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Range Bounding with Taylor Models for Global Optimization

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Abstract: Taylor models provide enclosures of functional dependencies by a polynomial and an interval remainder bound that scales with a high power of the domain width, allowing a far-reaching suppression of the dependency problem. For the application to range bounding, one observes that the resulting polynomials are more well-behaved than the original function; in fact, merely naively evaluating them in interval arithmetic leads to a quadratic range bounder that is frequently noticeably superior to other second order methods.

However, the particular polynomial form allows the use of other techniques. We review the linear dominated bounder (LDB) and the quadratic fast bounder (QFB). LDB often allows an exact bounding of the polynomial part if the function is monotonic. If it does not succeed to provide an optimal bound, it still often provides a reduction of the domain simultaneously in all variables. Near interior minimizers, where the quadratic part of the local Taylor model is positive semidefinite, QFB minimizes the quadratic contribution to the lower bound of the function, avoiding the infamous cluster effect for validated global optimization tasks.

Some examples of the performance of the bounders for unconstrained global optimization problems are given, beginning with various common toy problems of the community, and also including a rather challenging Lennard-Jones problem.

Key-Words: Taylor model, Global optimization, Linear dominated bounder LDB, Quadratic fast bounder QFB, COSY-GO.

1 Linear Dominated Bounder

The linear dominated bounder (LDB) introduced in [2] is based on the fact that for Taylor models with sufficiently small remainder bound, the linear part of the Taylor model dominates the behavior, and this is also the case for range bounding. The linear dominated bounder utilizes the linear part as a guideline for iterative domain reduction to bound Taylor models.

LDB Algorithm

Wlog, find the lower bound of minimum of a Taylor model $P + I$ in D.

(1) Re-expand P at the mid-point c of D, call the resulting polynomial P_m and the centered domain D_1.

(2) Turn the linear coefficients L_i's of P_m all positive by suitably flipping coordinate directions, call the resulting polynomial P_+.

(3) Compute the bound of the linear (I_1) and nonlinear (I_h) parts of P_+ in D_n. The minimum is bounded by $[M, M_{in}] := \underline{I}_1 + I_h$. If applicable, lower M_{in} by the left end value and the mid-point value.

(a) If $d = \text{width}([M, M_{in}]) > \varepsilon$, set D_{n+1} such that $\forall i$, if $L_i > 0$ and $\text{width}(D_{n+1,i}) > d/L_i$, then $\overline{D}_{n+1,i} := \underline{D}_{n,i} + d/L_i$. Re-expand P_+ at the mid-point c of D_{n+1}. Prepare the new coefficients L_i's. Go to 3.

(b) Else, M is the lower bound of minimum.

Any errors associated with re-expansion and

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estimating point values are included in the remainder error bound interval. If f is monotonic, the exact bound is often obtained with high accuracy. If only a threshold cutoff test is needed, the resulting domain reduction or elimination is often superior. The reduction of the domain of interest works multi-dimensionally and automatically, and the observed domain reduction rate is thus often fast. Even when there is no linear part in the original Taylor model, by shifting the expansion point, normally a linear part is introduced.

2 Quadratic Fast Bounder

The natural next idea of Taylor model bounding is to utilize the quadratic part of P, and a preliminary scheme of a quadratic dominated bounder (QDB) is discussed in [2]. For the task of global optimization in practice, an efficient bounding of the quadratic part in the vicinity of interior minimizers is important. Around an isolated interior minimizer, the Hessian of a function f is positive definite, so the purely quadratic part of a Taylor model $P + I$ which locally represents f, has a positive definite Hessian matrix H. The actual definiteness can be tested in a validated way using the common LDL or extended Cholesky decomposition. The quadratic fast bounder (QFB) provides a lower bound of a Taylor model cheaply when the purely quadratic part is positive definite. It is based on the following observation.

Let $P + I$ be a given Taylor model in D, and let H be the Hessian matrix of P. We decompose the polynomial P into two parts via

$$P + I = (P - Q) + I + Q.$$

Then a lower bound for $P + I$ is obtained as

$$l(P + I) = l(P - Q) + l(Q) + l(I).$$

For QFB, we choose

$$Q = Q_{x_0} = \frac{1}{2}(x - x_0)^t H(x - x_0)$$

with any $x_0 \in D$. If H is positive semidefinite, $l(Q_{x_0}) = 0$, and the value 0 is attained. The remaining $P - Q_{x_0}$ does not contain pure quadratic terms anymore, but consists of linear as well third and higher order terms $P_{>2}$. If x_0 is chosen to be the minimizer of the quadratic part P_2 of P in D, then x_0 is also a minimizer of the remaining linear part (a consequence of the Kuhn-Tucker conditions), and so the lower bound estimate is optimally sharp. Thus by choosing x_0 close enough to the minimizer of P_2 in D, a contribution of $P_2 - Q_{x_0}$ to the lower bound can be very small. For a given P_2 in D, x_0 can be determined inexpensively by an iterative scheme to search a series of $x_0^{(i)}$ in the direction of $-\nabla P_2$ while limiting $x_0^{(i)}$ to stay inside D.

3 Validated Global Optimizer COSY-GO

For the example problems of validated global optimization in the next sections, we apply three branch-and-bound methods available in the code COSY-GO[4]. The first one is the Taylor model-based optimizer utilizing the LDB and QFB algorithms (LDB/QFB). We compare the performance with two other optimizers; one based on mere interval bounding (IN) and one based on bounding with centered form (CF). The sub domain box list management is performed in the same way for all three optimizers. At each sub domain box step, the following tasks are performed.

- A function bound is estimated using the tools described below; if the lower bound is above the cutoff value, the box is eliminated; if not, the box is bisected.
- Bounding schemes are applied in a hierarchical manner. The mere interval bounding is estimated for all optimizers. If the interval bound fails to eliminate the box, the centered form bounding is performed for the CF optimizer. Likewise, for the LDB/QFB optimizer, if the interval bound fails, the naive Taylor model bound[3] based on interval evaluation of the Taylor polynomial is determined, and only when it fails, the LDB bound is determined. If it also fails and the quadratic part of the local Taylor model of the function is positive definite, the QFB bounding is performed.
- When the LDB bound fails, however, often the domain box can be reduced before bisection.

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- The cutoff value is updated. The mid-point value estimate is conducted for all optimizers.
- For the LDB/QFB optimizer, the linear and quadratic parts of the local Taylor model are utilized to guess a candidate for the global minimizer to obtain a better cutoff value estimate.

4 A One Dimensional Polynomial

The first example problem is to search the minimum of the polynomial

$$f(x) = 1 + x^5 - x^4$$

in $[0, 1]$, suggested by R. Moore[5]. The function has a shallow minimum at $x = 0.8$, and looks rather innocent as shown in Figure 1; but the dependency problem and the high order of the polynomial prevents the mere interval bounding method from being successful. Table 1 summarizes the performance of the three optimizers. The Taylor model LDB/QDB optimizer eliminates all sub domain boxes but the one containing the minimum in 17 steps, among which 8 steps are size reductions by LDB. There are at most 3 active boxes kept in the whole optimization process. On the other hand, the interval optimizer requires a total of 12471 steps, and retains 2591 small boxes. The centered form optimizer performs better than the interval optimizer, but cannot reach the performance of the LDB/QFB optimizer. The sub domain boxes active in each step are shown in Figure 1, and an example of LDB domain reduction can be seen in the processing of the parent box in step 5 to yield the bisected boxes appearing in steps 6 and 7. As seen later in Figure 2, the LDB domain reduction works favorably also in multidimensional cases.

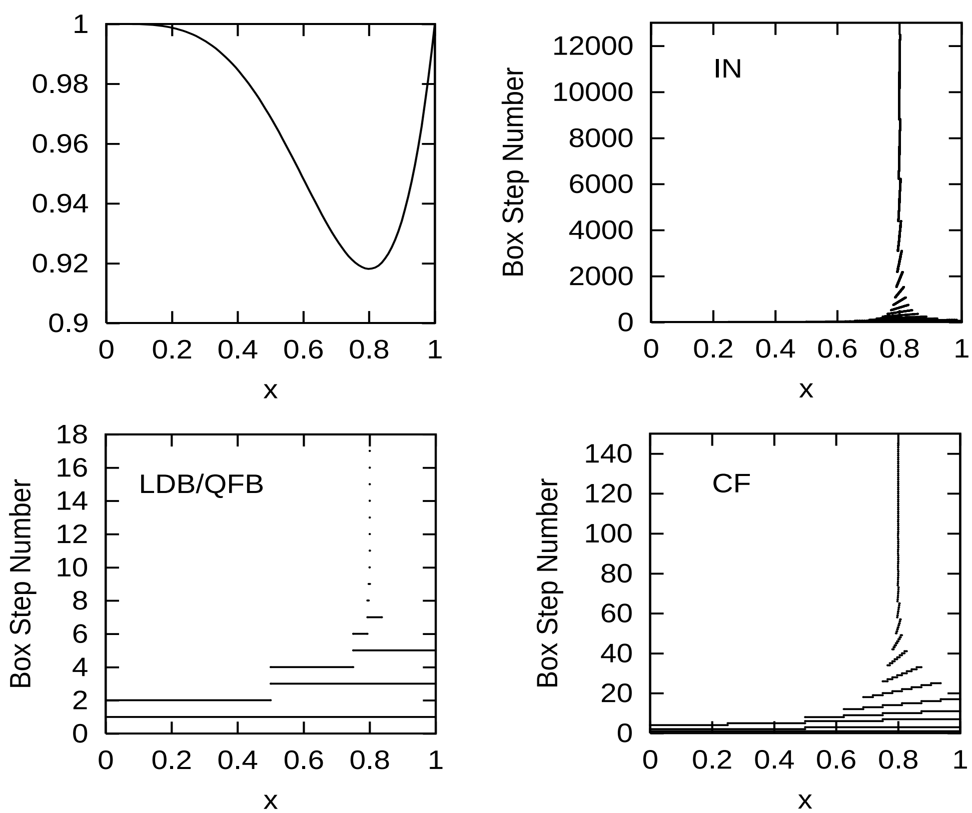

Figure 1: Global optimization of $f(x) = 1 + x^5 - x^4$ in $[0, 1]$ (top left). Sub domain boxes for minimum search are shown at each step: (top right) the interval, (bottom right) the centered form, and (bottom left) the LDB/QFB optimizers.

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	$f(x) = 1 + x^5 - x^4$ in $[0, 1]$			Beale function f_B in $[-4.5, 4.5]^2$		
	IN	CF	LDB/QFB	IN	CF	LDB/QFB
Total box processing steps	12471	145	17	3407	3285	353
Max number of active boxes	4044	11	3	236	234	52
Retained small boxes ($< 10^{-6}$)	2591	4	1	25	25	3
LDB domain reduction steps	–	–	8	–	–	108

Table 1: Performance of various optimizers.

5 The Beale Function

The next example is the Beale function[6]

$$f_B(x_1, x_2) = (1.5 - x_1(1 - x_2))^2 + \left(2.25 - x_1(1 - x_2^2)\right)^2 + \left(2.625 - x_1(1 - x_2^3)\right)^2 .$$

The problem is to find the minimum in the initial domain $[-4.5, 4.5] \times [-4.5, 4.5]$ with validation. The function has little dependency and the minimum 0 occurs at $(3, 0.5)$, however the very shallow behavior of the function makes a validated global optimization task difficult.

The performance of the optimizers is summarized in Figure 2 and Table 1. Square expressions in f_B are not utilized to simplify the arithmetic. We observe no advantage in the centered form optimizer compared to the interval optimizer. On the other hand, the LDB/QFB optimizer significantly outperformed both others because of more efficient box rejection and LDB domain size reduction.

6 The Lennard-Jones Potential Problem

For the last example, we choose a challenging problem and also compare actual performance with one of the leading global optimization tools, Baker Kearfott's GlobSol[1]. We consider the Lennard-Jones potential problem, describing an ensemble of n particles interacting pointwise with the potential

$$V = \sum_{i<j}^{n} V_{LJ}\left(r_i - r_j\right), \; V_{LJ}(r) = \frac{1}{r^{12}} - 2 \cdot \frac{1}{r^6}.$$

As seen in Figure 3, V_{LJ} has a shallow minimum of value -1 at $r = 1$, while having an extremely wide range of function values. In fact, the behavior of the function has a similarity to the 5th order polynomial discussed above.

We studied the following six and nine dimensional problems corresponding to $n = 4$ and $n = 5$.

For $n = 4$, four particles are positioned at

$$\vec{a}_1 = (0, 0, 0), \; \vec{a}_2 = (x_1, 0, 0),$$
$$\vec{a}_3 = (x_2, x_3, 0), \; \vec{a}_4 = (x_4, x_5, x_6)$$

with all the x_i's positive, and the objective function is

$$f_{n=4}(\vec{x}) = \sum_{i<j}^{n=4} V_{LJ}\left(r_i - r_j\right) + 6.$$

The minimum is expected to occur at $\vec{x}_{\min} = (1, 1/2, \sqrt{3}/2, 1/2, 1/(2\sqrt{3}), \sqrt{2/3})$ with a value of 0. In the initial search box

$$[0.8, 1.2] \times [0.4, 0.6] \times [0.7, 1.0]$$
$$\times [0.4, 0.6] \times [0.2, 0.4] \times [0.7, 1.0],$$

the LDB/QFB optimizer locates the minimizer

$$\begin{aligned}\vec{x}_{\min} \in\ & [0.999999236, 1.00000077]\\ \times\ & [0.499999236, 0.500000764]\\ \times\ & [0.866025161, 0.866025735]\\ \times\ & [0.499999236, 0.500000764]\\ \times\ & [0.288674163, 0.288675691]\\ \times\ & [0.816495956, 0.816497373]\end{aligned}$$

with the expected minimum value enclosed in a sharp interval as shown in Table 2. Both the interval and the centered form optimizers, however, failed to eliminate any sub box before reaching the limit of list length for sub domain box management. To provide performance comparison, we ran

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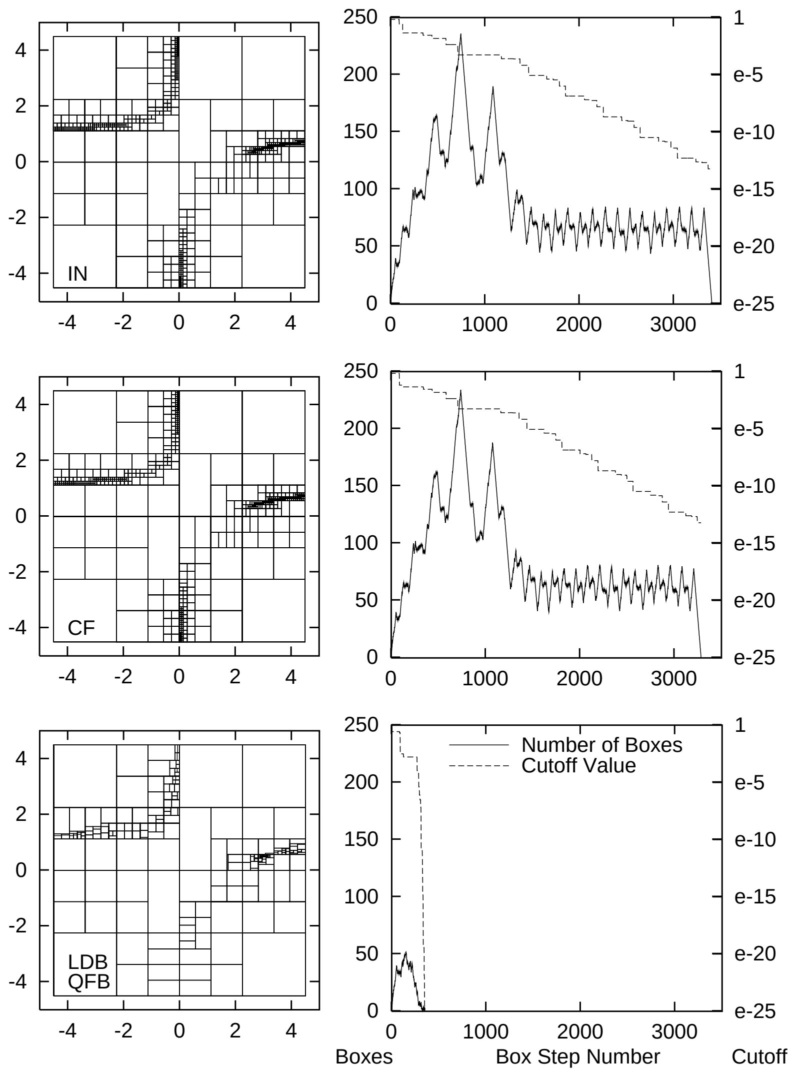

Figure 2: Minimum search for the Beale function in $[-4.5, 4.5]^2$ by the interval, the centered form, and the LDB/QFB optimizers. Left: sub domain boxes. Right: number of active boxes and cutoff value.

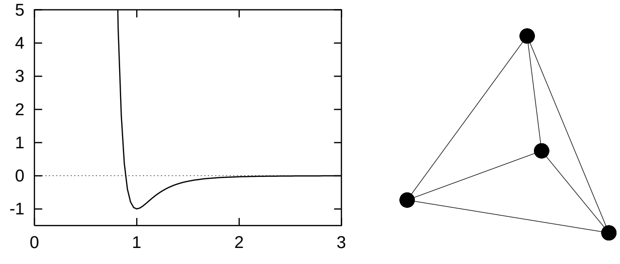

Figure 3: The Lennard-Jones potential $V_{LJ}(r)$ and four interacting particles.

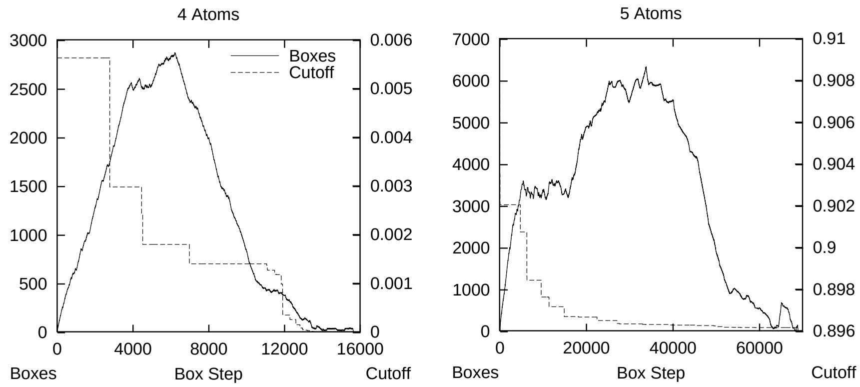

Figure 4: Performance of the Taylor model LDB/QFB optimizer for the Lennard-Jones potential problems.

	$n = 4$ (6D)		$n = 5$ (9D)	
	LDB/QFB	GlobSol	LDB/QFB	GlobSol
Total steps	15655	243911	69001	598491
Max boxes	2866	–	6321	–
Retained boxes ($< 10^{-6}$)	17	–	111	–
LDB reduction	2079	–	5153	–
CPU time	89 s	5833 s	1550 s	(> 259200 s)
Minimum	$[-6.8 \cdot 10^{-11}$ $, 1.5 \cdot 10^{-13}]$	$< 10^{-12}$	[0.896147584195 ,0.896147584293]	< 0.9046

Table 2: Performance for the 6D and 9D Lennard-Jones problems by LDB/QFB COSY-GO and GlobSol.

the same problem in GlobSol with its standard mode, and the result is listed in the table.

One more particle is added at $\vec{a}_5 = (x_7, x_8, x_9)$ with x_7,$x_8 > 0$, $x_9 < 0$, and the new objective function is

$$f_{n=5}(\vec{x}) = \sum_{i<j}^{n=5} V_{LJ}(r_i - r_j) + 10.$$

The original domain box is

$$\begin{aligned}&[0.9, 1.1] \times [0.45, 0.55] \times [0.8, 1.0]\\ \times&[0.45, 0.55] \times [0.25, 0.35] \times [0.75, 0.9]\\ \times&[0.45, 0.55] \times [0.25, 0.35] \times [-0.9, -0.75].\end{aligned}$$

The LDB/QFB optimizer locates the minimizer

$$\begin{aligned}\vec{x}_{\min} \in\ &[1.00145263, 1.00145417]\\ &\times [0.500726317, 0.500727845]\\ &\times [0.867283629, 0.867285157]\\ &\times [0.500726317, 0.500727845]\\ &\times [0.289093780, 0.289096070]\\ &\times [0.813335036, 0.813336183]\\ &\times [0.500726317, 0.500727845]\\ &\times [0.289093780, 0.289096070]\\ &\times [-0.813336183, -0.813335036],\end{aligned}$$

and the achieved enclosure of the minimum is listed in Table 2. The table and Figure 4 show the performance, and the comparison with GlobSol in the standard mode is provided as well. Apparently the Taylor model-based optimizer compares very favorably.

Acknowledgements

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References:

[1] R. B. Kearfott. *Rigorous Global Search: Continuous Problems*. Kluwer, 1996.

[2] K. Makino. *Rigorous Analysis of Nonlinear Motion in Particle Accelerators*. PhD thesis, Michigan State University, East Lansing, Michigan, USA, 1998. Also MSUCL-1093.

[3] K. Makino and M. Berz. Taylor models and other validated functional inclusion methods. *International Journal of Pure and Applied Mathematics*, 6,3:239–316, 2003. http://bt.pa.msu.edu/pub.

[4] K. Makino and M. Berz. COSY INFINITY version 9. *Nuclear Instruments and Methods*, in print.

[5] R. E. Moore. Private communication.

[6] More, Garbow, and Hillstrom. Testing unconstrained optimization software. *ACM Trans. Math. Software*, 7:17–41, 1981.