Interval methods for solving various kinds of quantified nonlinear problems

Bartłomiej Jacek Kubica

Institute of Control and Computation Engineering
Warsaw University of Technology
Poland

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What shall we consider?

- What (in particular) kind of problems can we solve using interval methods?
- What is the algorithm to solve them?
- How to make this algorithm efficient?
- How to parallelize it successfully?

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  - uncertain parameters,
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- My view: the interval analysis is an approach to seek points, satisfying a certain logical condition.

Problem under solution

Find **all** $x \in \mathbb{R}^n$, satisfying the condition $P(x)$, i.e.,
find the set $\{x \in \mathbb{R}^n | P(x)\}$.

where *P (x)* is a predicate formula with a free variable *x*, i.e., free variables: $x_1, \ldots, x_n$.

It can contain bound variables, also (we shall call them "parameters").

Previous papers

- Computability of the problem:
  - V. Kreinovich, B. J. Kubica, *From computing sets of optima, Pareto sets and sets of Nash equilibria to general decision-related set computations*, Journal of Universal Computer Science, Vol. 16, pp. 2657 – 2685 (2010).
- Early presentation:
  - B. J. Kubica, *A class of problems that can be solved using interval algorithms*, SCAN 2010, Computing, Vol. 94 (2-4), pp. 271 – 280 (2012).

Explanation

- Several researchers investigated solving quantified constraints using the interval approach.
  - Papers of Ratschan, 2002; Benhamou & Goualard, 2000; Shary, 2002; Goldsztejn & Jaulin, 2006 (not exclusively!) are particularly notable.

$$\{x \in X \mid (\forall t \in [t_0, t_f]) \ (f(x,t) \leqslant 0)\}$$

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    $$\{x \in X \mid (\forall t \in [t_0, t_f])\ (f(x,t) \leqslant 0)\}$$
- Also, other problems, traditionally solved by interval methods, can be formulated that way, e.g.:
  - global optimization: $\{x \in X \mid (\forall t \in X)\ (f(x) \leqslant f(t))\}$
  - Pareto sets seeking,
  - ...

Example problems

$$\{x \in X \mid h(x) = 0\}$$

$$\{x \in X \mid f(x) \in [\underline{y}, \overline{y}]\}$$

$$\{x \in X \mid (\forall t \in X)\ (f(x) \leqslant f(t))\}$$

$$\{x \in X \mid (\forall t \in X)\ (\forall i = 1, \ldots, N\ \ f_i(x) \leqslant f_i(t)) \vee (\exists i\ f_i(x) < f_i(t))\}$$

$$\{x \in X \mid (\forall i = 1, \ldots, n)\ (\forall x'_i \in \boldsymbol{x_i} \subseteq \mathbb{R}^{k_i})\ (f_i(x_{\setminus i}, x'_i) \geqslant f_i(x))\}$$

where:

$$X \subseteq \mathbb{R}^n, \quad h : \mathbb{R}^n \to \mathbb{R}^m, \quad f, f_1, \ldots f_N : \mathbb{R}^n \to \mathbb{R}$$

Proposed algorithm

- We shall use the name generalized branch-and-bound method or branch-and-bound type method.
- Several algorithms, described in the literature, are its specific instances:
  - Branch-and-bound method.
  - Branch-and-prune method.
  - “Nested” b&b or b&p (for parameters).
  - SIVIA – Set Inversion Via Interval Analysis (Jaulin, 1993).
  - PPS – Partitioning Parameter Set (дроблене параметров; Калмыков, 1982).

Generic algorithm

Lpos = {}; *Lverif* = {}; *Lcheck* = {};
// Phase I
while (there are boxes to consider) **do**
pop (***x***);
process (***x***); // using interval tools
if (***x*** was verified to contain a solution/a point satisfying some necessary conditions) **then** push (*Lverif*, ***x***);
else if (***x*** is verified not to contain solutions) **then**
if (***x*** may be necessary in phase II) **then** push (*Lcheck*, ***x***);
else discard ***x*;**
end if
if (***x*** was discarded or stored) **then** pop (***x***)**;**
else if (diam (***x***) < ε**) then** push (*Lpos*, ***x***);
else
bisect (***x***, ***x1***, ***x2***); push (***x2***); ***x*** = ***x1***;
end if
end while
// Phase II – verification of *P(x)* for stored solution candidates
for each (***x*** in *Lverif* *Lpos*) **do**
if (***x*** does not contain a solution) **then** discard ***x***;
end for each

What does the algorithm result in?

- Two lists:
  - **`Lverif`** – the list of boxes verified (certified) to contain a solution,
  - **`Lpos`** – the list of boxes possibly containing a solution.
- What conditions have to be verified so that the solution was “verified”?
- There can be more than two lists, in general:
  - Some conditions are verified, some are not.
  - We classify points of the domain int more than two classes.

Algorithm's other details

- In what order do we process boxes? Does the order matter?
- How do we store boxes?
- What tools do we use to process a box?
- What information is needed to process a box in phase I?
- What information is needed to verify a box in phase II?
- In particular, what boxes do we store in *Lcheck* – if any?

Algorithm's other details

- All depends on the problem under solution.
- Does the presence of solution in one area have influence on its presence elsewhere?
  - For equations systems – not really.
  - For optimization problems – it does (the optimum occurs to be local, only, if we have found a better point elsewhere).
  - For seeking Pareto sets – also.
  - ...
- Obviously, rejection/reduction tests rely on the problem under solution, also.

How to store boxes?
The simplest case.

- The order of processing boxes does not matter.
  - Equations systems, CSPs, etc.
- Then, we can use any structure – a stack, queue, pool, etc.
- Parallelization is (relatively) easy.
- Some frameworks allow us to store the boxes implicitly, using the task queue (e.g., Intel TBB).
- Sufficient (not necessary!) condition: no bound occurrences of the variable x (i.e., no quantifiers range over its domain).

How to store boxes? More sophisticated cases.

- For, e.g., global optimization, the order, in which we process boxes, matters – and we know in what way.
- A priority queue is suitable.
- Parallelization is more difficult (but TBB has a class `priority_queue`).
- For some problems the order matters, but in a complicated way, difficult to predict.
  - E.g., Nash equilibria computing.
  - In my implementations, I used ordinary queues.
  - A potential for improvement, certainly.

Tools to process a box

- Order of function approximation:
  - 0th order tools – comparing function values.
  - 1st order tools – use of gradients.
  - 2nd order tools – use of Hesse matrices.
  - Higher order tools ?
- Operations:
  - Simply, comparing function values.
  - Several versions of the interval Newton operator (*componentwise*, GS) – on various levels.
  - Various constraint satisfaction methods (consistency enforcing, SIVIA, etc.).
  - ...

The information stored

- For equations systems, CSPs, etc. – no additional info is needed – boxes only (i.e., only local information).
- Global optimization – upper bound on the global minimum; a single number; no *Lcheck* list needed.
- Pareto sets seeking – we store the approximation of the Pareto frontier; a set of several points, changing frequently.
  - Tricky – especially for parallel implementations.
  - Simple 0^{th} order tools are inefficient.
  - Still, the list *Lcheck* is not needed (only a set of points in the criteria space).

The information stored

- A difficult problem – seeking Nash points or strong Nash points of a continuous game.
- To verify a solution, we need to compare players' utilities for boxes located in proper places of the search domain.
  - For “plain” Nash points – in proper subspaces; for strong ones – in the whole domain.
- An interval tree is an option (suggested in my earlier papers).
- Storing the boxes on the *Lcheck* list seems a better solution.

Three important example problems

- Seeking Nash points and strong Nash points of a continuous game.
- Seeking all local (including global) optima of a function.

My papers on games solutions seeking

- B. J. Kubica, A. Woźniak, *An interval method for seeking the Nash equilibria of non-cooperative games*, PPAM 2009, LNCS, Vol. 6068, pp. 446 – 455 (2010).
- B. J. Kubica, A. Woźniak, *Applying an interval method for a four agent economy analysis*, PPAM 2011, LNCS, Vol. 7204, pp. 477 – 483 (2012).
- B. J. Kubica, A. Woźniak, *Interval methods for computing various refinements of Nash equilibria*, SCAN 2012, unpublished.
- B. J. Kubica, A. Woźniak, *Interval methods for computing strong Nash equilibria of continuous games*, SING10 (2014), submitted to *Operations Research and Decisions*.

Solution concepts

John Forbes Nash Jr.
Nash equilibrium, 1950

Robert John (Yisrael) Aumann.
Strong Nash equilibrium, 1959

Picture from: http://commons.wikimedia.org/wiki/File:John_Forbes_Nash,_Jr._and_Robert_Aumann.jpg

Computing the solutions

- Nash points can use be defined by the following system of conditions:

$$\forall i = 1, \ldots, n \quad \forall x_i \in \boldsymbol{x_i} \subseteq \mathbb{R}^{k_i}$$

$$q_i\left(x_1^*, \ldots, x_{i-1}^*, x_i, x_{i+1}^*, \ldots, x_n^*\right) \geqslant q_i\left(x_1^*, \ldots, x_n^*\right)$$

- Hence, strong Nash points:

$$\forall I \subseteq \{1, \ldots, n\} \quad \forall x_I \in \boldsymbol{x_I} \subseteq \mathbb{R}^{k_i}$$

$q_i\left(x_{\setminus I}^*, x_I\right)$ does not dominate $q_i\left(x_1^*, \ldots, x_n^*\right)$

where x_I denotes a subvector, consisting of components of x with indexes from the set I.

Necessary conditions for Nash points

- Well determined ($N = \sum_i k_i$ equations and total N variables).
- The Jacobi matrix is composed of rows of Jacobi matrices of systems $\nabla q_i(x_1, \ldots, x_n) = 0$

$$
\begin{array}{cccc}
\dfrac{\partial q_1(x)}{\partial x_1} = 0, & \dfrac{\partial q_1(x)}{\partial x_2} = 0, & \cdots & \dfrac{\partial q_1(x)}{\partial x_n} = 0, \\
\dfrac{\partial q_2(x)}{\partial x_1} = 0, & \dfrac{\partial q_2(x)}{\partial x_2} = 0, & \cdots & \dfrac{\partial q_2(x)}{\partial x_n} = 0, \\
\vdots & \vdots & \cdots & \vdots \\
\dfrac{\partial q_n(x)}{\partial x_1} = 0, & \dfrac{\partial q_n(x)}{\partial x_2} = 0, & \cdots & \dfrac{\partial q_n(x)}{\partial x_n} = 0.
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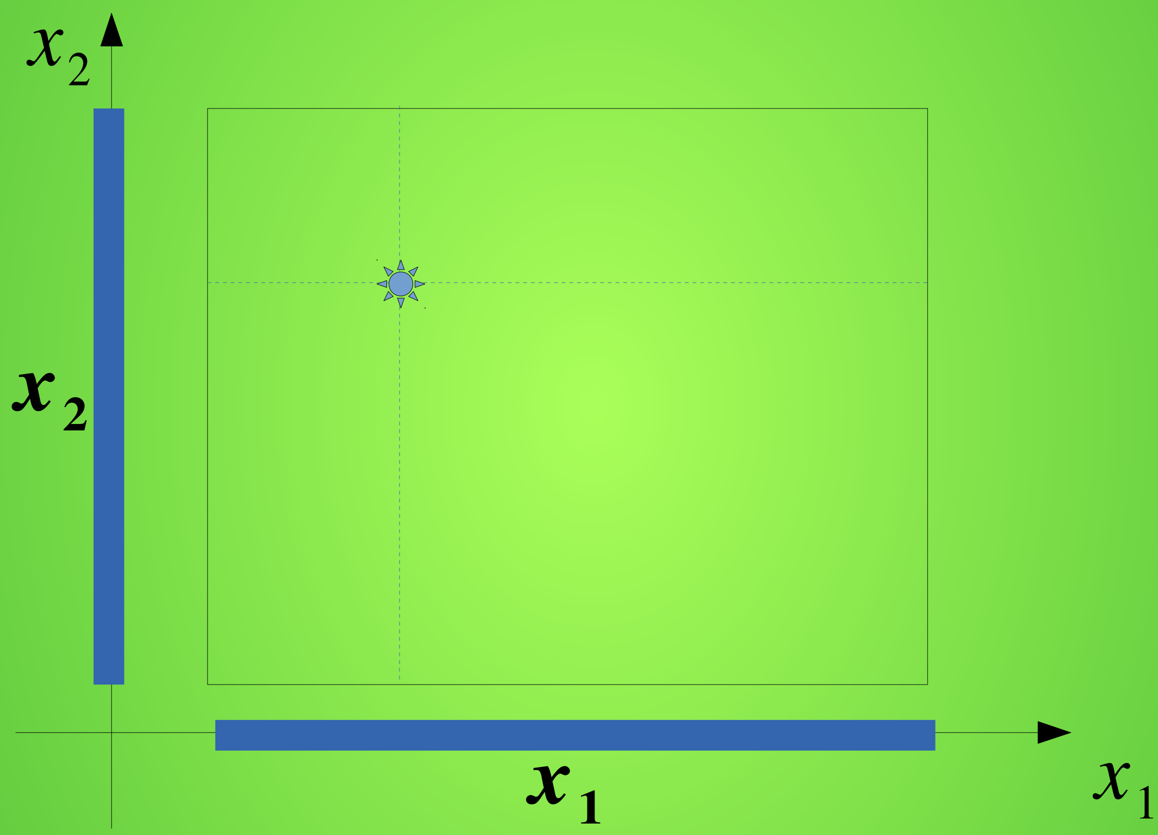
Necessary conditions for strong Nash points

- Necessary conditions:
  - All conditions for ordinary Nash points hold!
  - And there are additional ones.
- So, the system is overdetermined.
  - That is the reason (at least one of them) why SNEs exist so rarely.
  - It will not be possible to compute verified results using the interval Newton operator.
- What are these necessary conditions, specifically?
- We assume *i*-th player controls the variable $x_i \in X_i \subseteq \mathbb{R}$; extension to the general case is straightforward.

What do we check in phase II?

Consider the case with two players and $x_{1,}\, x_2 \in \mathbb{R}$



$$\forall\, x_1 \in \boldsymbol{x_1} \quad q_1(x_{1,} x_2^*) \geqslant q_1(x_1^*, x_2^*),$$

$$\forall\, x_2 \in \boldsymbol{x_2} \quad q_2(x_1^*, x_2) \geqslant q_2(x_1^*, x_2^*),$$

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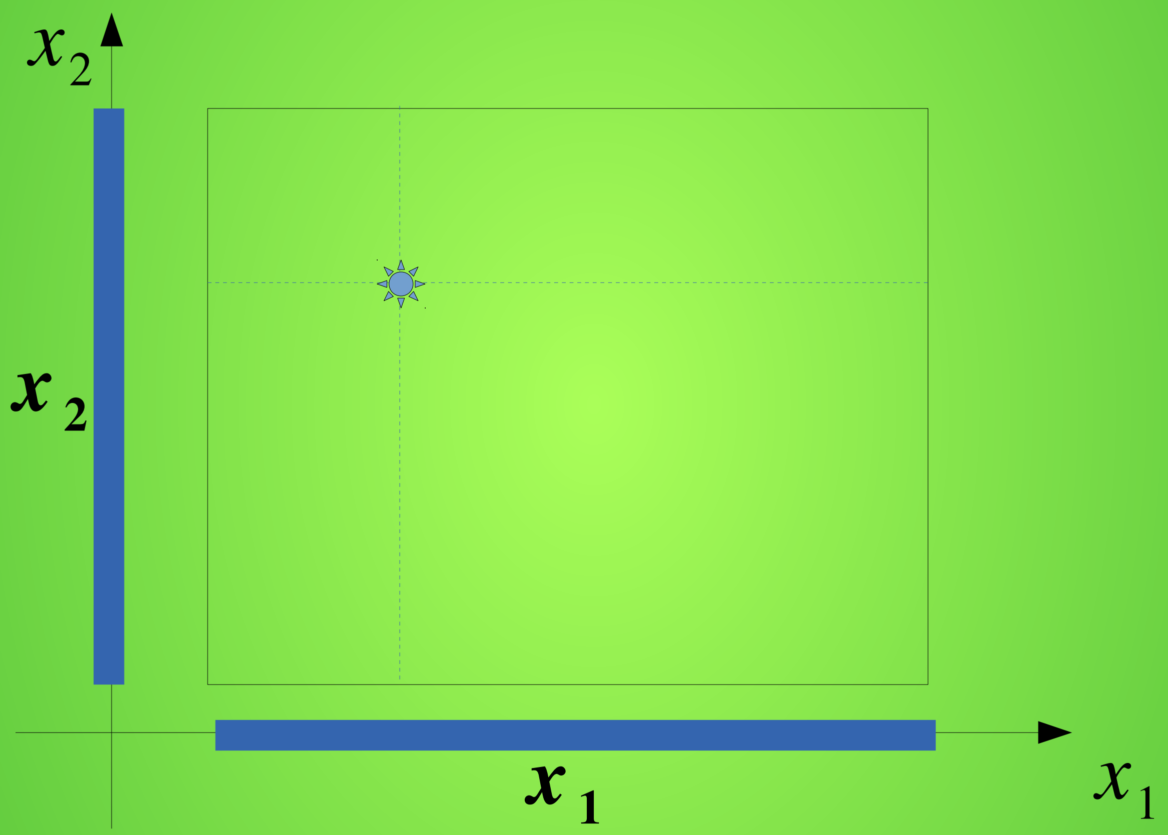

$$\forall\, x_1 \in \boldsymbol{x}_{1,} \quad x_2 \in \boldsymbol{x}_2 \qquad q_1(x_{1,} x_2) \geqslant q_1(x_1^*, x_2^*) \text{ or } x_1 \neq x_1^*,$$

$$q_2(x_{1,} x_2) \geqslant q_2(x_1^*, x_2^*) \text{ or } x_2 \neq x_2^*$$

Third important example: seeking local optima

$$\{x \in X \mid (\exists \delta > 0) \wedge (\forall t \in X \wedge d(x,t) < \delta)\ (f(x) \leqslant f(t))\}$$

- Find all local (and global) minima (or maxima).
- Should not be confused, e.g., with seeking an ε-optimal solution! $\{x \in X \mid (\forall t \in X)\ (f(x) \leqslant f(t) + \varepsilon)\}$
- The problem was rarely considered, up to now (and usually for very specific cases):
  - K. Villaverde, V. Kreinovich, *A linear-time algorithm that locates local extrema of a function of one variable from interval measurement results*, Interval Computations 4, pp. 176 – 194 (1993).
  - E. Lyager, *Finding local extremal points by using parallel interval methods*, Interval Computations, Vol. 3, pp. 63 – 80 (1994).
  - Ch. Eick, K. Villaverde, *Robust algorithms that locate local extrema of a function of one variable from interval measurement results: A remark*, Reliable Computing, Vol 2(3), pp. 213 – 218 (1996).

Third important example: seeking local optima

$$\{x \in X \mid (\exists \delta > 0) \wedge (\forall t \in X \wedge d(x,t) < \delta)\ (f(x) \leqslant f(t))\}$$

- Important potential applications:
  - Potential games (no pun intended) – local optima of the potential function are Nash equilibibira.
  - NMR spectroscopy – local maxima of the spectrum show, for which frequency the nucleus resonates.
  - Radio-astronomy – local maxima of the ray show where astronomical objects are located.
  - …
- How is the problem related to global optimization?

Comparison

Seeking global optima

- Efficient 0^{th} order tools (comparing function values).
- Global information on the minimum's upper bound.
- Boxes with smaller lower bound should be processed earlier.
- Phase II simple, but necessary.

Seeking local optima

- No 0^{th} order tools (function values are irrelevant).
- No global information.
- Order of boxes processing – irrelevant.
- No phase II.

- 1^{st} and higher order tools – very similar.

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- There is a great deal of interval tools.
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- All of them give guaranteed (verified) results.
- None of them are intelligent *per se*!
- It is crucial to develop a heuristic to:
  - choose the interval tools adequate for a specific box,
  - arrange them,
  - parameterize them.

How to make the branch-and-bound-type method efficient?

- The author devoted several papers to design heuristics for two problems:
  - Nonlinear equations systems – especially seeking all solutions of underdetermined systems.
  - Seeking Pareto sets of a multicrietia problem.
- Many tools & versions; several papers.
- We present two topics:
  - Choosing the coordinate for bisection.
  - Initial exclusion phase – for nonlinear systems.

Underdetermined systems

- B. J. Kubica, *Interval methods for solving underdetermined nonlinear equations systems*, SCAN 2008, Reliable Computing, Vol. 15, pp. 207 – 217 (2011).
- B. J. Kubica, *Performance inversion of interval Newton narrowing operators*, KAEiOG 2009, Zeszyty Naukowe PW. Elektronika, Vol. 169, pp. 111 – 119 (2009).
- B. J. Kubica, *Shared-memory parallelization of an interval equations systems solver – comparison of tools*, KAEiOG 2009, *ibidem*, pp. 121 – 128.
- B. J. Kubica, *Intel TBB as a tool for parallelization of an interval solver of nonlinear equations systems*, ICCE internal report, 09-02, 2010.
- B. J. Kubica, *Tuning the multithreaded interval method for solving underdetermined systems of nonlinear equations*, PPAM 2011, LNCS, Vol. 7204, pp. 467 – 476 (2012).
- B. J. Kubica, *Excluding regions using Sobol sequences in an interval branch-and-prune method for nonlinear systems*, SCAN 2012, Reliable Computing, Vol. 19 (4), pp. 385 – 397 (2014).
- B. J. Kubica, *Using quadratic approximations in an interval method of solving underdetermined and well-determined nonlinear systems*, PPAM 2013, LNCS 8385, pp. 623 – 633 (2014).
- B. J. Kubica, *Presentation of a highly tuned multithreaded interval solver for underdetermined and well-determined nonlinear systems. Empirical evaluation of innovations*, Numerical Algorithms, submitted.

Pareto sets computing

- B. J. Kubica, A. Woźniak, *Interval methods for computing the Pareto-front of a multicriterial problem*, PPAM 2007, LNCS, Vol. 4967, pp. 1382 – 1391 (2008).
- B. J. Kubica, A. Woźniak, *A multi-threaded interval algorithm for the Pareto-front computation in a multi-core environment*, PARA 2008 Proceedings, LNCS, Vol. 6126 (not published, yet???).
- B. J. Kubica, A. Woźniak, *Optimization of the multi-threaded interval algorithm for the Pareto-set computation*, Journal of Telecommunications and Information Technology, Vol. 1, pp. 70 – 75 (2010).
- B. J. Kubica, A. Woźniak, *Using the second-order information in Pareto-set computations of a multi-criteria problem*, PARA 2010 Proceedings, LNCS, Vol. 7134, pp. 137 – 148 (2012).
- B. J. Kubica, A. Woźniak, *Computing Pareto-sets of multicriteria problems using interval methods*, presented at SCAN 2010, unpublished.
- B. J. Kubica, A. Woźniak, *Tuning the interval algorithm for seeking Pareto sets of multi-criteria problems*, PARA 2012, LNCS, Vol. 7782, pp. 504 – 517 (2013).

Underdetermined systems – tools used in my solver

- Interval Newton operators – we switch between the componentwise and Gauss-Seidel operators; a proper heuristic to choose.
  - BC3 for large (a heuristic to tell, which are large!) boxes.
- Using a quadratic approximation for boxes likely to contain singular points or otherwise hard for the Newton operator; a heuristic to decide.
- Initial exclusion phase, using 0^{th} order information, only.
- Two advanced policies to choose the bisection direction.

Bisection

- Often, it is assumed that bisection should minimize the diameter of the objective function on resulting boxes.

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- An example of such heuristic is MaxSmear (Shary, 1992; Ratz, 1992; Ratz & Csendes, 1995).
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  - Works reasonably well for well-determined equations systems.
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  - Works very well for optimization problems.
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- In my opinion, the objective of bisection should be defined in a different way: give boxes that are **easy to process** by the used **interval tools**.

Bisection

- For equations solving, the main tool is some kind of the interval Newton operator.
- So, for a single equation in two variables, it might seem reasonable to choose the minimal smear.
- But the convergence...
- A proper policy should take into account several criteria.
- For several, advanced tools, such a policy cannot be too simple...

Bisection

- For example, the heuristic of Kubica, 2012:

find index *j_max* and diameter *w_max* of the longest component;
find index *j_min* and diameter *w_min* of the shortest component;
find index *j_max_nonred* and diameter *w_max_nonred* of the longest component **not reduced** by the latest use of the Newton;
if ((Newton operator reduced no component) or (*w_max* > 1.5 * *w_max_nonred*)) **then return** *j_max*;
else if (*w_max_nonred* > 8 * *w_min*) **then return** *j_max_nonred*;
find index *j* and diameter *w* of the component with the smallest maximal absolute value in all rows of the Jacobi matrix;
if (*w* > 0.1) **then return** *j*;
else return *j_max_noned*;

- My new paper proposes a new, yet different heuristic...

Bisection

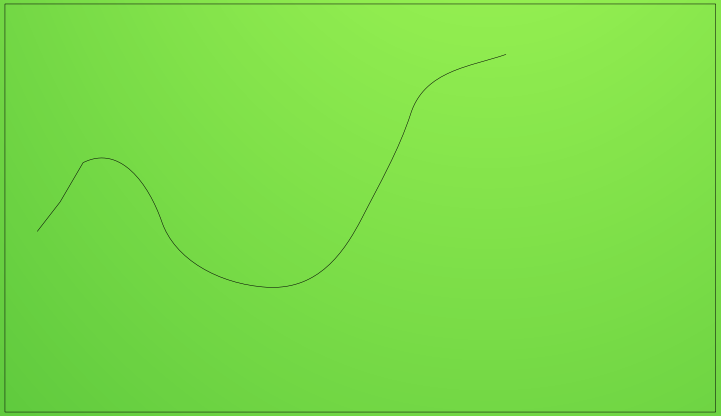
- For Pareto sets seeking, the proper heuristic is quite different:

find the index i of the criterion with maximal distance from the set in the criteria space;
find the index j and diameter w of the component with maximal smear with respect to criterion i;
find the index j_max and diameter w_max of the component with maximal diameter;
if ($w\_max < 8 * w$) **then return** j;
else return j_max;

- Reasons: different interval tools, used in the algorithm.

Underdetermined systems

- Initial exclusion phase – motivation:
  - Interval Newton operators are powerful, but relatively expensive.
  - Large boxes, encountered in the early stages of the b&p algorithm can rarely be reduced by the Newton operator.
  - We should apply these operators only for boxes close to the solution set.
  - Large regions of the domain can be discarded using function values, only.



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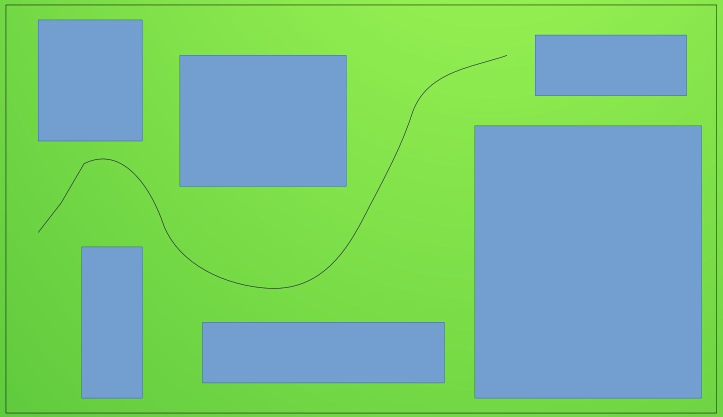
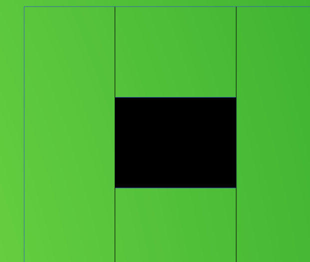


Underdetermined systems

- Initial exclusion phase – essence:
  - Before starting the actual branch-and-prune method, we generate a given number (n^2 ; n or $2n$ in earlier versions) of points, using the Sobol sequence.
  - Around the points we generate boxes, not containing solutions (procedure of Сергей П. Шарый for the linearized equation + ε-inflation; if $f(x) \in [-\varepsilon, \varepsilon]$, the point is ignored).
  - We exclude the boxes from the domain and start the b&p algorithm on their completion.
  - The procedure does not require using derivatives (global values are used for the Shary's procedure), so it is not computationally intensive.
  - Sobol sequences can be generated simply and efficiently (there are open libraries!).

Underdetermined systems



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- There is the procedure of R.B. Kearfott for a single box; it generates at most 2 *n* boxes.
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Underdetermined systems

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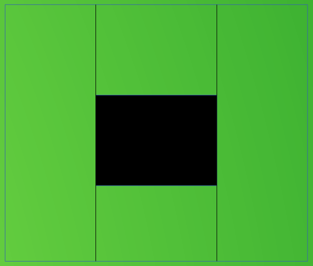
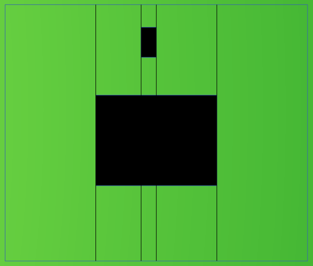
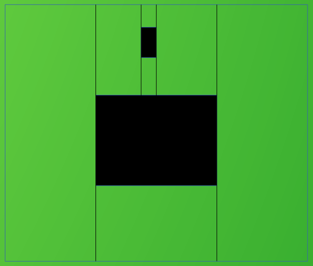
- There is the procedure of R.B. Kearfott for a single box; it generates at most 2 *n* boxes.
- It can be applied several times subsequently, but:
  - It would not be parallel.
  - The result would depend on the order of boxes exclusion.
  - The generated box set could be very large.
  - Often, boxes have peculiar shapes (long and flat), their shapes are unrelated to function values.
  - Hence, actually, sometimes expanding the exclusion boxes decreases the performance.







Underdetermined systems

- Boxes might be sorted with respect to decreasing Lebesgue measure, but it solves the problem rarely.
- The satisfying solution:
  - We use task parallelism. Each task is to cut from a specific box a list of excluded boxes.
  - From this list we choose the box with the largest (wrt the Lebesgue measure) intersection with the box from which we do the exclusion.
  - Boxes, created in the exclusion process, become basis for new tasks (obviously, their lists of excluded boxes are shorter by one than for the parent task).
  - Far fewer boxes are created and the parallelism is natural.
  - All functions $f_i(\cdot)$ are used for exclusion.

Underdetermined systems

- For each function, after the ε-inflation, variables, not occurring in its formula, are set to their whole domain.
- We exclude the box for $f_i(\cdot)$, for which we obtained the largest Lebesgue measure.
- There is a threshold value not to exclude to many boxes (128 worked well, but it is a magical constant, obviously).

• Intel TBB allows an elegant implementation:

- We use the concept of **`tbb::parallel_do`**.
- Boxes, created in the exclusion process, become basis for new tasks – using **`tbb::parallel_do_feeder`**.
- Lists of boxes are represented as **`std::vector`** (**`tbb::concurrent_vector`** does not have the method **`pop_back`**).
- Counter of excluded boxes it represented as **`tbb::atomic`**.

Underdetermined systems – computational times

Problem	GS only	PPAM 2011	PPAM 2011 + BC3	Full algorithm
Broyden 16	21 851s (6h 4min 11s)	6112 s (101min 52s)	644 s (10min 44s)	70 s (1 min 10 s)
Bratu 30	broken > 7h	broken > 7h	3 s	4 s
Brent 10	2604 s (43min 24s)	97 s (1min 37s)	43 s	18 s
Hippopede	21 s	2 s	under 1 s	1 s
5R planar	81 s	65 s	63 s	59 s

Parallelization

- We already discussed that, but – to sum up.
- Parallelization is simplest, when:
  - the order of boxes processing is irrelevant and
  - no global information is needed.
- Such problems are, i.a.:
  - equations systems,
  - CPSs,
  - seeking all local optima.
- The box list can be stored implicitly – e.g., Intel TBB.
- Parallelization with OpenMP simple, also – particularly for OpenMP 3 (the **`task`** directive), but not only.

Shared memory

- For global optimization:
  - The order of boxes matters – a priority queue is needed.
  - Global information on the upper bound on the global minimum (a single floating-point number).
- Parallelization is more difficult, but the difference is minor:
  - Applying TBB not that natural (the class **`tbb::priority_queue`** might be useful!).
  - The global minimum upper bound should be protected by a mutex (or something similar).
- Pareto sets seeking:
  - We have to store the Pareto frontier – sounds scary...
  - Difficult choice of a box to process.

Shared memory

- Parallel Nash points seeking:
  - Several shared lists.
  - In my resent implementation the boxes are stored in a queue – can we do better?
  - Second phase is very important...
  - … and difficult – it requires a nested branch-and-bound procedure for each solution to (verify it).

- Local memory:
  - Box migration.
  - Termination detection.
  - Much more difficult if we need shared information.

Summary

- Interval methods can be applied for a wide class of problems, described by predicate formulae.
- Various kinds of these problems can be solved by some instances of the generalized branch-and-bound method.
- Details depend on the specific problem. They are difficult (or impossible) to determine automatically – a human is needed.
- For the efficiency, it is crucial to develop a proper heuristic to choose and parameterize the interval tools.
- The branch-and-bound-type methods parallelize well, but not trivially; some knowledge is needed to do it properly.