

Taylor Series Models in Deterministic Global Optimization

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1 Deterministic Global Optimization

Deterministic global optimization involves exhaustive search over the domain; the domain is subdivided (“branching”), and those subdomains that cannot possibly contain global minimizers are rejected. For example, if the problem is the unconstrained problem

$$\begin{array}{l} \text{minimize } \phi(x) \\ \text{subject to } x \in \mathbf{x}, \end{array} \tag{1}$$

then evaluating ϕ at a particular point x gives an upper bound for the global minimum of ϕ over the region \mathbf{x} . Some method is then used to bound the range of ϕ over subregions $\tilde{\mathbf{x}} \subset \mathbf{x}$. If the lower bound $\underline{\phi}$, so obtained, for ϕ over $\tilde{\mathbf{x}}$ has $\underline{\phi} > \phi(x)$, then $\tilde{\mathbf{x}}$ may be rejected as not containing any global optima; see Figure 1 for the situation in one dimension.

A simple interval evaluation $\phi(\tilde{\mathbf{x}})$ of ϕ over $\tilde{\mathbf{x}}$ is sometimes a practical way of obtaining the lower bound. (See [4], [5], or a number of other introductory expositions.) However, there are some functions for which interval evaluation gives an extreme overestimation, and other techniques are necessary. One such function arises from Gritton’s second problem, a chemical engineering model that J. D. Seader pointed out to the author. In Gritton’s problem, the eighteen solutions of $f(x) = 0$ in $[-12, 8]$ are sought, where f is defined by

$$\begin{aligned} f(x) = & -371.93625x^{18} - 791.2465656x^{17} + 4044.944143x^{16} \\ & + 978.1375167x^{15} - 16547.8928x^{14} + 22140.72827x^{13} \\ & - 9326.549359x^{12} - 3518.536872x^{11} + 4782.532296x^{10} \\ & - 1281.47944x^9 - 283.4435875x^8 + 202.6270915x^7 - 16.17913459x^6 \\ & - 8.88303902x^5 + 1.575580173x^4 + 0.1245990848x^3 \\ & - 0.03589148622x^2 - 0.0001951095576x + 0.0002274682229. \end{aligned}$$

Such examples can sometimes be treated by careful tessellation and use of point evaluations, as explained in [6]. However, a more elegant way would be if sharper

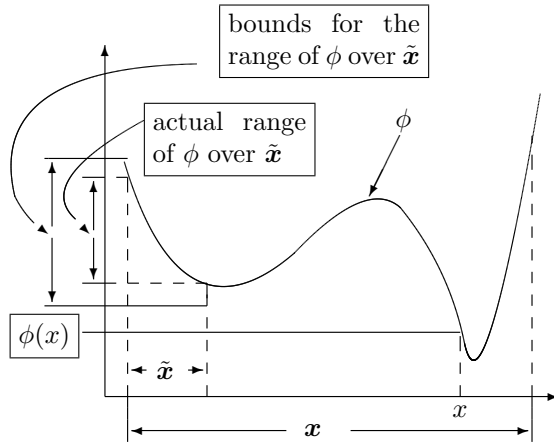


Figure 1: Rejecting $\tilde{\mathbf{x}}$ because of a high objective value

bounds on the range could be easily obtained. We will thoroughly investigate Taylor models for this purpose.

2 Taylor Models

Oversimplifying, Taylor models are models of the form $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ of the form

$$\phi(x) \in P_m(x) + \mathbf{E}(x), \quad (2)$$

where $P_m(x)$ is a degree- m polynomial in the n variables $x \in \mathbb{R}^n$ and \mathbf{E} is an interval that encompasses the truncation error. Early work in interval computations did not indicate that Taylor models were promising. In particular, if one merely evaluated P_m with interval arithmetic over a box (i.e. over an interval vector) \mathbf{x} , then the difference between the width of $P_m(\mathbf{x}) + \mathbf{E}(\mathbf{x})$ and the width of the actual range of ϕ over \mathbf{x} decreases no faster than the square of the widths of \mathbf{x} , a rate that can already be achieved with $m = 2$. A higher convergence order can be achieved if the range of P_m can be estimated accurately, but computing such an estimation is NP-complete in the length of the expression defining P_m ; see [7, Ch. 3 and Ch. 4].

However, Berz et al have found Taylor models to be highly effective at computing low-overestimation enclosures of the range of functions [8]. Berz' group has applied such models successfully to the analysis of stability of particle beams in accelerators [2], and has advocated its use for global optimization in general [8]. In an informal communication, Berz and Makino illustrated that the overestimation in Gritton's problem can be reduced by many orders of magnitude simply by approximating the degree-18 function with its degree-5 Taylor polynomial. This indicates that additional careful study of Taylor models in general deterministic global optimization algorithms is warranted.

3 Global Optimization and Taylor Models

In this work, we study the effectiveness of Taylor models in enhancing the utility of the GlobSol [3, 5] interval global optimization package. Where possible, we embed the high-quality automatic differentiation structure and Fortran libraries provided by Berz et al [1, 2]. Both the behavior for particular range estimations and the behavior of the overall global optimization algorithm is compared with test cases that utilize simple interval arithmetic.

References

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