SONIC

A Solver and Optimizer for Nonlinear Problems based on Interval Computations

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Contents

What is SONIC

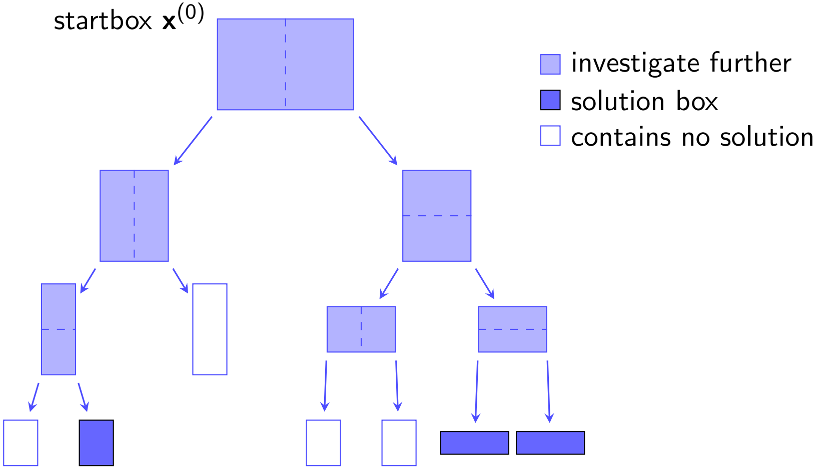
SONIC– A **S**olver and **O**ptimizer for **N**onlinear Problems based on **I**nterval **C**omputations

- rigorous solver for nonlinear systems
- developed at RWTH Aachen and University of Wuppertal
- initially for dynamic systems in chemical processes

Features

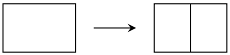
- written in `C++`
- portability and performance by different interval libraries: choice between `C-XSC`, `filib++`
- parallel versions for distributed and shared memory (MPI, OpenMP)
- solver for optimization problems
- handling of unbounded intervals

Branch and Bound



Subdivison

- subdivision using gaps caused by division
- choice of subdivision direction:
  - subdivide direction with largest width
  - search zeros near boundary
  - search direction with highest influence on function value
  - hybrid strategy
- choice of subdivision point:
  - bisect at midpoint



  - shift bisection point

- iterated subdivision

Contractors

Aim: Contract or discard a given box

- Constraint propagation
- Taylor refinement
- Interval Newton method
- Taylor models

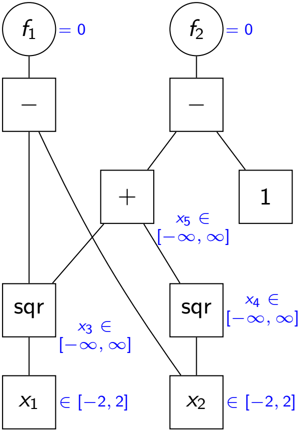
Constraint propagation

Consider system

$$f_1(x) = x_1^2 - x_2 = 0$$

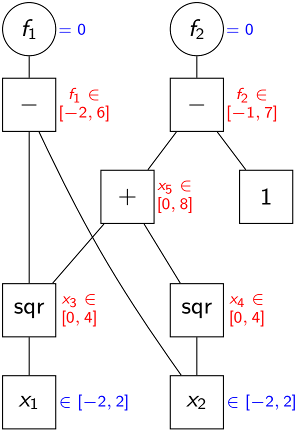
$$f_2(x) = x_1^2 + x_2^2 - 1 = 0$$

with $x \in [-2, 2]^2$



Constraint propagation

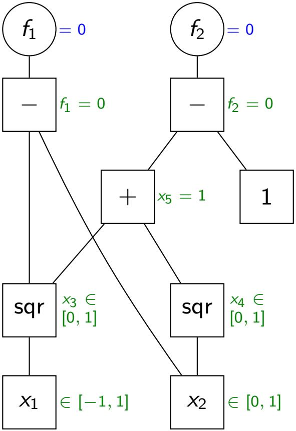
Forward sweep corresponds to the natural interval evaluation



Constraint propagation

Backward sweep yields narrower bounds:

$$0 = f_1 = x_3 - x_2$$
$$\Leftrightarrow x_3 = f_1 + x_2 \in$$
$$(0 + [-2, 2]) \cap [0, 4] = [0, 2]$$
$$\dots$$
$$x_1 = \pm\sqrt{x_3} \in [-1, 1]$$
$$x_2 = \pm\sqrt{x_4} \in [0, 1]$$



Taylor refinement

Gain sharper enclosure by Taylor expansion for $f : \mathcal{D} \subseteq \mathbb{R}^n \to \mathbb{R}$:

$$f(\mathbf{x}) \subseteq f(c) + \sum_{i=1}^{n} \mathbf{s_i} \cdot (\mathbf{x_i} - c_i)$$

$$\mathbf{x_i'} := \mathbf{x_i} \cap \left(c_i - \left(f(c) + \sum_{\substack{j=1 \\ j \neq i}}^{n} \mathbf{s_j} \cdot (\mathbf{x_j} - c_j) \right) \oslash \mathbf{s_i} \right), \qquad i = 1 \dots n$$

with some center $c \in x$ and slope vector s

Interval Newton method

Refines or discards box

$$\mathbf{f}(\mathbf{x}) \subseteq f(c) + \mathbf{S}(\mathbf{x} - c)$$

$$-f(c) = \mathbf{S}(x^* - c)$$

- solve with Gauß-Seidel-approach
- several preconditioners available
- can be used to verify the existence of a (unique) solution

Algorithm 1 Application scheme for contractors (box $\mathbf{x}$)

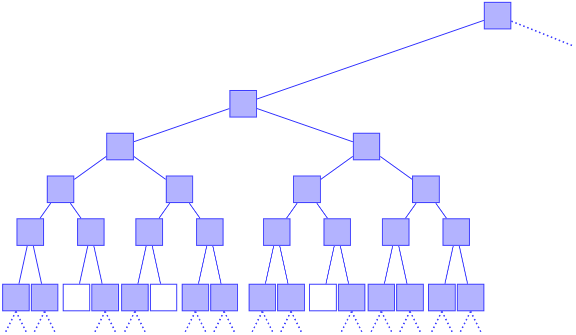
```
if CP is enabled then apply CP
if x cannot contain a solution then discard x
if Taylor refinement of first order is enabled then
    apply Taylor refinement of first order
    if CP is enabled then apply CP
end if
if x cannot contain a solution then discard x
if Taylor refinement of second order is enabled then
    apply Taylor refinement of second order
    if CP is enabled then apply CP
end if
if x cannot contain a solution then discard x
if Newton method is enabled then
    apply Newton method
    if CP is enabled then apply CP
end if
if x cannot contain a solution then discard x
```

Verification

Aim: Prove existence or uniqueness of a solution in a given box

- Newton test
  - apply one step of the interval Newton method
  - proofs uniqueness
- Miranda test
  - compare sign of function values on opposite facets
- Borsuk test
- topological degree test

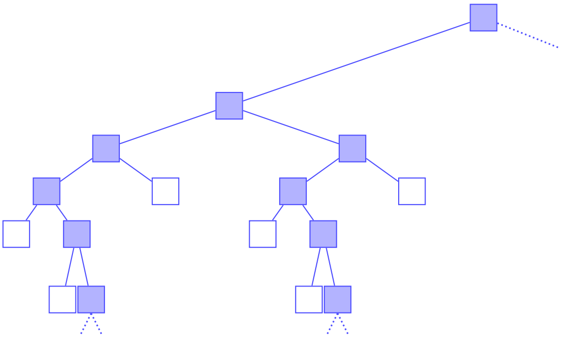
Problem: Too many boxes...



no discarding of boxes

many boxes → slow

Problem: Too many boxes...



Taylor models discard boxes

fewer boxes left to investigate

Taylor models

Idea: Enclosure of a function over its course

based on the works by Berz, Hoefkens and Makino

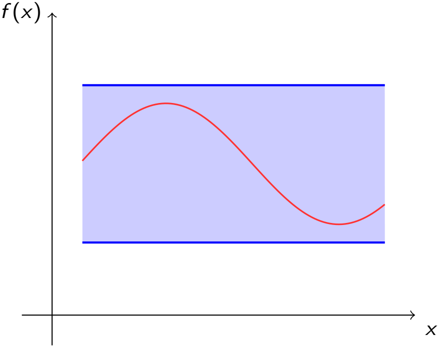
Consists of

- domain $\mathcal{D} \in \mathbb{R}^v$
- reference point $x_0 \in \mathcal{D}$
- Taylor polynomial $P_n : \mathcal{D} \to \mathbb{R}^w$ of order n
- remainder interval $R \in \mathbb{IR}^w$

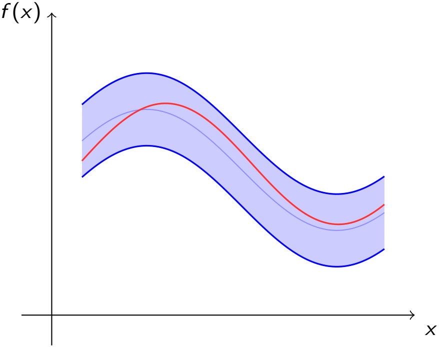
Inclusion property for all $x \in \mathcal{D}$:

$$f(x) \in P_n(x) + R$$

Function enclosures



Enclosure by a box ...



... and a Taylor Model

Properties of Taylor models

- sharper enclosure over relatively large domain
  $\Rightarrow$ avoids subdivisons
- the remainder interval scales with the $(n+1)$-st order of the magnitude of $\mathcal{D}$
- reduced impact of the dependency problem
- number of coefficients for a polynomial of order n with v variables: $\frac{(n+v)!}{n! \cdot v!}$

Taylor models in SONIC

Usage of Taylor models as a contractor in SONIC:

Algorithm 2 Usage of Taylor models as a contractor (box x)

1: build Taylor model T over x
2: compute evaluation $B(T)$ of T
3: **if** $0 \notin B(T)$ **then**
4: discard x
5: **end if**

Results

Observations for the naive usage of Taylor models:

- computation time increases significantly
- most time is consumed on the buildup of the TM
- very few boxes get discarded
- natural function evaluation of Taylor polynomial causes overestimations
  $\rightarrow$ linear dominated bounder

Inverse Taylor models

Taylor models $T = (P_n, x_0, \mathcal{D}, R)$ and $S = (G_n, y_0, \Delta, \Omega)$

S *left-inverse Taylor model* for T if

- $G_n \circ P_n =_n \mathcal{I}$
- $P_n(x_0) = y_0$
- $f \in T \Rightarrow f(\mathcal{D}) \subset \Delta$
- $B(G_n(T) - I) \subsetneq \Omega$

Theorem

Let $T = (P_n, x_0, \mathcal{D}, R)$ and $S = (G_n, y_0, \Delta, \Omega)$ be given Taylor models such that S is a left-inverse Taylor model for T. Assume that $f \in T$ is invertible over $\mathcal{D}$.

Then there is $g \in S$ such that $g = f^{-1}$ on $f(\mathcal{D})$.

Newton method with inverse Taylor models

Algorithm 3 Newton method with taylor models ()

$k := 0$
repeat
    build n-th order Taylor model $T^{(k)}$
    over $D^{(k)}$ with reference point $mid(D^{(k)})$
    compute left-inverse Taylor model $S^{(k)}$ for $T^{(k)}$
    $D^{(k+1)} := D^{(k)} \cap S^{(k)}(0)$
    if $D^{(k+1)} = \emptyset$ **then**
        discard box
    end if
    $k := k + 1$
until $D^{(k)}$ accurate enough

Properties

Properties of the inverse TM Newton method:

- faster speed of convergence
- larger domain of convergence
- less domain splitting required
- less impact of dependency problem and cancellation errors

Future plans

- web interface
- graphical output

Contact

For questions write to

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