Relaxing kindly and efficiently

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based on joint works with
D. Skipper (USNA) and E. Speakman (U. Mich.)
Context: Global optimization

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Several key paradigms: convex vs nonconvex? polynomials? (partially-)separable?
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Considerable ‘generic’ software available via modeling languages (e.g., GAMS, AMPL, JuMP):

- **Approach I**: B&B, Outer approx, hybrid approaches [aimed at finding optima of convex instances] (e.g., Bonmin, SBB, KNITRO, AlphaECP, DICOPT)

- **Approach II**: Spatial B&B/Global optimization [aimed at finding optima of nonconvex instances] (e.g., Baron, Couenne, SCIP, ANTIGONE)
Spatial Branch-and-Bound

Spatial branch-and-bound is a global-optimization strategy successfully aimed at “factorable” formulations:

- $\sin(x)$
- $|x|$
- $ax$
- $x^p$
- $\log(x)$
- $x + y$
- $x \times y$
- $x \times y \times z$, etc.

In this way a function is kept as a DAG, with the leaves being model variables. We must be able to bound the graph of every library function (on an interval or a square domain) with a convex set. Bounds at the leaves propagate up, bounds at the root propagate down. The DAGs and the leaf bounds end up giving us a convex relaxation of our formulation. Branching is done by subdividing the (interval) domain of a variable.
Spatial Branch-and-Bound

Spatial branch-and-bound is a global-optimization strategy successfully aimed at “factorable” formulations:

- functions are built up from a library of functions of 1, 2 and sometimes 3 variables: \( \sin(x) \), \(|x|\), \(a^x\), \(x^p\), \(\log(x)\), \(x + y\), \(x \times y\), \(xy\), \(x \times y \times z\), etc.
- in this way a function is kept as a DAG, with the leaves being model variables.
- we must be able to bound the graph of every library function (on an interval or a square domain) with a convex set.
- bounds at the leaves propagate up, bounds at the root propagate down.
- the DAGS and the leaf bounds end up giving us a convex relaxation of our formulation.
- branching is done by subdividing the (interval) domain of a variable
Branching and re-convexifying
Two spatial branch-and-bound issues

- Functions should be twice continuously differentiable, as is technically required by most NLP solvers to give fast local convergence.

  E.g., root functions $x^p$, with $0 < p < 1$ are not smooth at 0.

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- Functions should be twice continuously differentiable, as is technically required by most NLP solvers to give fast local convergence.

  E.g., root functions $x^p$, with $0 < p < 1$ are not smooth at 0.


- How should we build our DAGS? Where to branch?

  E.g., $x \times y \times z = xyz = (xy)z = (xz)y = (yz)x$.

1st Topic
A class of almost well-behaved univariate functions

We suppose that $f(w), w \geq 0$ has the following properties: $f(0) = 0$, $f'(0)$ is undefined (and maybe even blows up as we tend toward 0), $f$ is increasing and concave, and $f(w)$ is twice continuously differentiable for $w > 0$
A class of almost well-behaved univariate functions

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Goal

Find an underestimator that mimics $f$, but is twice continuously differentiable (and maybe has a controlled derivative everywhere).
Natural polynomial smoothing

Motivated by the case of $f(w) = \sqrt{w}$ addressed by D’Ambrosio, Fampa, Lee and Vigerske, we define a smooth approximation for $f$ as follows:

$$g(w) = \begin{cases} 
Aw^3 + Bw^2 + Cw, & 0 \leq w \leq \delta \\
 f(w), & w > \delta,
\end{cases}$$

where

$$A = \frac{f(\delta)}{\delta^3} - \frac{f'(\delta)}{\delta^2} + \frac{f''(\delta)}{2\delta},$$

$$B = -\frac{3f(\delta)}{\delta^2} + \frac{3f'(\delta)}{\delta} - f'''(\delta),$$

$$C = \frac{3f(\delta)}{\delta} - 2f'(\delta) + \frac{\delta f''(\delta)}{2}.$$
Piecewise smooth at $\delta$

**Observation 1**

*By construction, $g$ has $g(0) = 0$, $g(\delta) = f(\delta)$, $g'(\delta) = f'(\delta)$ and $g''(\delta) = f''(\delta)$; i.e. $g$ is twice continuously differentiable.*
Summary of Results

Extending results of D’Ambrosio, Fampa, Lee and Vigerske (for $f(w) = \sqrt{w}$):

- We demonstrate that $g$ is not always increasing and concave.
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- We give a sufficient condition on $f$ (satisfied by some natural functions) so that $g$ is increasing and concave. New in SCIP 3.2!
- We demonstrate that $g$ is a lower bound for $f$ when $f$ is an “integer-root” function: $f(w) = w^{1/q}$, for integer $q \geq 2$.
- We demonstrate that $g$ is a tighter bound than the simpler “shifted root” for lots of integer-root functions: $f(w) = w^{1/q}$, integer $2 \leq q \leq 10,000$. 

![Graph showing the comparison of $g$ and $f$ for different values of $q$.]
Example 2 (where $g$ is not concave and increasing)

For $\epsilon > 0$, let

$$f(w) := \begin{cases} 
\sqrt{w - 1} - \sqrt{\epsilon} + \frac{1+\epsilon}{2\sqrt{\epsilon}}, & w \geq 1 + \epsilon; \\
\frac{1}{2\sqrt{\epsilon}} w, & w < 1 + \epsilon.
\end{cases}$$

- $f(0) = 0$, $f$ is twice differentiable, increasing, and concave on $[0, +\infty)$
- Our sufficient condition for $g$ to be increasing and concave is not satisfied when $\epsilon = 1/10$, $\phi = 1/100$, and $\delta = 1 + \epsilon + \phi$. 

In fact, $g(w)$ is decreasing and convex for $0 < w < \epsilon$. Can modify the example (adding a bit of $\sqrt{w}$) to make $f$ strictly concave and also nondifferentiable at 0.
Example 2 (where \( g \) is not concave and increasing)

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- \( f(0) = 0 \), \( f \) is twice differentiable, increasing, and concave on \([0, +\infty)\).
- Our sufficient condition for \( g \) to be increasing and concave is not satisfied when \( \epsilon = 1/10 \), \( \phi = 1/100 \), and \( \delta = 1 + \epsilon + \phi \).
- In fact, \( g(w) \) is decreasing and convex for \( 0 < w < \epsilon \).
- Can modify the example (adding a bit of \( \sqrt{w} \)) to make \( f \) strictly concave and also nondifferentiable at 0.
Theorem 3 (sufficient condition)  

On $[\delta, +\infty)$, let $f$ be increasing and differentiable, with $f'$ non-increasing (decreasing); $f(0) = 0$, and $f$ twice differentiable at $\delta$. If

$$f''(\delta) \geq \frac{2}{\delta} \left( f'(\delta) - \frac{f(\delta)}{\delta} \right),$$

then $g$ is increasing and concave (strictly concave) on $[0, +\infty)$. 
Increasing and concave

**Theorem 3 (sufficient condition)**

On \([\delta, +\infty)\), let \(f\) be increasing and differentiable, with \(f'\) non-increasing (decreasing); \(f(0) = 0\), and \(f\) twice differentiable at \(\delta\). If

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f''(\delta) \geq \frac{2}{\delta} \left( f'(\delta) - \frac{f(\delta)}{\delta} \right),
\]

then \(g\) is increasing and concave (strictly concave) on \([0, +\infty)\).

**Corollary 4 (roots)**

For \(f(w) = w^p\), \(0 < p < 1\), \(g\) is increasing and strictly concave on \([0, +\infty)\).

\[f(w) = w^{1/3}, \, \delta = 0.0001\]
Example 5 (not only roots)

Let \( f(w) := \log(1 + w) \), \( w \geq 0 \). To verify that the sufficient condition is satisfied for \( \delta > 0 \), we consider the expression \( f''(\delta) - \frac{2}{\delta} \left( f'(\delta) - \frac{f(\delta)}{\delta} \right) \), which simplifies to

\[
\frac{2(1 + \delta)^2 \log(1 + \delta) - 3\delta^2 - 2\delta}{\delta^2 (1 + \delta)^2}.
\]

The denominator of this expression is positive so we focus on the numerator, which we define to be \( k(\delta) \). The second derivative of the numerator, \( k''(\delta) = 4 \log(1 + \delta) \), is positive for \( \delta > 0 \), implying that the \( k'(\delta) = 4(1 + \delta) \log(1 + \delta) - 4\delta \) increases from \( k'(0) = 0 \). Therefore, \( k(\delta) \) likewise increases from \( k(0) = 0 \). We conclude that the sufficient condition is satisfied for \( \delta > 0 \). Note that we can add \( \sqrt{w} \) to \( f \) to get an example that is not differentiable at 0.
Lower bound and better

Theorem 6 (Lower bound)

For \( f(w) := w^p \), with \( p = 1/q \) for integer \( q \geq 2 \), we have \( g(w) \leq f(w) \) for all \( w \in [0, +\infty) \).
Lower bound and better

Theorem 6 (Lower bound)

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How do we compare to a simpler “shift” smoothing for roots?

Theorem 7 (Better lower bound)

For \( f(w) := w^p \), with \( p = 1/q \) and \( 2 \leq q \leq 10,000 \), for all \( \delta > 0 \),

\[
g(w) \geq h(w) := (w + \lambda)^p - \lambda^p, \quad w \in [0, \infty),
\]

when \( \lambda \) is chosen so that \( g'(0) = h'(0) \).
Lower bound: proof summary

We seek to express \((f - g)(w)\) as a product of factors that are nonnegative for \(0 \leq w \leq \delta\):

\[
(f - g)(w) = w^p - \frac{d^{p-3}}{2}(p^2 - 3p + 2)w^3 \\
+ d^{p-2}(p^2 - 4p + 3)w^2 - \frac{d^{p-1}}{2}(p^2 - 5p + 6)w
\]
Lower bound

We reparameterize $f - g$ to arrive at a polynomial in $t$: $0 \leq t \leq L$, where $L = \delta^{1/q}$:

$$(f - g)(t) = \frac{t}{2q^2 L^{3q-1}} \left(2q^2 L^{3q-1} - (6q^2 - 5q + 1)L^{2q} t^{q-1} + (6q^2 - 8q + 2)L^q t^{2q-1} - (2q^2 - 3q + 1)t^{3q-1}\right)$$
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We discover that $(L - t)^3$ is a factor of $(f - g)(t)$. For example, for $q = 3$, we have:

$$(f - g)(t) = \frac{t}{18L^8}(18L^5 + 54L^4t + 68L^3t^2 + 60L^2t^3 + 30Lt^4 + 10t^5)(L - t)^3$$

Notice that the remaining factor has all positive coefficients. This turns out to be the case for all integers $q \geq 2$. 
Lower bound

For integer $q \geq 2$, we find that $(f - g)(t) = \frac{t}{2q^2 L^{3q-1}} Q_q(L - t)^3$, where $Q_q$ has the following $3q - 3$ terms:

$$\left(\begin{array}{c} i + 2 \\ 2 \end{array}\right) a L^{3q-4-i} t^i, \quad 0 \leq i \leq q - 2;$$

$$\left[ \left(\begin{array}{c} i + 2 \\ 2 \end{array}\right) a - \left(\begin{array}{c} i - q + 3 \\ 2 \end{array}\right) b \right] L^{3q-4-i} t^i, \quad q - 1 \leq i \leq 2q - 2;$$

$$\left[ \left(\begin{array}{c} i + 2 \\ 2 \end{array}\right) a - \left(\begin{array}{c} i - q + 3 \\ 2 \end{array}\right) b + \left(\begin{array}{c} i - 2q + 3 \\ 2 \end{array}\right) c \right] L^{3q-4-i} t^i, \quad 2q - 1 \leq i \leq 3q - 4.$$

where

$$a = 2q^2$$

$$b = 6q^2 - 5q + 1$$

$$c = 6q^2 - 8q + 2$$
Lower bound

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The first type of coefficients are obviously positive: \( \binom{i+2}{2} aL^{3q-4-i} \).

For the second type of coefficients, we extend the discrete function of \( i \) that describes the coefficients to a function on a continuous domain with the same endpoints:

\[
C_2(x) = \frac{1}{2} (x + 2)(x + 1)a - \frac{1}{2} (x - q + 2)(x - q + 1)b, \quad x \in [q - 1, 2q - 2].
\]

We can see that \( C''_2(x) = -4q^2 + 5q - 1 \) is negative for \( q > 1 \). Therefore, \( C_2(x) \) is concave with \( C_2(q - 1) > 0 \) and \( C_2(2q - 2) > 0 \).
Lower bound

For the **third type of coefficients**, we again consider the continuous extension of the coefficients:

\[
C_3(x) = \frac{1}{2}(x + 2)(x + 1)a - \frac{1}{2}(x - q + 3)(x - q + 2)b \\
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We can see that \( C'_3(x) = (2q^2 - 3q + 1)x - (6q^3 - 14q^2 + \frac{21}{2}q - \frac{5}{2}) \) is negative for \( x < 3q - \frac{5}{2} \).
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We can see that \(C'_3(x) = (2q^2 - 3q + 1)x - (6q^3 - 14q^2 + \frac{21}{2}q - \frac{5}{2})\) is negative for \(x < 3q - 5/2\).

In particular, \(C_3(x)\) is decreasing on the interval \([2q - 1, 3q - 4]\) to \(C_3(3q - 4) = 2q^2 - 3q + 1\), which is positive for \(q > 1\).
Theorem 7 (Better lower bound)

For \( f(w) := w^p \), with \( p = 1/q \) and \( 2 \leq q \leq 10,000 \), for all \( \delta > 0 \),

\[
  g(w) \geq h(w) := (w + \lambda)^p - \lambda^p, \quad w \in [0, \infty),
\]

when \( \lambda \) is chosen so that \( g'(0) = h'(0) \).

Proof: We calculate the shift constant \( \hat{\lambda} \) in terms of \( \delta \):

\[
  \hat{\lambda} = (f')^{-1}(g'(0)) = \delta \left( \frac{p^2 - 5p + 6}{2p} \right)^{\frac{1}{p-1}}.
\]

As in the previous proof, we apply a sequence of substitutions to express \( g - h \) as a polynomial.
Better lower bound

We obtain

\[(g - h)(u) = \frac{\gamma}{2q^2} K(u)\]

\[= \frac{\gamma}{2q^2} \left[ d (u^q - Q^q)^3 - c (u^q - Q^q)^2 + b (u^q - Q^q) - a(u - Q) \right],\]

for \(Q \leq u \leq (1 + Q^q)^{1/q}\), where \(a, b, c,\) and \(d\) are defined as before, and

\[Q := \left( \frac{2q}{6q^2 - 5q + 1} \right)^{1/(q-1)} \quad \text{and} \quad u := \left( \frac{w}{\gamma^q + Q^q} \right)^{1/q}.\]

It is obvious that \(K\) has a root at \(Q\). In fact, \(K\) has a double root at \(Q\), which we verify by showing that \(K'\) also has a root at \(Q\).
Better lower bound

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In order to prove that \(K(u) \geq 0\) for \(u \in (Q, (1 + Q^q)^{1/q})\), it suffices to show that there are no roots in the interval \((Q, (1 + Q^q)^{1/q})\).
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In order to prove that $K(u) \geq 0$ for $u \in (Q, (1 + Q^q)^{1/q})$, it suffices to show that there are no roots in the interval $(Q, (1 + Q^q)^{1/q})$.

In fact, we prove that the only root in the interval

$$(0, (1 + Q^q)^{1/q}) \supseteq (Q, (1 + Q^q)^{1/q})$$

is the double root at $Q$. 
Better lower bound

Using a known technique, we apply the Möbius transformation

\[ K \left( \frac{(1 + Q^q)^{1/q}}{v + 1} \right) \]

to express \( K, u \in (0, (1 + Q^q)^{1/q}) \), as a function of \( v \) over the interval \((0, \infty)\).
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to express $K, u \in (0, (1 + Q^q)^{1/q})$, as a function of $v$ over the interval $(0, \infty)$.

Note that when $v = 0$, $K \left( \frac{(1 + Q^q)^{1/q}}{v + 1} \right) = K \left( (1 + Q^q)^{1/q} \right)$, and as $v \to \infty$, $K \left( \frac{(1 + Q^q)^{1/q}}{v + 1} \right) \to K(0)$. 
Better lower bound

For each integer $2 \leq q \leq 10,000$, we employ Mathematica to calculate the coefficients of the transformed polynomial and verify that there are exactly two sign changes when listed in standard form.
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The same bound applies to the number of roots of $K(u)$ in the interval $(0, (1 + Q^q)^{1/q})$.

Therefore, the double root at $Q$ is the only root of $K(u)$ in the interval $(0, (1 + Q^q)^{1/q})$. □
2nd Topic
Factorable functions → Expression DAGs

A function can often be ‘factored’ in different ways. For example:

\[ x_1 x_2 \sin(x_1 x_3) \times x_1 x_2 \sin(x_1 x_3) \times \sin(x_1 x_3) \times \sin(x_1 x_3) \times x_1 x_3 \]

The performance of sBB depends on how we build such DAGs. Let’s explore analytically how to build good expression DAGs.
How should we convexify \( f = x_1x_2x_3, \; x_i \in [a_i, b_i] \)?

One possibility is the true trilinear hull

\[ \mathcal{P}_H := \text{conv} \{ (f, x_1, x_2, x_3) : x_i \in [a_i, b_i] \} \]

Let \( O_i := a_i(b_j b_k) + b_i(a_j a_k) \). Then we can construct a labeling such that \( O_1 \leq O_2 \leq O_3 \). Therefore, without loss of generality, we can assume that

\[ a_1b_2b_3 + b_1a_2a_3 \leq a_2b_1b_3 + b_2a_1a_3 \leq a_3b_1b_2 + b_3a_1a_2. \quad (\Omega) \]
How should we convexify $f = x_1 x_2 x_3$, $x_i \in [a_i, b_i]$?

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Let $O_i := a_i (b_j b_k) + b_i (a_j a_k)$. Then we can construct a labeling such that $O_1 \leq O_2 \leq O_3$. Therefore, without loss of generality, we can assume that

$$a_1 b_2 b_3 + b_1 a_2 a_3 \leq a_2 b_1 b_3 + b_2 a_1 a_3 \leq a_3 b_1 b_2 + b_3 a_1 a_2. \quad (\Omega)$$

### Theorem 8

$$\text{Vol}_{\mathcal{P}_H} = (b_1 - a_1)(b_2 - a_2)(b_3 - a_3) \times$$

$$(b_1 (5b_2 b_3 - a_2 b_3 - b_2 a_3 - 3a_2 a_3)$$

$$+ a_1 (5a_2 a_3 - b_2 a_3 - a_2 b_3 - 3b_2 b_3)) / 24$$
Proof sketch

- $\mathcal{P}_H$ has 8 vertices
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- Assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
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- include one more vertex at a time, by determining which facets of the current polytope are seen
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- do all of this in a judicious order
- continuity argument to handle the cases of some \( a_i = 0 \)

It turns out that for \( a_i > 0 \), \( \mathcal{P}_H \) is a simplicial polytope, the “type” of which was cataloged by Grünbaum and Sreedharan (1967) when they characterized the combinatorial types of all simplicial polytopes on 8 vertices in dimension 4.
Picture of $\mathcal{P}_H$

- start with the blue simplex
- then the red point sees only one facet, so we calculate the pyramid over that facet.
- Then the remaining two green points can be added separately (they each see different parts), and we build the relevant pyramids
The inequality description of $\mathcal{P}_H$ is “heavy”

Another possibility is “double McCormick”.

For $f = x_1 x_2$, we have McCormick: The convexification of the feasible points $(f, x_1, x_2)$ arises from the following inequalities, by multiplying out and substituting $f$ for all instances of $x_1 x_2$.

\[
(x_1 - a_1)(x_2 - a_2) \geq 0, \quad (x_1 - a_1)(b_2 - x_2) \geq 0, \\
(b_1 - x_1)(x_2 - a_2) \geq 0, \quad (b_1 - x_1)(b_2 - x_2) \geq 0.
\]
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$$
(x_1 - a_1)(x_2 - a_2) \geq 0, \quad (x_1 - a_1)(b_2 - x_2) \geq 0,
(b_1 - x_1)(x_2 - a_2) \geq 0, \quad (b_1 - x_1)(b_2 - x_2) \geq 0.
$$

**Double McCormick:** Consider the monomial $f = x_i x_j x_k$, and assume that we first group the variables $x_i$ and $x_j$. We let $w_{ij} = x_i x_j$, and so $f = w_{ij} x_k$. Next we write down the two McCormick relaxations. Then we project out $w_{ij}$, and consider the polytopes $\mathcal{P}_k \subset \mathbb{R}^4$ versus the trilinear hull $\mathcal{P}_H$. 
Double McCormick Inequalities

\[ w = x_1 x_2, \quad f = wx_3 \]

\[
\begin{align*}
    w - a_2 x_1 - a_1 x_2 + a_1 a_2 & \geq 0 \\
    -w + b_2 x_1 + a_1 x_2 - a_1 b_2 & \geq 0 \\
    -w + b_2 x_1 - b_1 x_2 - b_1 a_2 & \geq 0 \\
    w - b_2 x_1 - b_1 x_2 + b_1 b_2 & \geq 0 \\
    f - a_3 w - a_1 a_2 x_3 + a_1 a_2 a_3 & \geq 0 \\
    -f + b_3 w + a_1 a_2 x_3 - a_1 a_2 b_3 & \geq 0 \\
    -f + a_3 w + b_1 b_2 x_3 - b_1 b_2 a_3 & \geq 0 \\
    f - b_3 w - b_1 b_2 x_3 + b_1 b_2 b_3 & \geq 0
\end{align*}
\]
Double McCormick Inequalities

\[ w = x_1 x_2, \quad f = wx_3 \]

\[
\begin{align*}
  & w - a_2 x_1 - a_1 x_2 + a_1 a_2 \geq 0 \\
  & -w + b_2 x_1 + a_1 x_2 - a_1 b_2 \geq 0 \\
  & -w + a_2 x_1 + b_1 x_2 - b_1 a_2 \geq 0 \\
  & w - b_2 x_1 - b_1 x_2 + b_1 b_2 \geq 0 \\
  & f - a_3 w - a_1 a_2 x_3 + a_1 a_2 a_3 \geq 0 \\
  & -f + b_3 w + a_1 a_2 x_3 - a_1 a_2 b_3 \geq 0 \\
  & -f + a_3 w + b_1 b_2 x_3 - b_1 b_2 a_3 \geq 0 \\
  & f - b_3 w - b_1 b_2 x_3 + b_1 b_2 b_3 \geq 0 
\end{align*}
\]

System Projected Back Into \( \mathbb{R}^4 \) (\( w \) removed)

\[
\begin{align*}
  & f - a_2 a_3 x_1 - a_1 a_3 x_2 - a_1 a_2 x_3 + 2a_1 a_2 a_3 \geq 0 \\
  & f - a_2 b_3 x_1 - a_1 b_3 x_2 - b_1 b_2 x_3 + a_1 a_2 b_3 + b_1 b_2 b_3 \geq 0 \\
  & f - b_2 a_3 x_1 - b_1 a_3 x_2 - a_1 a_2 x_3 + a_1 a_2 a_3 + b_1 b_2 a_3 \geq 0 \\
  & f - b_2 b_3 x_1 - b_1 b_3 x_2 - b_1 b_2 x_3 + 2b_1 b_2 b_3 \geq 0 \\
  & -f + b_2 b_3 x_1 + a_1 b_3 x_2 + a_1 a_2 x_3 - a_1 a_2 b_3 - a_1 b_2 b_3 \geq 0 \\
  & -f + a_2 b_3 x_1 + b_1 b_3 x_2 + a_1 a_2 x_3 - a_1 a_2 b_3 - b_1 a_2 b_3 \geq 0 \\
  & -f + b_2 a_3 x_1 + a_1 a_3 x_2 + b_1 b_2 x_3 - a_1 b_2 a_3 - b_1 b_2 a_3 \geq 0 \\
  & -f + a_2 a_3 x_1 + b_1 a_3 x_2 + b_1 b_2 x_3 - b_1 a_2 a_3 - b_1 b_2 a_3 \geq 0 \\
  & a_i \leq x_i \leq b_i, \quad i = 1, 2, 3 
\end{align*}
\]
Extra extreme points

We need the following twelve points in $\mathbb{R}^4$, where $j := i + 1 \pmod{3}$ and $k := i + 2 \pmod{3}$:

\[
v_1^9 := \begin{bmatrix} \theta_1^1 \\ \theta_2^2 \\ a_2 \\ b_3 \end{bmatrix}, \quad v_1^{10} := \begin{bmatrix} \theta_1^3 \\ \theta_1^4 \\ b_2 \\ a_3 \end{bmatrix}, \quad v_1^{11} := \begin{bmatrix} \theta_1^5 \\ \theta_2^6 \\ b_2 \\ a_3 \end{bmatrix}, \quad v_1^{12} := \begin{bmatrix} \theta_1^7 \\ \theta_2^8 \\ a_2 \\ b_3 \end{bmatrix},
\]

\[
v_2^9 := \begin{bmatrix} \theta_2^1 \\ b_1 \\ \theta_2^2 \\ a_3 \end{bmatrix}, \quad v_2^{10} := \begin{bmatrix} \theta_2^3 \\ a_1 \\ \theta_2^4 \\ b_3 \end{bmatrix}, \quad v_2^{11} := \begin{bmatrix} \theta_2^5 \\ a_1 \\ \theta_2^6 \\ b_3 \end{bmatrix}, \quad v_2^{12} := \begin{bmatrix} \theta_2^7 \\ b_1 \\ \theta_2^8 \\ a_3 \end{bmatrix},
\]

\[
v_3^9 := \begin{bmatrix} \theta_3^3 \\ b_1 \\ a_2 \\ \theta_3^4 \end{bmatrix}, \quad v_3^{10} := \begin{bmatrix} \theta_3^1 \\ a_1 \\ b_2 \\ \theta_3^2 \end{bmatrix}, \quad v_3^{11} := \begin{bmatrix} \theta_3^7 \\ a_1 \\ b_2 \\ \theta_3^8 \end{bmatrix}, \quad v_3^{12} := \begin{bmatrix} \theta_3^5 \\ b_1 \\ a_2 \\ \theta_3^6 \end{bmatrix},
\]
where:

\[ \theta^1_i = a_i a_j a_k + \frac{a_j (b_k - a_k) (b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta^2_i = a_i + \frac{a_j (b_i - a_i) (b_k - a_k)}{b_j b_k - a_j a_k}, \]

\[ \theta^3_i = a_i a_j a_k + \frac{a_k (b_j - a_j) (b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta^4_i = a_i + \frac{a_k (b_j - a_j) (b_i - a_i)}{b_j b_k - a_j a_k}, \]

\[ \theta^5_i = \frac{b_j a_k (a_i b_j b_k - a_i a_j b_k - b_i a_j a_k + b_i a_j b_k)}{b_j b_k - a_j a_k}, \quad \theta^6_i = a_i + \frac{b_j (b_i - a_i) (b_k - a_k)}{b_j b_k - a_j a_k}, \]

\[ \theta^7_i = \frac{a_j b_k (b_i b_j a_k - b_i a_j a_k - a_i b_j a_k + a_i b_j b_k)}{b_j b_k - a_j a_k}, \quad \theta^8_i = a_i + \frac{b_k (b_j - a_j) (b_i - a_i)}{b_j b_k - a_j a_k}. \]
where:

\[
\begin{align*}
\theta_1^i &= a_i a_j a_k + \frac{a_j(b_k - a_k)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_2^i = a_i + \frac{a_j(b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k}, \\
\theta_3^i &= a_i a_j a_k + \frac{a_k(b_j - a_j)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_4^i = a_i + \frac{a_k(b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k}, \\
\theta_5^i &= \frac{b_j a_k (a_i b_j b_k - a_i a_j b_k - b_i a_j a_k + b_i a_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_6^i = a_i + \frac{b_j (b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k}, \\
\theta_7^i &= \frac{a_j b_k (b_i b_j a_k - b_i a_j a_k - a_i b_j a_k + a_i b_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_8^i = a_i + \frac{b_k (b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k}.
\end{align*}
\]

**Theorem 9**

The smallest double-McCormick is \( \mathcal{P}_3 \) (then \( \mathcal{P}_2 \), then \( \mathcal{P}_1 \)), and

\[
\text{Vol}_{\mathcal{P}_3} = \text{Vol}_{\mathcal{P}_H} + \frac{(b_1 - a_1)(b_2 - a_2)^2(b_3 - a_3)^2 (5(a_1 b_1 b_2 - a_1 b_1 a_2) + 3(b_2^2 a_2 - a_1^2 b_2))}{24(b_1 b_2 - a_1 a_2)}.
\]
Proposition 10

With $\mathcal{P}_H$ and branching on any $x_i$, branching at the midpoint of $[a_i, b_i]$ always yields the least volume.

Theorem 11

With $\mathcal{P}_H$ and midpoint branching, branching on $x_1$ gives the least volume, and branching on $x_3$ gives the greatest volume.
Proposition 10

With $\mathcal{P}_H$ and branching on any $x_i$, branching at the midpoint of $[a_i, b_i]$ always yields the least volume.

Theorem 11

With $\mathcal{P}_H$ and midpoint branching, branching on $x_1$ gives the least volume, and branching on $x_3$ gives the greatest volume.

Proposition 12

Using $\mathcal{P}_3$ and branching on $x_3$, the least volume after branching is obtained by branching at the midpoint of $[a_3, b_3]$.

Theorem 13

For $i = 1, 2$ and using the relaxation $\mathcal{P}_3$, the total volume of the relaxations after branching on $x_i$ is a convex function in the branching point $c_i$, over the domain $[a_i, b_i]$. Moreover, the minimum occurs to the right of the midpoint.