + \bar{y}. \quad (16)$$

The procedure used here to solve for $\bar{y}$ is Hansen and Smith's Method 4 [5]. In [4] Hansen presents a refinement procedure which may improve a given interval solution.

If (13) holds, then $\bar{N}_2(x^0, \bar{x})$ contains a stationary point x^* of f , and x^* is the unique such point in $\bar{x}$. Furthermore, if $f''(x)$ is positive definite for any $x \in \bar{x}$, then $f''(x)$ is positive definite on $\bar{x}$; and x^* minimizes f over $\bar{x}$. The interval bound (14) on the difference $f(x^0) - f(x^*)$ holds if $x^0 \in \bar{x}^I$ and/or $\bar{N}_2(x^0, \bar{x}) \subseteq \bar{x}^I$, and is easily obtained from the calculation of $\bar{N}_2(x^0, \bar{x})$. This follows since (12), (14), and (16) imply that

$$x^0 - \bar{N}_2(x^0, \bar{x}) = \bar{f}(\bar{x}, \bar{x})^{-1} \cdot f'(x^0) = -\bar{y}$$

and therefore

$$f(x^0) - f(x^*) \in -\frac{1}{2} f'(x^0)^T \cdot \bar{y}.$$

It cannot be overemphasized how much the usefulness of the above results depends on the availability of good interval extensions and good numerical methods for calculating an interval determinant and solving an interval linear system.

4. Unconstrained Signomial Programs

Many optimization problems, especially in engineering design [13], can be formulated as an unconstrained nonlinear program where the objective function f , a signomial [12], can be written as

$$f(x) = \sum_{t=1}^m c_t \prod_{i=1}^n x_i^{a_{ti}}. \quad (18)$$

Here x is a positive vector in R^n , and the coefficients c_t and exponents a_{ti} are arbitrary real numbers. If all the coefficients c_t are positive, then f is a posynomial [2]; and has a unique stationary point which is the global minimizer. Defining the exponent vectors $a_t = (a_{t1}, \dots, a_{tn})$ and substituting $z = \log x$, f can be rewritten as

$$f(z) = \sum_{t=1}^m s_t(z)$$

where the single-term functions, s_t , are defined as

$$s_t(z) = c_t \exp(a_t^T \cdot z), \quad t=1, \dots, m.$$

For an interval $[u, w]$, define $\exp([u, w]) = [\exp(u), \exp(w)]$; and for positive $[u, w]$, define $\log([u, w]) = [\log(u), \log(w)]$.

Given a positive vector $\bar{x}$, the corollary requires an interval extension of the Hessian

$$f''(z) = \sum_{t=1}^m s_t(z) a_t \cdot a_t^T$$

on $\bar{z} = \log \bar{x}$. Since each s_t is monotonic, an interval extension $\bar{s}_t(\bar{z})$, is easily obtained by computing s_t in interval arithmetic. Then the definition of an interval extension, the inclusion monotonicity of interval arithmetic, and Theorems 4.1 and 4.2 by Moore [8, p. 19] imply that

$$\bar{f}''(\bar{z}, \bar{z}) = \sum_{t=1}^m \bar{s}_t(\bar{z}) a_t \cdot a_t^T \quad (19)$$

is a continuous interval extension of $f''(z)$ evaluated on $\bar{z}$. The above procedure is computationally attractive, however, different methods exist which might yield sharper results.

As an example consider the minimum-cost design of the hypothetical chemical plant introduced in Section 1. The procedure will be illustrated on two intervals $\bar{z} = \log \bar{x}$ containing the (approximate) stationary point

$$z^* = \log x^* = \log \begin{pmatrix} 694.9 \\ 35.56 \\ 1.187 \end{pmatrix} = \begin{pmatrix} 6.5437 \\ 3.5712 \\ 0.17143 \end{pmatrix} \quad (20)$$

obtained using Dembo's algorithm [1] for signomial programs. This will permit a comparison between the interval bounds on the difference $f(z^0) - f(z^*)$ with the actual values. Note that since $f''(z^*)$ is positive definite, if $\bar{f}''(\bar{z}, \bar{z})$ is nonsingular in the interval sense, then $f''(z)$ is positive definite on $\bar{z}$.

Table 2 presents results where the interval on the original design variables $\bar{x}$ equals a ± 2.5 percent symmetric deviation around x^* given in (20), that is,

$$\bar{x} = x^* \pm 0.025 x^* = \begin{pmatrix} [677.48, 712.24] \\ [34.671, 36.450] \\ [1.1573, 1.2167] \end{pmatrix}.$$

Substituting $\bar{z} = \log \bar{x}$ and computing the interval Hessian (19) yields

$$\bar{f}''(\bar{z}, \bar{z}) = \begin{pmatrix} [338.20, 376.31] & [229.05, 249.39] & 0 \\ [229.05, 249.39] & [434.68, 475.56] & [257.74, 284.86] \\ 0 & [257.74, 284.86] & [521.61, 562.26] \end{pmatrix}.$$

Calculating the interval determinant defined by (15) yields

$$\det \bar{f}''(\bar{z}, \bar{z}) = [1.6802(10^7), 4.6121(10^7)].$$

Therefore, $f''(z)$ is positive definite on $\bar{z}$, and the interval Newton operator

$$\bar{N}_2(z^0, \bar{z}) = z^0 - \bar{f}''(\bar{z}, \bar{z})^{-1} \cdot f'(z^0) \quad (21)$$

is well defined. As discussed in the previous section, $\bar{N}_2(z^0, \bar{z})$ is calculated by solving the interval linear system

$$\bar{f}''(\bar{z}, \bar{z}) \cdot y = -f'(z^0) \quad (22)$$

for an interval solution $\bar{y}$ and augmenting z^0 to obtain $\bar{N}_2(z^0, \bar{z}) = z^0 + \bar{y}$.

The results for three different points $z^0 = \log x^0$ (where $x^0 = x^* + 0.005 x^*$, $x^* + 0.01 x^*$, $x^* + 0.02 x^*$) are given in Table 2, and in each case

$\bar{N}_2(z^0, \bar{z}) \subseteq \bar{z}$. Therefore, in each case the existence of a stationary point z^* in $\bar{N}_2(z^0, \bar{z})$ has been verified, z^* is the unique stationary point in $\bar{z}$ and z^* minimizes f over $\bar{z}$. Furthermore, since in each case z^0 lies in the interior of $\bar{z}$, the interval bound

$$f(z^0) - f(z^*) \leq -\frac{1}{2} f'(z^0)^T \cdot \bar{y} \quad (23)$$

holds; and since z^* is known in this example, the bound can be compared with the actual value. Note that as the distance between z^0 and z^*

Table 2

INTERVAL ON ORIGINAL DESIGN VARIABLES

$$\bar{x} = x^* + .025x^*$$

Point x_0	Interval Newton Operator Eq. (21)	$\bar{z} = \log \bar{x}$	Interval Bound Eq. (23)	Actual Difference $f(z_0) - f(z^*)$
1. $x^* + .005x^*$				
$= \begin{bmatrix} 698.33 \\ 35.738 \\ 1.1929 \end{bmatrix}$	$\begin{bmatrix} [6.5400, 6.5464] \\ [3.5668, 3.5739] \\ [.16905, .17372] \end{bmatrix}$	$\begin{bmatrix} [6.5183, 6.5685] \\ [3.5459, 3.5960] \\ [.14611, .19613] \end{bmatrix}$	$[0.14345, .049467]$	.029138
2. $x^* + .01x^*$				
$= \begin{bmatrix} 701.81 \\ 35.916 \\ 1.1989 \end{bmatrix}$	$\begin{bmatrix} [6.5360, 6.5489] \\ [3.5626, 3.5768] \\ [.16630, .17568] \end{bmatrix}$	$\begin{bmatrix} [6.5183, 6.5685] \\ [3.5459, 3.5960] \\ [.14611, .19613] \end{bmatrix}$	$[.058156, .20003]$	.11609
3. $x^* + .02x^*$				
$= \begin{bmatrix} 708.76 \\ 36.271 \\ 1.2107 \end{bmatrix}$	$\begin{bmatrix} [6.5278, 6.5533] \\ [3.5546, 3.5828] \\ [.16079, .17951] \end{bmatrix}$	$\begin{bmatrix} [6.5183, 6.5685] \\ [3.5459, 3.5960] \\ [.14611, .19613] \end{bmatrix}$	$[.23244, .79913]$	.46185

becomes larger, the interval solution $\bar{y}$ to (22) becomes wider; and hence the interval Newton operator and the interval bound become wider.

Table 3 presents results with the same points x^0 and where the interval $\bar{x}$ equals a ± 5 percent deviation around x^* , that is,

$$\bar{x} = x^* \pm 0.05 x^* = \begin{pmatrix} [660.11, 729.61] \\ [33.782, 37.338] \\ [1.1276, 1.2464] \end{pmatrix}.$$

Substituting $\bar{z} = \log \bar{x}$ and computing (19) yields

$$\bar{f}''(\bar{z}, \bar{z}) = \begin{pmatrix} [319.64, 395.86] & [219.15, 259.81] & 0 \\ [219.15, 259.81] & [415.82, 497.78] & [245.61, 300.06] \\ 0 & [245.61, 300.06] & [502.72, 584.23] \end{pmatrix}.$$

Again, $f''(z)$ is positive definite on $\bar{z}$ since (15) yields

$$\overline{\det \bar{f}''(\bar{z}, \bar{z})} = [0.41092(10^7), 6.3177(10^7)].$$

However, the requirement: $\bar{N}_2(z^0, \bar{z}) \subseteq \bar{z}$ only holds in the first case where $z^0 = \log(x^* + 0.005 x^*)$. In cases 2 and 3, the combination of the width of $\bar{z}$ and the distance between z^0 and z^* cause the method to fail.

All basic interval arithmetic operations were performed using Zoltan's single-precision rounded interval arithmetic package [15]. Other numerical procedures yielding tighter interval extensions, or better methods for solving an interval linear system should produce even better results.

Table 3
INTERVAL ON ORIGINAL DESIGN VARIABLES

$$\bar{x} = x^* + .05x^*$$

Point x^0	Interval Newton Operator Eq. (21)	$\bar{z} = \log \bar{x}$	Interval Bound Eq. (23)	Actual Difference $f(z^0) - f(z^*)$
1. $x^* + .005x^*$				
$= \begin{bmatrix} 698.33 \\ 35.738 \\ 1.1929 \end{bmatrix}$	$\begin{bmatrix} [6.5152, 6.5678] \\ [3.5374, 3.5922] \\ [.15090, .18059] \end{bmatrix}$	$\begin{bmatrix} [6.4924, 6.5926] \\ [3.5199, 3.6201] \\ [.12013, .22022] \end{bmatrix}$	$[-.074331, .19180]$	.029138
2. $x^* + .01x^*$				
$= \begin{bmatrix} 701.81 \\ 35.916 \\ 1.1989 \end{bmatrix}$	$\begin{bmatrix} [6.4862, 6.5917] \\ [3.5035, 3.6141] \\ [.12983, .18880] \end{bmatrix}$	$\begin{bmatrix} [6.4924, 6.5926] \\ [3.5199, 3.6201] \\ [.12013, .22022] \end{bmatrix}$	$\bar{N}_2(z^0, \bar{z}) \not\subseteq \bar{z}$	.11609
3. $x^* + .02x^*$				
$= \begin{bmatrix} 708.76 \\ 36.271 \\ 1.2107 \end{bmatrix}$	$\begin{bmatrix} [6.4282, 6.6386] \\ [3.4364, 3.6590] \\ [.08789, .20492] \end{bmatrix}$	$\begin{bmatrix} [6.4924, 6.5926] \\ [3.5199, 3.6201] \\ [.12013, .22022] \end{bmatrix}$	$\bar{N}_2(z^0, \bar{z}) \not\subseteq \bar{z}$	.46185

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