Introduction of auxiliary variables into an interval function for improving its monotonicity-based evaluation

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Interval Analysis

- An interval \([x] = [a; b] = \{x \in \mathbb{R} | a \leq x \leq b\}\) represents the domain of a variable \(x\).

- A box \([B]\) is a vector of intervals defining the search space.

- Basic interval operators for \([x] = [a; b]\) and \([y] = [c; d]\).
  \[\begin{align*}
  [x] \text{op} [y] &= \{x \text{ op } y | x \in [x], y \in [y]\} \\
  [x] + [y] &= [a + c; b + d] \\
  [x] - [y] &= [a - d; b - c] \\
  [x] \times [y] &= [\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)] \\
  [x]/[y] &= [a; b] \times [1/d, 1/c], 0 \notin [y].
  \end{align*}\]
An interval extension \([f([x], [y], ..)]\) encloses all the values of \(f(x, y, ..)\) for \(\{x, y, ..\} \in \{[x], [y], ..\}\), that is:

\[
[f([B])] \supseteq \{f(X)/X \in [B]\}
\]

The natural interval extension of a function \(f\) is obtained replacing each variable for its domain and applying interval arithmetics. For example:
\(f(x, y) = x^2 - x + y\) and \([x] = [1; 5]\), \([y] = [-3; 4]\).

The natural extension of \(f\) is:
\([f([x], [y])] = [1; 5]^2 - [1; 5] + [-3; 4] = [-7; 28]\)

If a variable occurs more than once in a function, the natural extension overestimates the true range (dependency problem). The true range of \([f]\) is \([-3; 24]\).
The monotonicity of a function $f$ in $[\mathcal{B}]$ can be used to compute sharper interval extensions of $f$ eliminating the dependency problem in the monotonic variables ($x$ s.t. $\frac{\partial f}{\partial x} \geq 0$ or $\frac{\partial f}{\partial x} \leq 0$, $\forall X \in [\mathcal{B}]$).

Consider the function $f(X) = f(x_1, .., x_k)$

- $x_1, .., x_i$ are monotonic increasing.
- $x_{i+1}, .., x_j$ are monotonic decreasing.
- The evaluation by monotonicity of $f$ in the box $[\mathcal{B}] = \{[x_1], ..,[x_k]\}$ is given by:
  - $f_{min} = \overline{f}(x_1, .., \underline{x_i}, \overline{x_{i+1}}, .., \underline{x_j}, [x_{j+1}], .., [x_k])$
  - $f_{max} = \underline{f}(\underline{x_1}, .., \overline{x_i}, \underline{x_{i+1}}, .., \overline{x_j}, [x_{j+1}], .., [x_k])$
  - $[f]_M([\mathcal{B}]) = [f_{min}, f_{max}]$
Consider the function \( f(x, y) := x^2 - x + y \) with domains \([x] = [1; 5]\) and \([y] = [-3; 4]\).

The natural extension \([f]\) of \( f \) is:

\[
[f]([1; 5], [-3; 4]) = [1; 5]^2 - [1; 5] + [-3; 4] = [-7; 28]
\]

The evaluation by monotonicity \([f]_M\) of \( f \):

\[
[f]_M ([1; 5], [-3; 4]) = [-3; 24]
\]
The evaluation by monotonicity is sharper than (or equivalent to) the natural extension if at least one variable is monotonic and has multiple occurrences.
Contributions

- Improving the evaluation by monotonicity $[f]_M([\mathbf{B}])$ when a variable $x$ is not monotonic in $[\mathbf{B}]$ using a so-called **Occurrence Grouping (OG)**:
  - Function $f$ is transformed in $f^*$.
  - $f^*$ replace all the occurrences of $x$ in $f$ by auxiliary variables: $x_a$, $x_b$ or $x_c$.
  - $x_a$ and $x_b$ are monotonic variables in $f^*$
    $\rightarrow [f^*]_M([\mathbf{B}^*]) \subseteq [f]_M([\mathbf{B}])$.

- Finding a OG that minimizes a Taylor-based estimation of $W([f^*]_M)$.
Outline

1. Introduction
2. Occurrence Grouping
3. An Efficient OG Algorithm
4. Experiments
Consider the function \( f(x) = x^2 + x^3 + 7x + x^4 - 2x \) with \([x] = [-1; 1] \Rightarrow x \) is not monotonic in \([B]\).

The **OG** method consists in transforming \( f(x) \) in a new function \( f^*(x_a, x_b, x_c) \), replacing the occurrences of \( x \) by \( x_a, x_b \) or \( x_c \), s.t.

\[
\frac{\partial f}{\partial x_a} \geq 0, \quad \frac{\partial f}{\partial x_b} \leq 0, \quad \forall \{x_a, x_b, x_c\} \in [B^*] \quad ([g](x_a) \geq 0, \ [g](x_b) \leq 0)
\]

and \([x_a] = [x_b] = [x_c] = [x]\).

A possible OG for \( f \):

\[
f^* = x_b^2 + x_c^3 + 7x_a + x_a^4 - 2x_b
\]

where \([g](x_a) = [3; 11] \geq 0\) and \([g](x_b) = [-4; 0] \leq 0\)
Occurrence Grouping (Example 2/2)

\[
f = x^2 + x^3 + 7x + x^4 - 2x
\]

\[
f^* = x_b^2 + x_c^3 + 7x_a + x_a^4 - 2x_b
\]

- The natural extension \( f[B] \) is \([-10; 12]\).
- The evaluation by monotonicity \( f^*[B^*] \) is \([-8; 12]\).
Proposition

Let $f^*$ be the result of applying an OG procedure to a function $f$ for one non-monotonic variable. Then:

the evaluation by monotonicity of $f^*$ is sharper than the evaluation by monotonicity of $f$.

$[f^*]^M \subseteq [f]^M \subseteq [f]$
The Optimization Problem

- The objective of OG is to sharpen, as much as possible, the evaluation by monotonicity of a function \( f \) in a box \([\mathcal{B}]\).
- We want to minimize the width \( W \) of the interval: \([f^*]_M\).
- Using Taylor series we can represent an overestimation of \([f^*]_M\) as an interval \([W_{f^*}] \supseteq W\):

Overestimation of the width of \([f^*]_M\)

\[
[W_{f^*}] = \sum_{i=1}^{k} \left[ w([x_i]) \times \left( [g](x_{ia}) - [g](x_{ib}) + \sum_{j=1}^{\#x_{ic}} |[g](x_{ic}^{(j)})| \right) \right]
\]

\([g](x_{iz})\) is the interval gradient of \( x_{iz} \) in \([\mathcal{B}]\).
Observations

- $[W_{f^*}]$ is an interval and overestimates the width $W$ of $[f^*]_M$.
- A good **heuristic approach** to minimize $W$ is minimizing $\overline{W_{f^*}}$ and $\underline{W_{f^*}}$ at the same time.
- The optimal grouping is **independent for each variable** (every term in the sum is related to only one variable).
- The minimization of $\overline{W_{f^*}}$ and $\underline{W_{f^*}}$ can be reduced to the minimization of $\overline{G}$ and $\underline{G}$ for each variable $x \in X$, where:

$$
\overline{G} = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x_c} \left|[g](x_c^{(j)})\right|_{max} \right)
$$

$$
\underline{G} = \left( [g](x_a) - \overline{g}([x_b]) + \sum_{j=1}^{\#x_c} \left|[g](x_c^{(j)})\right|_{min} \right)
$$
The Optimization Problem

Minimize: $\overline{G}, \underline{G}$

\[
\overline{G} = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x} r_{c_j} \cdot |g(x_j)|_{max} \right)
\]

\[
\underline{G} = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x} |g(x_j)|_{min} \right)
\]

subject to:

\[
[g](x_a) = \sum_{j=1}^{\#x} r_{a_j} \cdot [g](x_j) \geq 0, \quad [g](x_b) = \sum_{j=1}^{\#x} r_{b_j} \cdot [g](x_j) \leq 0
\]

\[
r_{a_j} + r_{b_j} + r_{c_j} = 1
\]

\[
r_{a_j}, r_{b_j}, r_{c_j} = \{0, 1\}
\]
The problem is **discrete and likely NP-hard**: each occurrence of $x$ is replaced by $x_a$, $x_b$ or $x_c$.

If we replace each variable $x$ in $X$ by $r_a \cdot x_a + r_b \cdot x_b + r_c \cdot x_c$ in $f^*$ ($r_a, r_b, r_c \geq 0$ and $r_a + r_b + r_c = 1$):

- Natural extensions are equivalents: $[f] = [f^*]$.
- The new problem is **continuous and tractable**: each occurrence of $x$ is split into 3 parts that are replaced by $x_a$, $x_b$ and $x_c$.
- The relaxed problem has lower minimums.
The Optimization Problem

Minimize: $\overline{G}$, $G$

$$\overline{G} = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x} r_{c_j} \cdot |g(x_j)|_{max} \right)$$

$$G = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x} |g(x_j)|_{min} \right)$$

subject to:

$$[g](x_a) = \sum_{j=1}^{\#x} r_{a_j} \cdot [g](x_j) \geq 0, \quad [g](x_b) = \sum_{j=1}^{\#x} r_{b_j} \cdot [g](x_j) \leq 0$$

$$r_{a_j} + r_{b_j} + r_{c_j} = 1$$

$$r_{a_j}, r_{b_j}, r_{c_j} \geq 0$$
Proposition

For any variable \( x \), there exists a grouping \( \{ x_a, x_b, x_c \} \) such that:

\[
\bar{G}(x_a, x_b, x_c) \leq \bar{G}(x_{a_1}, x_{b_1}, x_{c_1}) \quad \text{and} \quad \underline{G}(x_a, x_b, x_c) \leq \underline{G}(x_{a_2}, x_{b_2}, x_{c_2})
\]

for all groupings \( \{ x_{a_1}, x_{b_1}, x_{c_1} \} \) and \( \{ x_{a_2}, x_{b_2}, x_{c_2} \} \). Where,

\[
\bar{G}(x_a, x_b, x_c) = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x_c} |[g](x_c^{(j)})|_{\text{max}} \right)
\]

\[
\underline{G}(x_a, x_b, x_c) = \left( [g](x_a) - [g](x_b) + \sum_{j=1}^{\#x_c} |[g](x_c^{(j)})|_{\text{min}} \right)
\]

subject to the previous constraints.
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Description of the algorithm

- Our algorithm finds a grouping that minimizes: $\overline{G}(x_a, x_b, x_c)$ and $G(x_a, x_b, x_c)$ at the same time.

- Let $x_m$ and $x_n$ be the sets of monotonic and non monotonic occurrences of a variable $x$ resp. There exists 3 possible cases:
  - $[g](x) > 0$ (or $[g](x) < 0$): the variable is monotone $\Rightarrow$ all the occurrences of $x$ are replaced by $x_a$ (or $x_b$).
  - $[g](x_m) \ni 0$: the variable is non monotone, each occurrence in $x_m$ is replaced by $r.x_a + (1 - r).x_b$.
  - $[g](x_m) > 0$ (or $[g](x_m) < 0$) and $[g](x) \ni 0$: the variable is non monotone, all the occurrences in $x_m$ and a part of the occurrences in $x_n$ are replaced by $x_a$ (or $x_b$).
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**Case:** \([g](x_m) \ni 0\)

1: \([g_{m+}, g_{m+}] \leftarrow [g](x_{m+})\)
2: \([g_{m-}, g_{m-}] \leftarrow [g](x_{m-})\)
3: \(\frac{g_{m+}g_{m-} + g_{m-}g_{m-}}{g_{m+}g_{m-} - g_{m-}g_{m+}}\)
4: \(r_1 \leftarrow \frac{g_{m+}g_{m+} + g_{m-}g_{m+}}{g_{m+}g_{m-} - g_{m-}g_{m+}}\)
5: \(r_2 \leftarrow \frac{g_{m+}g_{m+} + g_{m-}g_{m+}}{g_{m+}g_{m-} - g_{m-}g_{m+}}\)
6: 
7: **for all** \(x \in x_{m+} \textbf{ do } x \leftarrow (1 - r_1).x_a + r_1.x_b \textbf{ end for}**
8: **for all** \(x \in x_{m-} \textbf{ do } x \leftarrow r_2.x_a + (1 - r_2).x_b \textbf{ end for}**
9: **for all** \(x \in x_n \textbf{ do } x \leftarrow x_c \textbf{ end for}**
Case: $[g](x_m) > 0$ and $[g](x) \ni 0$

for all $x \in x_m$ do $x \leftarrow x_a$ end for

$x_n \leftarrow \text{AscOrder}(x_n, f_{order} = -[g](x)/[g](x))$

for all $x \in x_n$ do
    if $[g](x_a) + [g](x) \geq 0$ then
        $x \leftarrow x_a$
    else
        $r \leftarrow -[g](x_a)/[g](x)$
        $x \leftarrow r.x_a + (1 - r).x_c$
    end if
end for
Occurrence grouping v/s natural extension

Example:

- Consider $f(x) = x^2 + x^3 + 7x + x^4 - 2x$, $[x] = [-1; 1]$.
- The grouping algorithm convert $f$ into:
  $$f^* = x^2_a + x^3_a + 7x_a + \left(\frac{3}{4}x_a + \frac{1}{4}x_c\right)^4 - 2x_a$$
- The evaluation by monotonicity of $f^*$:
  $$[f^*]_M = [-4.94; 8]$$
  that is 40% sharper than
  $$[f] = [f]_M = [-10; 12]$$
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Experimentation

- Implementation in Ibex, C++.
- Interval solver using 3BCID + Interval Newton as contractors (3BCID).
- OG has been incorporated in two methods that use the evaluation by monotonicity.
  - Monotonicity test applied before the contractor (MonoTest).
  - MoHC, a monotonicity-based contractor, inside 3BCID (MoHC).
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We have proposed **Occurrence Grouping**, a new method to obtain sharper evaluations using monotonicity.

OG adds monotonicities of non-monotonic variables

\[ [f^*]_M \subseteq [f]_M. \]

We solve an overestimation of an interesting problem: **minimization of the width of the evaluation by monotonicity of** \( f^* \).

The results show that OG can produce considerable improvements.
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