Relaxing kindly and efficiently

Jon Lee

University of Michigan

July 2016

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

Context: Global optimization

$$\min_{x \in \mathbb{R}^n} \{ f_0(x) \; : \; f_i(x) \leq 0, \; i = 1, \ldots, m \}.$$

Context: Global optimization

$$\min_{x \in \mathbb{R}^n} \{ f_0(x) \ : \ f_i(x) \le 0,\ i = 1, \ldots, m \}.$$

Very relevant to the workshop theme!!!

Context: Global optimization

$$\min_{x \in \mathbb{R}^n} \{ f_0(x) \ : \ f_i(x) \leq 0, \ i = 1, \ldots, m \}.$$

Very relevant to the workshop theme!!!

Several key paradigms: convex vs nonconvex? polynomials? (partially-)separable?

Context: Global optimization

$$\min_{x \in \mathbb{R}^n} \{ f_0(x) \; : \; f_i(x) \leq 0, \; i = 1, \ldots, m \}.$$

Very relevant to the workshop theme!!!

Several key paradigms: convex vs nonconvex? polynomials? (partially-)separable?

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

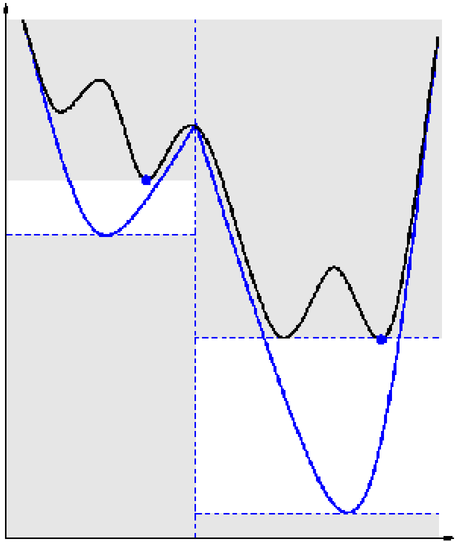
Spatial branch-and-bound is a global-optimization strategy successfully aimed at "factorable" formulations:

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, $\log(x)$, $x + y$, $x \times y$, x^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

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.

Daphne Skipper, Jon Lee. Virtuous smoothing for global optimization, arXiv:1605.05221; (extending work of D'Ambrosio, Fampa, Lee and Vigerske)

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.

  Daphne Skipper, Jon Lee. Virtuous smoothing for global optimization, arXiv:1605.05221; (extending work of D'Ambrosio, Fampa, Lee and Vigerske)

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

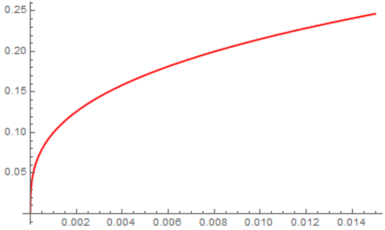
  E.g., $x \times y \times z = xyz = (xy)z = (xz)y = (yz)x$.

  Emily Speakman, Jon Lee. Quantifying double McCormick, arXiv:1508.02966, On sBB branching for trilinear monomials, GOW 2016.

1st Topic

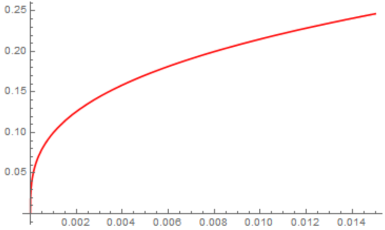
A class of almost well-behaved univariate functions

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

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 $w > 0$



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:

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

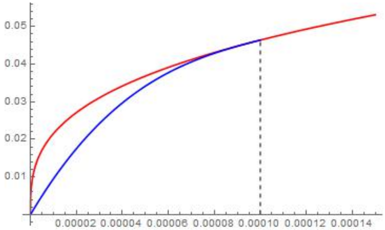
where

$$\begin{aligned} A &= \frac{f(\delta)}{\delta^3} - \frac{f'(\delta)}{\delta^2} + \frac{f''(\delta)}{2\delta}, \\ B &= -\frac{3f(\delta)}{\delta^2} + \frac{3f'(\delta)}{\delta} - f''(\delta), \\ C &= \frac{3f(\delta)}{\delta} - 2f'(\delta) + \frac{\delta f''(\delta)}{2}. \end{aligned}$$

Piecewise smooth at δ

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.

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.
- We give a sufficient condition on f (satisfied by some natural functions) so that g is increasing and concave. New in SCIP 3.2!

Summary of Results

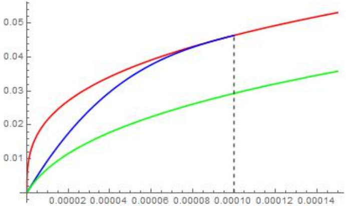
Extending results of D'Ambrosio, Fampa, Lee and Vigerske (for $f(w) = \sqrt{w}$):

- We demonstrate that g is not always increasing and concave.
- 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 $q \geq 2$.

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.
- 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 $2 \leq q \leq 10,000$.



Example 2 (where g is not concave and increasing)

For $\epsilon > 0$, let

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

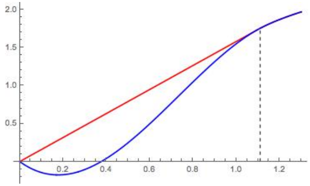
- $f(0) = 0$, f is twice differentiable, increasing, and concave on $[0, +\infty)$
- Our sufficient condition for g to be increasing and concave is not satisfied when $\epsilon = 1/10$, $\phi = 1/100$, and $\delta = 1 + \epsilon + \phi$.

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.



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* δ*. 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)

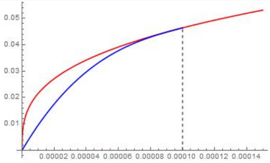
On $[\delta, +\infty)$, let f be increasing and differentiable, with f' non-increasing (decreasing); $f(0) = 0$, and f twice differentiable at δ. If

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

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

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)

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

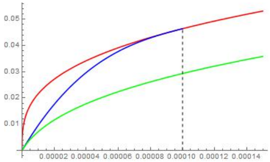
How do **we** compare to a simpler "shift" smoothing for roots?

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 λ 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 $L = \delta^{1/q}$:

$$(f-g)(t) = \frac{t}{2q^2L^{3q-1}}\Big(2q^2L^{3q-1} - (6q^2-5q+1)L^{2q}t^{q-1} + (6q^2-8q+2)L^q t^{2q-1} - (2q^2-3q+1)t^{3q-1}\Big)$$

Lower bound

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

$$(f-g)(t) = \frac{t}{2q^2L^{3q-1}}\Big(2q^2L^{3q-1} - (6q^2-5q+1)L^{2q}t^{q-1} + (6q^2-8q+2)L^qt^{2q-1} - (2q^2-3q+1)t^{3q-1}\Big)$$

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:

$$\begin{aligned} \binom{i+2}{2} a L^{3q-4-i} t^i, &\quad 0 \leq i \leq q-2; \\ \left[\binom{i+2}{2} a - \binom{i-q+3}{2} b\right] L^{3q-4-i} t^i, &\quad q-1 \leq i \leq 2q-2; \\ \left[\binom{i+2}{2} a - \binom{i-q+3}{2} b + \binom{i-2q+3}{2} c\right] L^{3q-4-i} t^i, &\quad 2q-1 \leq i \leq 3q-4. \end{aligned}$$

where

$$\begin{aligned} a &= 2q^2 \\ b &= 6q^2 - 5q + 1 \\ c &= 6q^2 - 8q + 2 \end{aligned}$$

Lower bound

It remains to show that each of the three types of coefficients is positive on its respective domain.

Lower bound

It remains to show that each of the three types of coefficients is positive on its respective domain.

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

Lower bound

It remains to show that each of the three types of coefficients is positive on its respective domain.

The first type of coefficients are obviously positive: $\binom{i+2}{2} a L^{3q-4-i}$.

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:

$$C_3(x) = \frac{1}{2}(x+2)(x+1)a - \frac{1}{2}(x-q+3)(x-q+2)b + \frac{1}{2}(x-2q+3)(x-2q+2)c, \quad x \in [2q-1, 3q-4].$$

Lower bound

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

$$C_3(x) = \frac{1}{2}(x+2)(x+1)a - \frac{1}{2}(x-q+3)(x-q+2)b + \frac{1}{2}(x-2q+3)(x-2q+2)c, \quad x \in [2q-1, 3q-4].$$

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 $x < 3q - 5/2$.

Lower bound

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

$$C_3(x) = \frac{1}{2}(x+2)(x+1)a - \frac{1}{2}(x-q+3)(x-q+2)b + \frac{1}{2}(x-2q+3)(x-2q+2)c, \quad x \in [2q-1, 3q-4].$$

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 $q > 1$. □

Better lower bound: proof summary

Theorem 7 (Better lower bound)

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

$$g(w) \ge h(w) := (w+\lambda)^p - \lambda^p, \;\; w \in [0,\infty),$$

when λ is chosen so that $g'(0) = h'(0)$.

Proof: We calculate the shift constant $\hat{\lambda}$ in terms of δ:

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

As in the previous proof, we apply a sequence of substitutions to express $g - h$ as a polynomial.

Better lower bound

We obtain

$$
\begin{aligned}
(g-h)(u) &= \frac{\gamma}{2q^2} K(u) \\
&= \frac{\gamma}{2q^2}\left[d\,(u^q - Q^q)^3 - c\,(u^q - Q^q)^2 + b\,(u^q - Q^q) - a(u - Q)\right],
\end{aligned}
$$

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

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

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

By the constructions of g and h, we have that $(g-h)((1+Q^q)^{1/q}) > 0$.

Better lower bound

By the constructions of g and h, we have that $(g - h)((1 + Q^q)^{1/q}) > 0$.

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 $(Q, (1 + Q^q)^{1/q})$.

Better lower bound

By the constructions of g and h, we have that $(g-h)((1+Q^q)^{1/q}) > 0$.

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 $(0, \infty)$.

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 $(0,\infty)$.

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.

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.

By Descartes' Rule of Signs, the transformed polynomial has no more than two positive roots.

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.

By Descartes' Rule of Signs, the transformed polynomial has no more than two positive roots.

The same bound applies to the number of roots of $K(u)$ in the interval $(0, (1+Q^q)^{1/q})$.

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.

By Descartes' Rule of Signs, the transformed polynomial has no more than two positive roots.

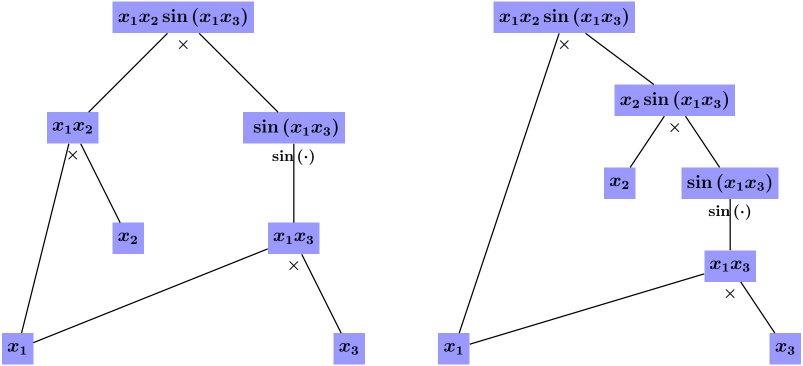
The same bound applies to the number of roots of $K(u)$ in the interval $(0, (1+Q^q)^{1/q})$.

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:



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 $f = x_1 x_2 x_3$, $x_i \in [a_i, b_i]$?

One possibility is the true trilinear hull

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

Let $\mathcal{O}_i := a_i(b_j b_k) + b_i(a_j a_k)$. Then we can construct a labeling such that $\mathcal{O}_1 \leq \mathcal{O}_2 \leq \mathcal{O}_3$. Therefore, without loss of generality, we can assume that

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

How should we convexify $f = x_1 x_2 x_3$, $x_i \in [a_i, b_i]$?

One possibility is the true trilinear hull

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

Let $\mathcal{O}_i := a_i(b_j b_k) + b_i(a_j a_k)$. Then we can construct a labeling such that $\mathcal{O}_1 \leq \mathcal{O}_2 \leq \mathcal{O}_3$. Therefore, without loss of generality, we can assume that

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

Theorem 8

$$\begin{aligned} Vol_{\mathcal{P}_H} = {} & (b_1 - a_1)(b_2 - a_2)(b_3 - a_3) \times \\ & (b_1(5b_2 b_3 - a_2 b_3 - b_2 a_3 - 3a_2 a_3) \\ & \quad + a_1(5a_2 a_3 - b_2 a_3 - a_2 b_3 - 3b_2 b_3))/24 \end{aligned}$$

Proof sketch

- $\mathcal{P}_H$ has 8 vertices

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen: nonnegativity of multivariate polynomials

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen: nonnegativity of multivariate polynomials
- build (simplicial) pyramids over these facets, always keeping track of facets that come and go

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen: nonnegativity of multivariate polynomials
- build (simplicial) pyramids over these facets, always keeping track of facets that come and go
- do all of this in a judicious order

Proof sketch

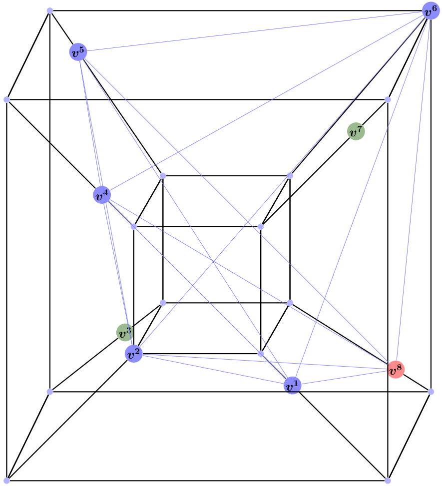
- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen: nonnegativity of multivariate polynomials
- build (simplicial) pyramids over these facets, always keeping track of facets that come and go
- do all of this in a judicious order
- continuity argument to handle the cases of some $a_i = 0$

Proof sketch

- $\mathcal{P}_H$ has 8 vertices
- assume that all $a_i > 0$. Now start with a simplex, 5 of the vertices, and calculate the volume as a determinant
- include one more vertex at a time, by determining which facets of the current polytope are seen: nonnegativity of multivariate polynomials
- build (simplicial) pyramids over these facets, always keeping track of facets that come and go
- 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 $x_1 x_2$.

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

The inequality description of $\mathcal{P}_H$ is "heavy"

Another possibility is "double McCormick".

For $f = x_1x_2$, 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_1x_2.

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

Double McCormick: Consider the monomial $f = x_ix_jx_k$, and assume that we first group the variables x_i and x_j. We let $w_{ij} = x_ix_j$, 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

Double McCormick Inequalities

$$\underline{w = x_1 x_2, \quad f = w x_3}$$

$$w - a_2 x_1 - a_1 x_2 + a_1 a_2 \geq 0$$

$$-w + b_2 x_1 + a_1 x_2 - a_1 b_2 \geq 0$$

$$-w + a_2 x_1 + b_1 x_2 - b_1 a_2 \geq 0$$

$$w - b_2 x_1 - b_1 x_2 + b_1 b_2 \geq 0$$

$$f - a_3 w - a_1 a_2 x_3 + a_1 a_2 a_3 \geq 0$$

$$-f + b_3 w + a_1 a_2 x_3 - a_1 a_2 b_3 \geq 0$$

$$-f + a_3 w + b_1 b_2 x_3 - b_1 b_2 a_3 \geq 0$$

$$f - b_3 w - b_1 b_2 x_3 + b_1 b_2 b_3 \geq 0$$

Double McCormick Inequalities

Double McCormick Inequalities

$$\underline{w = x_1 x_2, \quad f = w x_3}$$

$$w - a_2 x_1 - a_1 x_2 + a_1 a_2 \geq 0$$
$$-w + b_2 x_1 + a_1 x_2 - a_1 b_2 \geq 0$$
$$-w + a_2 x_1 + b_1 x_2 - b_1 a_2 \geq 0$$
$$w - b_2 x_1 - b_1 x_2 + b_1 b_2 \geq 0$$
$$f - a_3 w - a_1 a_2 x_3 + a_1 a_2 a_3 \geq 0$$
$$-f + b_3 w + a_1 a_2 x_3 - a_1 a_2 b_3 \geq 0$$
$$-f + a_3 w + b_1 b_2 x_3 - b_1 b_2 a_3 \geq 0$$
$$f - b_3 w - b_1 b_2 x_3 + b_1 b_2 b_3 \geq 0$$

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

$$f - a_2 a_3 x_1 - a_1 a_3 x_2 - a_1 a_2 x_3 + 2 a_1 a_2 a_3 \geq 0$$
$$f - a_2 b_3 x_1 - a_1 b_3 x_2 - b_1 b_2 x_3 + a_1 a_2 b_3 + b_1 b_2 b_3 \geq 0$$
$$f - b_2 a_3 x_1 - b_1 a_3 x_2 - a_1 a_2 x_3 + a_1 a_2 a_3 + b_1 b_2 a_3 \geq 0$$
$$f - b_2 b_3 x_1 - b_1 b_3 x_2 - b_1 b_2 x_3 + 2 b_1 b_2 b_3 \geq 0$$
$$-f + b_2 b_3 x_1 + a_1 b_3 x_2 + a_1 a_2 x_3 - a_1 a_2 b_3 - a_1 b_2 b_3 \geq 0$$
$$-f + a_2 b_3 x_1 + b_1 b_3 x_2 + a_1 a_2 x_3 - a_1 a_2 b_3 - b_1 a_2 b_3 \geq 0$$
$$-f + b_2 a_3 x_1 + a_1 a_3 x_2 + b_1 b_2 x_3 - a_1 b_2 a_3 - b_1 b_2 a_3 \geq 0$$
$$-f + a_2 a_3 x_1 + b_1 a_3 x_2 + b_1 b_2 x_3 - b_1 a_2 a_3 - b_1 b_2 a_3 \geq 0$$
$$a_i \leq x_i \leq b_i, \quad i = 1, 2, 3$$

Extra extreme points

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

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

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

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

where:

$$\theta_i^1 = a_i a_j a_k + \frac{a_j(b_k - a_k)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_i^2 = a_i + \frac{a_j(b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k},$$

$$\theta_i^3 = a_i a_j a_k + \frac{a_k(b_j - a_j)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_i^4 = a_i + \frac{a_k(b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k},$$

$$\theta_i^5 = \frac{b_j a_k(a_i b_j b_k - a_i a_j b_k - b_i a_j a_k + b_i a_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_i^6 = a_i + \frac{b_j(b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k},$$

$$\theta_i^7 = \frac{a_j b_k(b_i b_j a_k - b_i a_j a_k - a_i b_j a_k + a_i b_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_i^8 = a_i + \frac{b_k(b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k}.$$

where:

$$\theta_i^1 = a_i a_j a_k + \frac{a_j(b_k - a_k)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_i^2 = a_i + \frac{a_j(b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k},$$

$$\theta_i^3 = a_i a_j a_k + \frac{a_k(b_j - a_j)(b_i b_j b_k - a_i a_j a_k)}{b_j b_k - a_j a_k}, \quad \theta_i^4 = a_i + \frac{a_k(b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k},$$

$$\theta_i^5 = \frac{b_j a_k(a_i b_j b_k - a_i a_j b_k - b_i a_j a_k + b_i a_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_i^6 = a_i + \frac{b_j(b_i - a_i)(b_k - a_k)}{b_j b_k - a_j a_k},$$

$$\theta_i^7 = \frac{a_j b_k(b_i b_j a_k - b_i a_j a_k - a_i b_j a_k + a_i b_j b_k)}{b_j b_k - a_j a_k}, \quad \theta_i^8 = a_i + \frac{b_k(b_j - a_j)(b_i - a_i)}{b_j b_k - a_j a_k}.$$

Theorem 9

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

$$Vol_{\mathcal{P}_3} = Vol_{\mathcal{P}_H} + \frac{(b_1 - a_1)(b_2 - a_2)^2(b_3 - a_3)^2\left(5(a_1 b_1 b_2 - a_1 b_1 a_2) + 3(b_1^2 a_2 - a_1^2 b_2)\right)}{24(b_1 b_2 - a_1 a_2)}.$$

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.