Interval methods for solving underdetermined nonlinear equations systems

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Nonlinear problems

- Finding <u>all</u> solutions of underdetermined problems:
  - A few authors mention this problem, but they do not consider it in details (R. B. Kearfott, L. Kolev, M. Gavriliu).
  - A few papers about finding a <u>single</u> solution of the underdetermined system.
  - R. B. Kearfott's paper on homotopy methods.
  - A few papers about Pareto-front computation.
- What we consider in this presentation ?
  - Algorithms.
  - Theoretical analysis and background.
  - Engineering problems.

Algorithms for underdetermined problems

- Branch-and-bound method.
- Rejection/reduction tests – interval Newton operators:
  - interval Gauss-Seidel operator,
  - interval componentwise Newton operator,
  - Krawczyk operator.
- The algorithm computes:
  - the list of small boxes that possibly contain a segment of the solution manifold,
  - the list of boxes verified to contain a segment of the solution manifold.

How to use interval Newton operators ?

- Interval componentwise Newton:
  - We choose the equation *i* and variable *j* for the operator.
    - A list of pairs (*i*, *j*) is created at the beginning of the program and remains constant.
    - A list of pairs (*i*, *j*) is created for each box.
- Interval Gauss-Seidel:
  - Hansen proposed a technique for verifying feasibility in constrained optimization problems – variable choosing with Gauss elimination with full pivoting.
- Krawczyk operator:
  - A suitable preconditioning matrix may used – e.g. the Moore-Penrose pseudoinverse midpoint preconditioner.

Interval componentwise Newton operator

How to choose pairs (i, j) ?

- According to the idea of Herbort and Ratz, two lists are created – L1 for the use of Newton operator in ordinary and L2 – in extended interval arithmetic.
- L2 contains one pair for each variable – the equation for which the corresponding Jacobi matrix element has the longest diameter.
- L1 can contain more or less pairs and is constructed in one of several ways.

Interval componentwise Newton operator

- Herbort and Ratz original method
  - Fill L1 with all pairs (i, j) for which the corresponding element $\boldsymbol{J}_{ij}$ of the (interval-valued) Jacobi matrix is a non-zero; elements closer to the diagonal go first.
- Goualard method
  - Compute the following matrix and compute the maximum weighted matching:

$$W_{ij} = \begin{cases} \text{Mag}\,\boldsymbol{J}_{ij} & \text{if } 0 \in \boldsymbol{J}_{ij} \\ \text{Mig}\,\boldsymbol{J}_{ij} + \max_i \text{Mag}\,\boldsymbol{J}_{ij} & \text{otherwise} \end{cases}$$

- Gauss elimination with full pivoting on the midpoint matrix.
- GE with full pivoting on the Goualard matrix W.

Auxiliary theorems

Consider an equation $\sum_{j=1}^{n} \boldsymbol{a}_j \boldsymbol{x}_j = \boldsymbol{b}$.

Suppose the lower bound $\underline{x_k}$ of $\boldsymbol{x}_k$ has been improved by operator: $\boldsymbol{x}_k^{\boldsymbol{new}} = (\boldsymbol{b} - \sum_{j \neq k} \boldsymbol{a}_j \boldsymbol{x}_j) / \boldsymbol{a}_k$

Then: if $\boldsymbol{a}_k \boldsymbol{a}_l > 0$ then $\underline{x_l}$ cannot be further improved,

if $\boldsymbol{a}_k \boldsymbol{a}_l < 0$ then $\overline{x_l}$ cannot be further improved,

from this equation.

If the upper $\overline{x_k}$ bound has been improved, the relations are analogous.

Auxiliary theorems

In particular, if $\boldsymbol{x}_k^{new} \subset \operatorname{int} \boldsymbol{x}_k$ then no other improvement is possible form this equation before improvements from other ones.

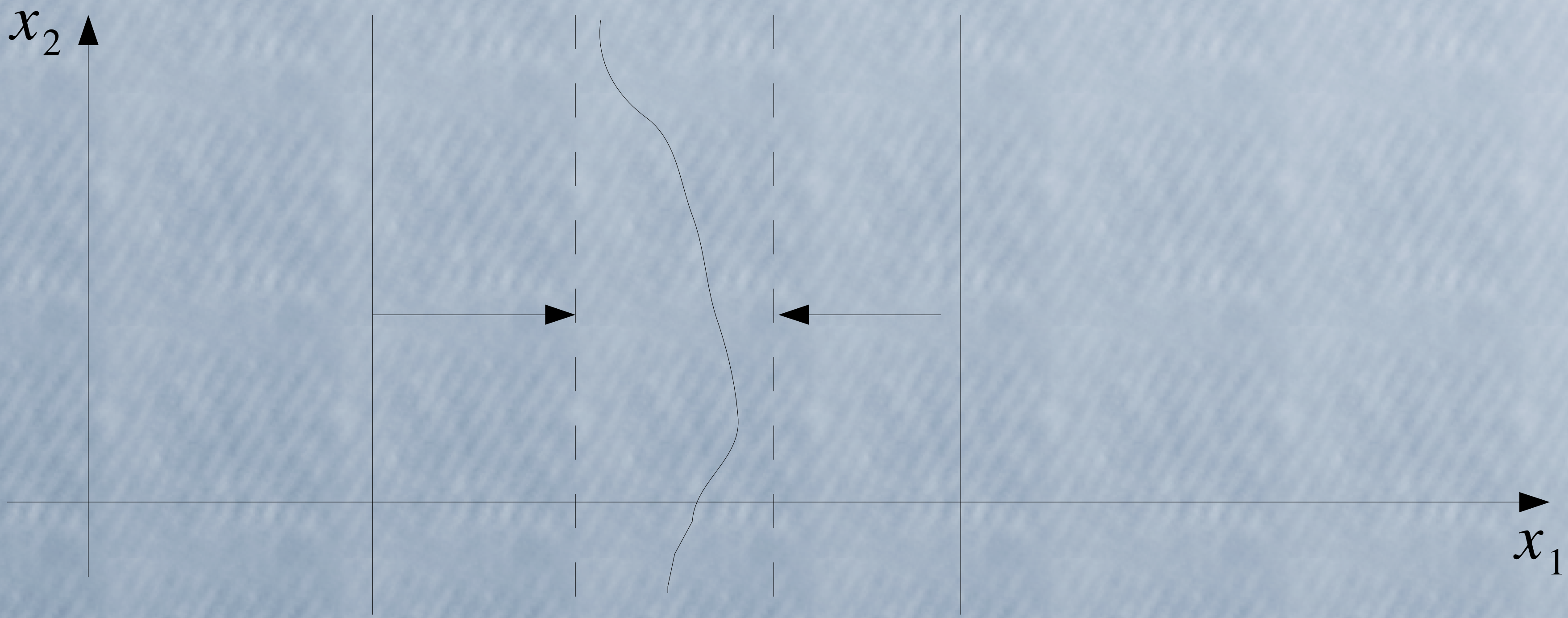
Please note that the above theorems were proven for the GS operator.

For the N_{cmp} operator the improvement is possible, but not probable.

Main theorem

Suppose we obtained $N_{cmp}(\boldsymbol{x}, \mathrm{f}, i, j) \subset \mathrm{int}\, \boldsymbol{x_j}$ for n variables x_{j_k}, $j_k \in J$.

Then: $\forall k \notin J \ \forall x \in \boldsymbol{x_k} \ \ \forall j \in J \ \exists ! x \in \boldsymbol{x_j} \quad f(x) = 0$



The same holds for the GS operator for one row.

Note on the margin

In particular the previous theorem implies that if we obtain $N_{cmp}(\boldsymbol{x}, \mathrm{f}, i, j) \subset \operatorname{int} \boldsymbol{x}_{\boldsymbol{j}}$ for all variables of a square (i.e. well-determined) equations system, we can be sure it has a unique solution in $\boldsymbol{x}$.

And even this margin wouldn't be too narrow to contain the proof, probably.

(with apologies to Pierre de Fermat).

Please note that even Herbort & Ratz who developed the N_{cmp} operator did not seem to know this property. Also my previous works assumed it can only (dis)prove existence, but not uniqueness.

Back to underdetemined problems – computations breaking

There, both relations are fulfilled (an improbable case due to numerical imprecision):

$$\forall\, x_1 \in \boldsymbol{x_1} \quad \exists!\, x_2 \in \boldsymbol{x_2} \qquad f(x)=0$$

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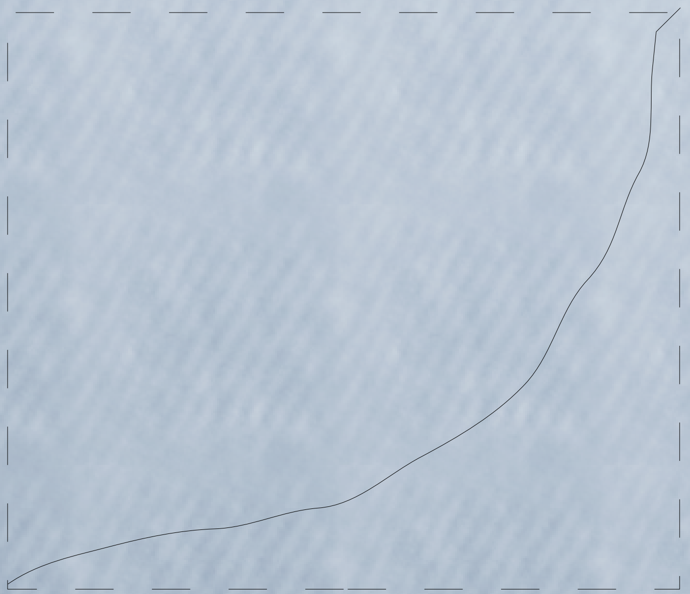

Should we bisect this box further or not ?

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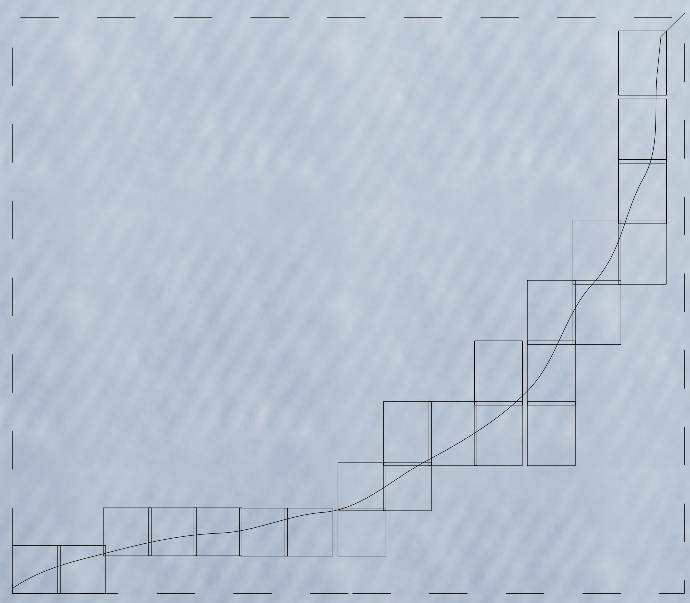


Should we bisect this box further or not ?

Possibly it would be better to have several small boxes...

Computational experiments

- Investigated methods:
  - Gauss-Seidel operator with Hansen's technique, i.e. Gauss elimination with full pivoting ("**GS+Hansen**"),
  - componentwise Newton operator with Herbort-Ratz heuristic used <u>once</u> ("**cmp+HR**"),
  - componentwise Newton operator with Goualard heuristic used <u>repeatedly</u> ("**cmp+Gou**"),
  - componentwise Newton operator with <u>repeatedly</u> choosing pairs by Gauss elimination with full pivoting on midpoint matrix ("**cmp+GE**"),
  - componentwise Newton operator with <u>repeatedly</u> choosing pairs by Gauss elimination with full pivoting on Goualard matrix ("**cmp+GouGE**").

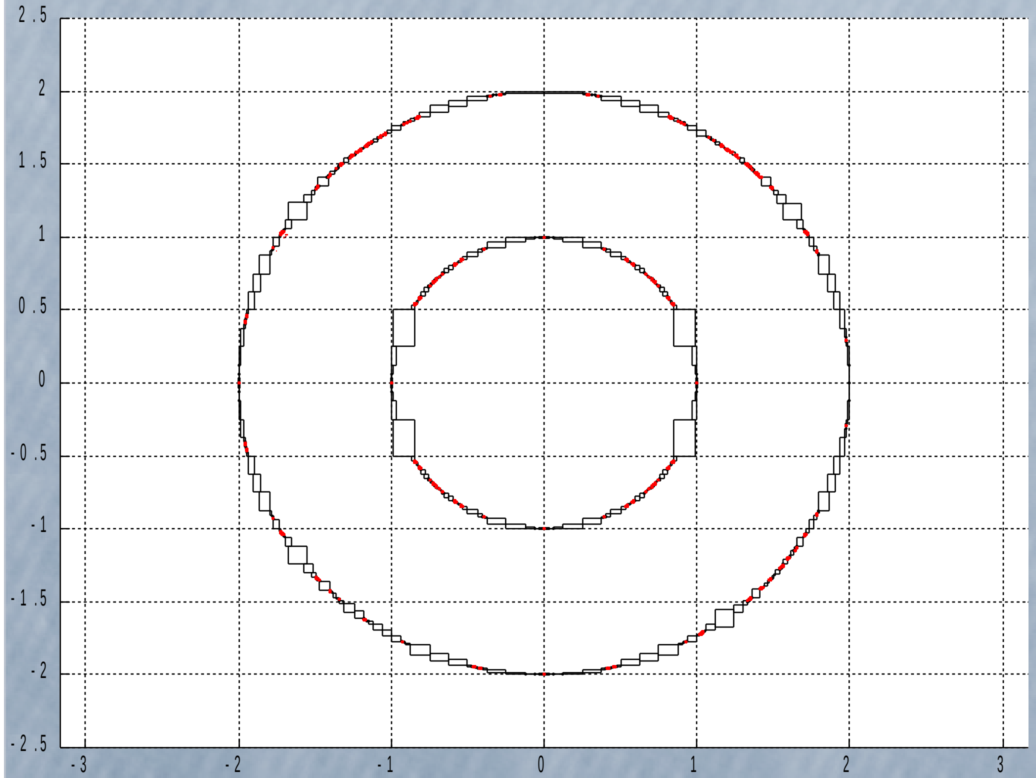
Computational experiments

- Processor Intel Core 2 Quad Q6600 2.4 GHz.
- Linux Slackware 2.6.21.5-smp operating system.
- GNU compiler 4.1.2.
- C-XSC 2.2.3 library for interval computations.
- The perfect weighted matching was computed using the Hungarian algorithm, implemented by John Weaver and distributed under GPL licence.

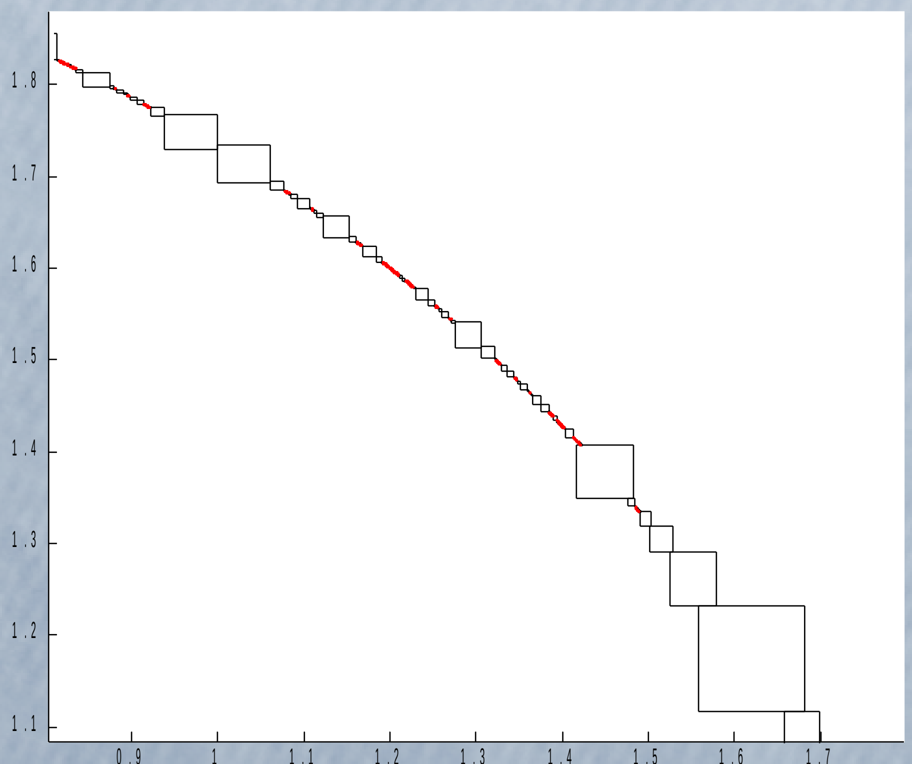
Computational results

"Two circles problem": $(x_1^2 + x_2^2 - 4)\cdot(x_1^2 + x_2^2 - 1) = 0$

$x_1, x_2 \in [-3, 5]$



GS+Hansen



zoom

Computational results

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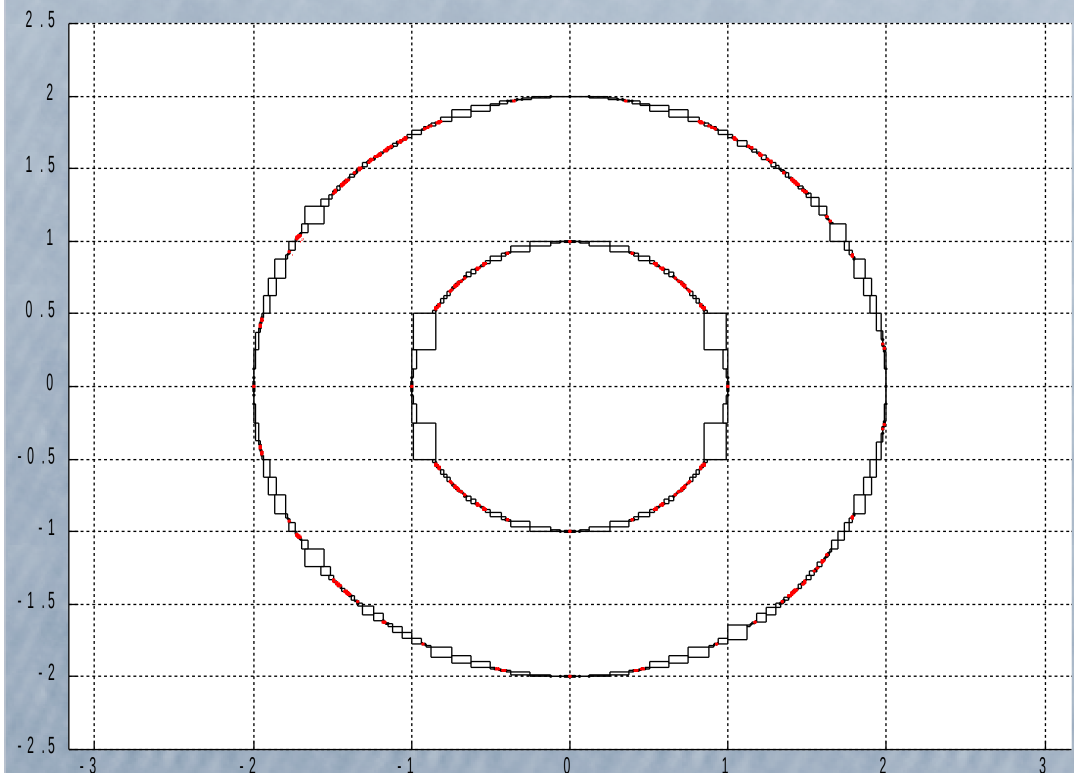
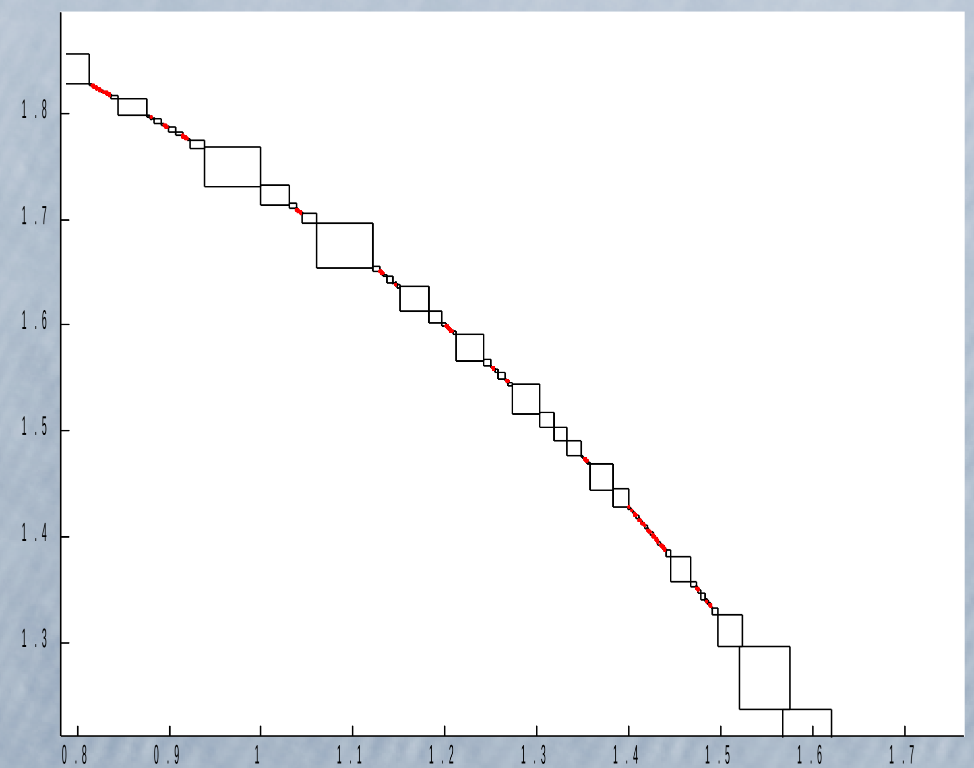


cmp+Gou



zoom

Thanks to Adam Wozniak for his help with preparing the figures.

Computational results

"Two circles problem".
One equation, two variables.

$\epsilon = 10^{-5}$

	Bisections	Possible	Verif.	P.-Lebes.	V.-Lebes.	Time(s)
GS+Hansen	69909	65605	3390	2.24e-6	0.58	3.9
cmp+HR	198552	191401	7080	6.70e-6	0.51	8.7
cmp+Gou	70571	66014	3614	2.04e-6	0.55	3.0
cmp+GE	70571	66014	3614	2.04e-6	0.55	2.9
cmp+GouGE	70571	66014	3614	2.04e-6	0.55	2.9

Computational results

Puma problem (inverse kinematics of a 3R robot).
8 equations with 8 unknowns.
One of classical benchmark problems.
http://www-sop.inria.fr/coprin/logiciels/ALIAS/Benches/benches.html

$$x_1^2 + x_2^2 = 0, \qquad x_i \in [-1, 1], \quad i = 1, \ldots, 8$$
$$x_3^2 + x_4^2 = 0$$
$$x_5^2 + x_6^2 = 0$$
$$x_7^2 + x_8^2 = 0$$
$$0.004731 \cdot x_1 \cdot x_3 - 0.3578 \cdot x_2 \cdot x_3 - 0.1238 \cdot x_1 - 0.001637 \cdot x_2 - 0.9338 \cdot x_4 + x_7 = 0$$
$$0.2238 \cdot x_1 \cdot x_3 + 0.7623 \cdot x_2 \cdot x_3 + 0.2638 \cdot x_1 - 0.07745 \cdot x_2 - 0.6734 \cdot x_4 - 0.6022 = 0$$
$$x_6 \cdot x_8 + 0.3578 \cdot x_1 + 0.004731 \cdot x_2 = 0$$
$$-0.7623 \cdot x_1 + 0.2238 \cdot x_2 + 0.3461 = 0$$

Computational results

Puma problem with 8 variables and 6 equations (last two dropped).

$\epsilon = 10^{-1}$

	Bisections	Possible	Verif.	P.-Leb.	V.-Leb.	Time(s)
GS+Hansen	125155	73848	400	3.91e-7	1.38e-08	74.7
cmp+HR	97823	70968	0	6.11e-7	-	41.2
cmp+Gou	208551	117144	16	8.86e-7	1.79e-11	84.6
cmp+GE	254712	136736	72	7.43e-7	5.32e-10	92.1
cmp+GouGE	253071	134496	88	8.29e-7	5.49e-10	95.6

Puma problem with 8 variables and 7 equations (but the last one).

$\epsilon = 10^{-3}$

	Bisections	Possible	Verif.	P.-Lebes.	V.-Lebes.	Time(s)
GS+Hansen	16879	9784	504	7.13e-24	3.39e-17	13.0
cmp+HR	406967	210760	56	4.60e-22	5.31e-15	193.3
cmp+Gou	919363	327420	60	8.04e-22	3.27e-20	422.9
cmp+GE	995668	351932	60	1.76e-21	3.29e-20	404.5
cmp+GouGE	1127947	385448	44	1.25e-21	8.46e-18	471.0

Parallelization

- Shared memory environment & OpenMP.
- The stack of boxes is shared between threads; a lock prevents it from race conditions.
- Each thread after bisection stacks one of the boxes and processes the other one.
- Statistics are computed using atomic operations (instead of each thread having its own object with statistics).
- A global variable denotes the number of threads that are not idle – used to finishing computations.

Parallelization – results

- A limited speedup was observed for a few threads (c. a. 2.5 – 3.5 for 4 threads).
- It seems the improvement should be more significant as operations that have to be synchronized are quick.
- Probably poor implementation of OpenMP in the GNU compiler is guilty.
- An implementation using POSIX threads will explain that (coming soon).

Conclusions

- Interval methods can be applied to underdetermined problems successfully, though such problems are more demanding than well-determined ones.
- Algorithms should differ (in several details) from the ones used for well-determined problems.
- Computational results are not conclusive about the choice of Newton operator variant.
  - GS operator with Hansen's heuristic preformed well,
  - Cmp. variants happened to be both better and worse than GS.
- Some theorems were presented.
- Several accelerations are possible (e.g. parallelization).