

Solving Nonconvex MINLPs

Summer School on Nonlinear Optimization with Mixed Integer and
Complementarity Constraints

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Solving Nonconvex MINLPs

- 1 Generic Relaxation Strategies
- 2 Spatial Branch-and-Bound
- 3 FBBT: Feasibility-Based Bound Tightening
- 4 OBBT: Optimality-Based Bound Tightening
- 5 Quadratically Constrained Optimization (QCO)
- 6 Solving Nonconvex MINLPs: Summary

Factorable Functions and MINLP

Consider MINLP with nonconvex, factorable $f(x, y)$ and $g(x, y)$

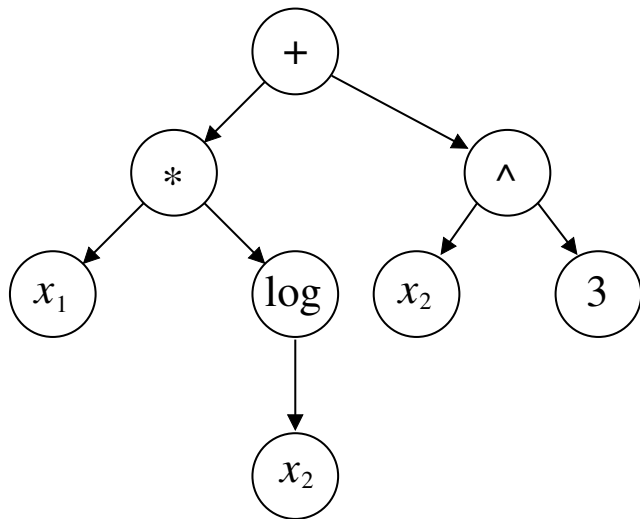
$$\underset{x}{\text{minimize}} \ f(x, y) \quad \text{subject to} \ g(x, y) \leq 0, \ y \in \mathbb{Z}^p$$

Definition (Factorable Function)

$g(x, y)$ is **factorable** iff expressed as sum of products of unary functions of a finite set $\mathcal{O}_{\text{unary}} = \{\sin, \cos, \exp, \log, |\cdot|\}$ whose arguments are variables, constants, or other functions, which are factorable.

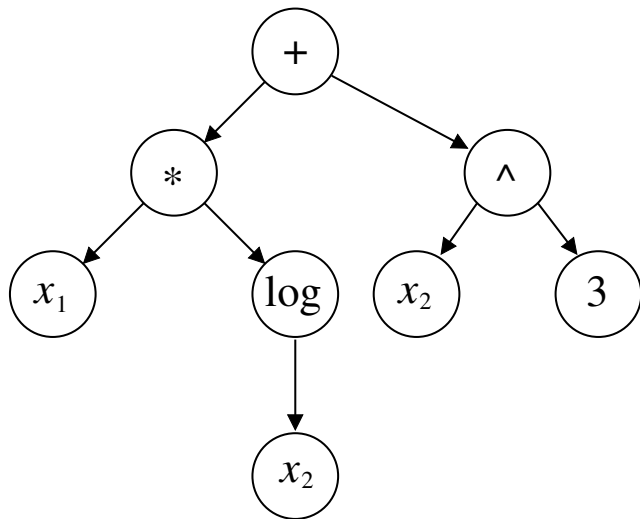
- Combination of functions from set of operators
 $\mathcal{O} = \{+, \times, /, ^, \sin, \cos, \exp, \log, |\cdot|\}$.
- Excludes integrals $\int_{\xi=x_0}^x h(\xi)d\xi$ and black-box functions
- Represented as expression trees

Expression Tree Example $f(x_1, x_2)$



What is $f(x_1, x_2)$?

Expression Tree Example $f(x_1, x_2)$



What is $f(x_1, x_2)$?

Expression tree of $f(x_1, x_2) = x_1 \log(x_2) + x_2^3$

Relaxations of Factorable Functions

MINLP with nonconvex, factorable $f(x, y)$ and $g(x, y)$

$$\underset{x}{\text{minimize}} \ f(x, y) \quad \text{subject to} \ g(x, y) \leq 0, \ y \in \mathbb{Z}^p$$

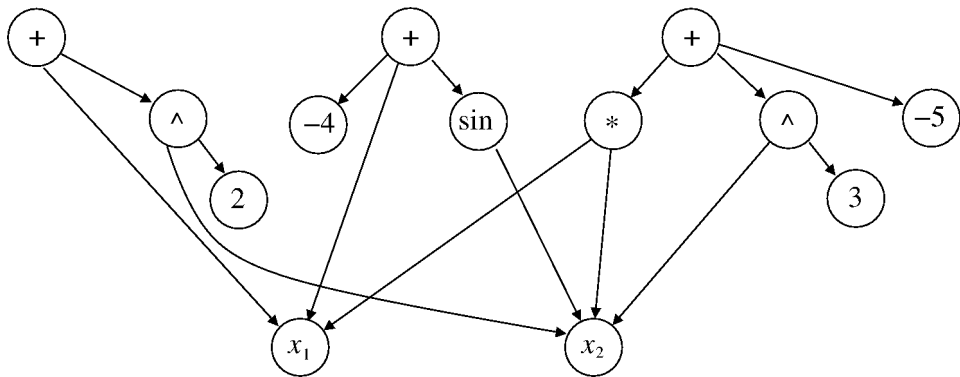
Combine expression trees of objective and constraints

- Root of each expression is $g_1(x, y), g_2(x, y), \dots, g_m(x, y)$, or $f(x, y)$
- Associated bounds: $[-\infty, 0]$ for $g_i(x, y)$, and $[-\infty, \bar{\eta}]$ for $f(x, y)$
- Leaf nodes of all trees represent variables (x, y)

$\Rightarrow$ gives **directed acyclic graph (DAG)**

Modeling languages (e.g. AMPL, GAMS) have DAG & solver API **Python not clear**

Example of DAG



$$\begin{aligned} \min & x_1 + x_2^2 \\ \text{s.t. } & x_1 + \sin x_2 \leq 4, \quad x_1 x_2 + x_2^3 \leq 5 \\ & x_1 \in [-4, 4] \cap \mathbb{Z}, \quad x_2 \in [0, 10] \cap \mathbb{Z}. \end{aligned}$$

Three nodes without entering arcs for objective & constraints

NB: $y = x_2$

Example of Reformulation of Factorable MINLP

$$\begin{aligned} \min \quad & x_1 + x_2^2 \\ \text{s.t.} \quad & x_1 + \sin x_2 \leq 4, \quad x_1 x_2 + x_2^3 \leq 5 \\ & x_1 \in [-4, 4] \cap \mathbb{Z}, \quad x_2 \in [0, 10] \cap \mathbb{Z}. \end{aligned}$$

Reformulation with **uni-/bi-variate nonconvex terms** (factorable)

$$\begin{array}{l|l|l|l|l} \min & x_9 & & & \\ \text{s.t.} & x_3 = \sin x_2 & x_7 = x_5 + x_6 - 5 & 0 \leq x_2 \leq 10 & 0 \leq x_6 \leq 1000 \\ & x_4 = x_1 + x_3 - 4 & x_8 = x_2^2 & -1 \leq x_3 \leq 1 & -45 \leq x_7 \leq 0 \\ & x_5 = x_1 x_2 & x_9 = x_1 + x_8 & -9 \leq x_4 \leq 0 & 0 \leq x_8 \leq 100 \\ & x_6 = x_2^3 & -4 \leq x_1 \leq 4 & -40 \leq x_5 \leq 40 & -4 \leq x_9 \leq 104 \\ & x_1, x_2, x_5, x_6, x_7, x_8, x_9 \in \mathbb{Z}. & & & \end{array}$$

- Integrality inherited from function
- Bounds inherited from function

... decomposition non-unique!

Reformulation of Factorable MINLP

Theorem (Equivalence of Factorable Formulation)

MINLP and factorable MINLP are equivalent, i.e. optimal solutions to one can be transformed into optimal solution of the other.

Factorable form makes it easier to get convex relaxation:

- Nonconvex sets, $k = n + 1, n + 2, \dots, n + q$

$$\Theta_k = \{x \in \mathbb{R}^{n+q} : x_k = \vartheta_k(x), l \leq x \leq u, x_i \in \mathbb{Z}, i \in I\}$$

... nonconvex due to **nonlinear equality**

- Let $\Theta_k \subset \check{\Theta}_k$ & define **convex relaxation** ... **only look at simple sets!**

$$\begin{cases} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & x_k = \vartheta_k(x) & \forall k \\ & l_i \leq x_i \leq u_i & \forall i \end{cases}$$

$$\begin{cases} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & x \in \check{\Theta}_k & \forall k \\ & l_i \leq x_i \leq u_i & \forall i \end{cases}$$

Reformulation of Factorable MINLP

General convex relaxation with polyhedral sets $\check{\Theta}_k$:

$$\begin{cases} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & x \in \check{\Theta}_k & k = n+1, n+2, \dots, n+q \\ & l_i \leq x_i \leq u_i & i = 1, 2, \dots, n+q \end{cases}$$

Often expressed as polyhedral set $\check{\Theta}_k$ defined by $a^k \in \mathbb{R}^{m_k}$, $B^k \in \mathbb{R}^{m_k \times (n+q)}$, and $d^k \in \mathbb{R}^{m_k}$:

$$\check{\Theta}_k = \{x \in \mathbb{R}^{n+q} : a^k x_k + B^k x \geq d^k, l \leq x \leq u\},$$

Lower bounding LP relaxation for MINLP solvers

$$\begin{cases} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & a^k x_k + B^k x \geq d^k & k = n+1, n+2, \dots, n+q \\ & l_i \leq x_i \leq u_i & i = 1, 2, \dots, n+q \end{cases}$$

Construct polyhedral sets for simple functions, e.g. McCormick

Example of Polyhedral Relaxation

Constructing polyhedral relaxation

Look at simple functions

- Secants from interval end-points
- Tangents on convex parts

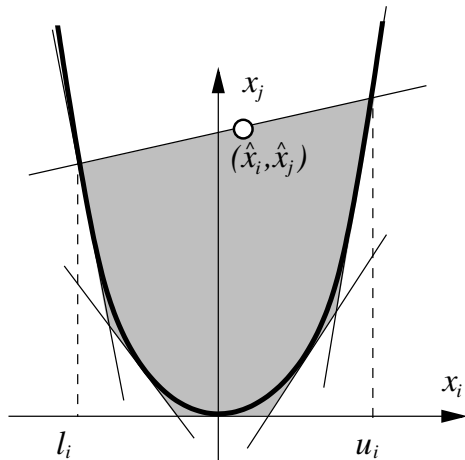
Exploit knowledge of convex/concave parts

Exercise (OA of bilinear terms)

Construct a convex relaxation of

$$\left\{ z = x_1 x_2 \mid l_i \leq x_i \leq u_i \right\}$$

Hint: Use $0 \leq (x_1 - l_1)(u_2 - x_2)$ etc.

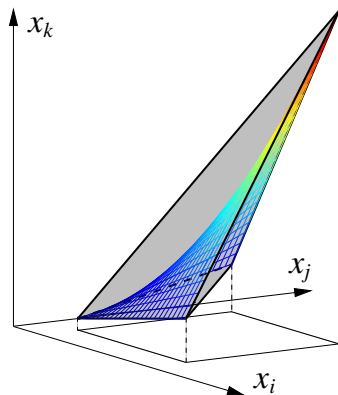


What about 2D functions?

Bilinear terms

For $B = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = x_1 x_2, x_1 \in [\ell_1, u_1], x_2 \in [\ell_2, u_2]\}$, convex hull given by *McCormick inequalities* [McCormick, 1976] & [Al-Khayyal and Falk, 1983]

$$\begin{aligned} \text{conv}(B) = \{ (x_1, x_2, x_3) \in \mathbb{R}^3 : \\ x_3 \geq \ell_2 x_1 + \ell_1 x_2 - \ell_2 \ell_1 \\ x_3 \geq u_2 x_1 + u_1 x_2 - u_2 u_1 \\ x_3 \leq \ell_2 x_1 + u_1 x_2 - \ell_2 u_1 \\ x_3 \leq u_2 x_1 + \ell_1 x_2 - u_2 \ell_1 \} \end{aligned}$$



These inequalities are added as convexification cuts after reformulation of problems which contain products of variables.

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Spatial Branch-and-Bound (BnB)

To separate solution of relaxation use **spatial BnB**

- Implicit enumeration technique like integer BnB
- Recursively define partitions of feasible set into two sets
- Use reformulation outlined above
- Solve LO relaxations ($\Rightarrow$ lower bounds)
... and nonconvex NLPs ($\Rightarrow$ upper bound if feasible)

Classic references & solvers:

- [Smith and Pantelides, 1997]
- [Sahinidis, 1996, Tawarmalani and Sahinidis, 2002] BARON
- [Belotti et al., 2009] Couenne ... **open-source in COIN-OR**
- [Mahajan et al., 2021] MINOTAUR ... **since 2026, ask Neeraj Kumar, open-source**

Ingredients of Spatial Branch-and-Bound (BnB)

Key ingredients of spatial BnB

- 1 Procedure to compute lower bound for subproblem
- 2 Procedure for partitioning feasible set of subproblem:
 $\text{NLP}(l^-, u^-)$ and $\text{NLP}(l^+, u^+)$

... generates tree **almost** like integer BnB

NLP node is subproblem: nonconvex $\text{NLP}(l, u)$

$$\left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & x_k = \vartheta_k(x) \quad k = n+1, n+2, \dots, n+q \\ & l_i \leq x_i \leq u_i \quad i = n+1, n+2, \dots, n+q \\ & l \leq x \leq u \end{array} \right. \quad (\text{NLP}(l, u))$$

... **nonconvex** restrictions of original MINLP on subtree $l \leq x \leq u$

Spatial Branch-and-Bound (BnB)

Linear lower bounding problem at **nonconvex** $\text{NLP}(I, u)$, e.g. $\text{LO}(I, u)$

$$\left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & x_{n+q} \\ \text{subject to} & a^k x_k + B^k x \geq d^k \quad k = n+1, n+2, \dots, n+q \\ & l_i \leq x_i \leq u_i \quad i = 1, 2, \dots, n+q \\ & x \in X. \end{array} \right. \quad (\text{LO}(I, u))$$

If $\text{LO}(I, u)$ infeasible, then prune node.

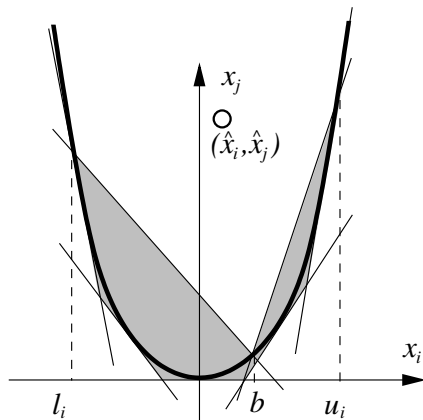
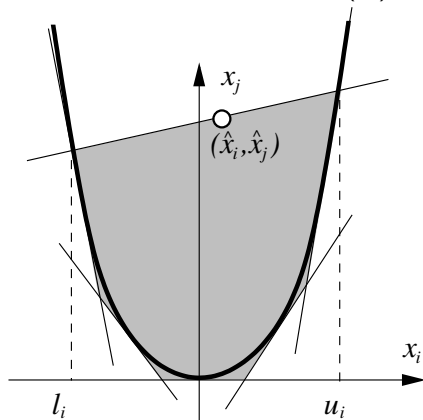
Otherwise, $\hat{x}$ optimal solution of $\text{LO}(I, u)$:

- If $\hat{x}$ feasible in $\text{NLP}(I, u)$ (hence MINLP), then fathom node (new incumbent)
- If $\hat{x}$ **not** feasible in $\text{NLP}(I, u)$ then ... branch ...
 - 1 $\hat{x}$ not integral, i.e., $\exists i \in I : \hat{x}_i \notin \mathbb{Z}$ **branch on integers first**
 - 2 Nonconvex constraint is violated, i.e.

$$\exists k \in \{n+1, n+2, \dots, n+q\} : \hat{x}_k \neq \vartheta_k(\hat{x}).$$

Branching for Spatial Branch-and-Bound

Branching example $x_k = \vartheta_k(x_i) = (x_i)^2$ violated



Branch-and-Bound for Nonconvex MINLP

Choose $\text{tol } \epsilon > 0$, set $U = \infty$, add $(\text{NLP}(-\infty, \infty))$ to heap $\mathcal{H}$.

while $\mathcal{H} \neq \emptyset$ **do**

 Remove $\text{NLP}(l, u)$ from heap: $\mathcal{H} = \mathcal{H} - \{\text{NLP}(l, u)\}$.

 Solve relaxation $\text{LO}(l, u) \Rightarrow$ solution $x^{(l,u)}$

 Possibly solve $\text{NLP}(l, u)$ for an upper bound

if $\text{LO}(l, u)$ is infeasible **then**

 | Prune node: infeasible

else if $f(x^{(l,u)}) > U$ **then**

 | Prune node; dominated by bound U

else if $x_i^{(l,u)}$ integral and $x_k = \vartheta_k(x)$, $\forall k$ **then**

 | Update incumbent : $U = f(x^{(l,u)})$, $x^* = x^{(l,u)}$.

else

 | $\text{BranchOnVariable}(x_i^{(l,u)}, l, u, \mathcal{H})$ or $\text{BranchOnConstraint}(x_k = \vartheta_k(x), l, u, \mathcal{H})$

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Tightening Bounds and Relaxations

Bound tightening to reduce range of bounds $x_i \in [l_i, u_i]$

... because **tighter bounds** $\Rightarrow$ **tighter relaxations** $\Rightarrow$ **smaller trees**

Conceptual Bound-Tightening Procedure

Feasible set $\mathcal{F} = \{x \in [l, u] : g(x) \leq 0, x_l \in \mathbb{Z}^p\}$

Solve $2n$ (global) optimization problems, given upper bound U on $f(x)$:

$$l'_i = \min\{x_i : x \in \mathcal{F}, f(x) \leq U\}; \quad u'_i = \max\{x_i : x \in \mathcal{F}, f(x) \leq U\}.$$

$2n$ nonconvex MINLPs $\Rightarrow$ use relaxations:

- 1 FBBT: feasibility-based bound tightening
- 2 OBBT: optimality-based bound tightening

FBBT: Feasibility-Based Bound Tightening

FBBT broadly used:

- Artificial intelligence community & constraint programming
- NLP solvers [[Messine, 2004](#)]
- MILO solvers [[Savelsbergh, 1994](#)]

Basic Principle of FBBT

Infer bounds on x_i from tighter bounds on x_j for $j \neq i$.

FBBT: Feasibility-Based Bound Tightening

Basic Principle of FBBT

Infer bounds on x_i from tighter bounds on x_j for $j \neq i$.

Example 1: $x_j = x_i^3$ and $x_i \in [l_i, u_i]$

- Tighten interval of x_j to $[l_j, u_j] \cap [l_i^3, u_i^3]$
- Tightened l'_j on $x_j \Rightarrow$ tighter $l'_i = \sqrt[3]{l_j}$ for x_i

Exercise ($x_3 = x_1 x_2$ with $(1, 1, 0) \leq (x_1, x_2, x_3) \leq (5, 5, 2)$)

- $l_1 = l_2 = 1 \Rightarrow l_3 = l_1 l_2 = 1 > 0$
- $u_3 = 2 \Rightarrow x_1 \leq \frac{u_3}{l_1}$ and $x_2 \leq \frac{u_3}{l_2} \Rightarrow u'_1 = u'_2 = 2 < 5$

Tightens McCormick underestimators ... try it!

FBBT: Feasibility-Based Bound Tightening: Affine Functions

FBBT for affine functions $x_k = a_0 + \sum_{j=1}^n a_j x_j$ for $k > n$

- $J^+ = \{j = 1, 2, \dots, n : a_j > 0\}$ positive coefficients
- $J^- = \{j = 1, 2, \dots, n : a_j < 0\}$ negative coefficients

$\Rightarrow$ valid bounds are ...

$$a_0 + \sum_{j \in J^-} a_j u_j + \sum_{j \in J^+} a_j l_j \leq x_k \leq a_0 + \sum_{j \in J^-} a_j l_j + \sum_{j \in J^+} a_j u_j$$

Bounds $[l_k, u_k]$ on x_k give new bounds on x_j , e.g. for $j \in J^+$

$$l'_j = \frac{1}{a_j} \left(l_k - \left(a_0 + \sum_{i \in J^+ \setminus \{j\}} a_i u_i + \sum_{i \in J^-} a_i l_i \right) \right)$$

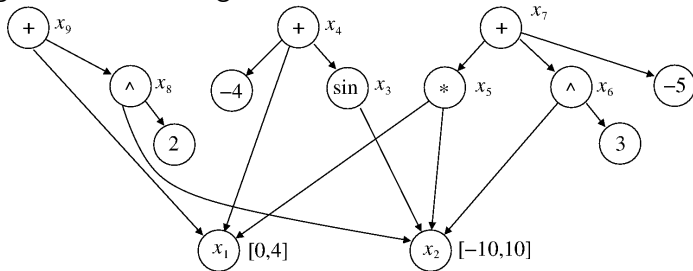
... similar for u'_j and $j \in J^-$

Better bounds from convex combination of inequalities, ... or solving more equations!

FBBT: Feasibility-Based Bound Tightening: Nonlinear Functions

For nonlinear functions, propagate bounds through DAG:

$$\begin{aligned} \min \quad & x_1 + x_2^2 \\ \text{s.t.} \quad & x_1 + \sin x_2 \leq 4 \\ & x_1 x_2 + x_2^3 \leq 5 \\ & x_1 \in [-4, 4] \cap \mathbb{Z} \\ & x_2 \in [0, 10] \cap \mathbb{Z}. \end{aligned}$$



Assume solution $\hat{x}$ found with $f(\hat{x}) = 10$:

- 1 $10 \geq x_9 := x_1 + x_8$ and $x_1 \geq -4$ imply $x_8 \leq 14 < 100$ tighter
- 2 Propagate to $x_8 = x_2^2$ implies $-\sqrt{14} \leq x_2 \leq \sqrt{14}$ tightens x_2

... no more tightening

In general propagate bounds until improvement tails off.

FBBT: Feasibility-Based Bound Tightening

Properties of FBBT

- Efficient and fast implementation for large-scale MINLP
- Can exhibit poor convergence, e.g. for $\alpha > 1$ consider:

$$\min x_1 \text{ s.t. } x_1 = \alpha x_2, x_2 = \alpha x_1, x_1 \in [-1, 1]$$

- Solution is $(0, 0)$
- **FBBT does not terminate in finite number of steps**
- Sequence of tighter bounds for $l = 1, 2, \dots$ with $\{[-\frac{1}{\alpha^l}, \frac{1}{\alpha^l}]\}_l \rightarrow (0, 0)$

... hence combine with other techniques

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OBBT: Optimality-Based Bound Tightening

Solving $\min / \max x_i$ s.t. $x \in \mathcal{F}$ (nonconvex MINLP) not practical

Instead, define (linear) relaxation

$$\mathcal{F}(l, u) = \left\{ x \in \mathbb{R}^{n+q} : \begin{array}{ll} a^k x_k + B^k x \geq d^k & k = n+1, n+2, \dots, n+q \\ l_i \leq x_i \leq u_i & i = 1, 2, \dots, n+q \end{array} \right\}.$$

Now get bounds on x_i for $i = 1, \dots, n$ by solving $2n$ LOs:

$$l'_i = \min\{x_i : x \in \mathcal{F}(l, u)\} \tag{1}$$

$$u'_i = \max\{x_i : x \in \mathcal{F}(l, u)\}$$

... only apply at root node, or small number of nodes ... or use convex relaxations

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Quadratically Constrained Optimization (QCO)

We want to solve a problem with quadratic objective function and one or more quadratic constraints:

$$\begin{aligned} \min \quad & x^T Q_0 x + b_0^T x \\ \text{s.t.} \quad & x^T Q_k x + b_k^T x \leq c_k \quad \forall k = 1, 2, \dots, m \\ & Ax \leq b \end{aligned}$$

If Q_0 and **all** Q_k are PSD, the problem is convex.

Otherwise, for a nonconvex QCO the standard B&C scheme would reformulate

- each term $q_{ij}x_i x_j$ using an **auxiliary** variable $z_{ij} = x_i x_j$
- each term $q_{ii}x_i^2$ using an **auxiliary** variable $z_{ii} = x_i^2$

Reformulation

Creates (**symmetric**) matrix of auxiliary variables, $Z = [z_{ij}]_{i \in N, j \in N}$, with $\frac{n(n+1)}{2}$ (obviously $z_{ij} = z_{ji}$).

The **reformulation** is as follows:

$$\begin{aligned} \min \quad & Q_0 \bullet Z + b_0^T x \\ \text{s.t.} \quad & Q_k \bullet Z + b_k^T x \leq c_k \quad \forall k = 1, 2, \dots, m \\ & z_{ij} = x_i x_j \quad \forall i, j = 1, 2, \dots, n, i \leq j \\ & Ax \leq b \end{aligned}$$

$Q \bullet Z$ is the sum over all element-wise products: $\sum_{i \in N, j \in N} q_{ij} x_i x_j$.

Sometimes these terms are also written $\text{tr}(QZ)$, *trace* of the matrix product QZ .

Reformulation

Rewrite the reformulation:

$$\begin{aligned} \min \quad & Q_0 \bullet Z + b_0^T x \\ \text{s.t.} \quad & Q_k \bullet Z + b_k^T x \leq c_k \quad \forall k = 1, 2, \dots, m \\ & z_{ij} = x_i x_j \quad \forall i, j = 1, 2, \dots, n, i \leq j \quad (*) \\ & Ax \leq b \end{aligned}$$

All constraints (*) are nonlinear and nonconvex.

They can be summarized in matrix constraint $Z = xx^T$, also nonconvex.

SDO Relaxation

Rewrite the matrix equation $Z = xx^T$ as $Z - xx^T = 0$.

- $Z - xx^T = 0$ implies $Z - xx^T \succeq 0$, which can be rewritten (Schur complement) as

$$\begin{pmatrix} 1 & x^T \\ x & Z \end{pmatrix} \succeq 0$$

- Unfortunately, $xx^T - Z \succeq 0$ is nonconvex and discarded.

Relaxation

We get a problem with linear constraints and one PSD constraint, i.e., a **semi-definite optimization (SDO)** problem.

$$\begin{aligned} \min \quad & Q_0 \bullet Z + b_0^T x \\ \text{s.t.} \quad & Q_k \bullet Z + b_k^T x \leq c_k \quad \forall j = 1, 2, \dots, m \\ & \begin{pmatrix} 1 & x^T \\ x & Z \end{pmatrix} \succeq 0 \\ & Ax \leq b \end{aligned}$$

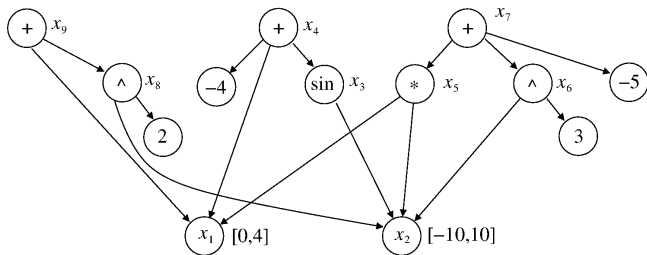
which is **convex**! Still a convex MINLP, if integer/binary variables added

Semidefinite relaxations play important role in optimization application

Good quality lower bounds, computationally more expensive to solve

Solving Nonconvex MINLPs: Summary and Take-Aways

- Generic relaxation of DAG
- Spatial branching to refine
- SDP relaxation of $Z = xx^T$



Two Classes of Bound Tightening using DAG

- Feasibility-based bound tightening
... propagate bounds through DAG: **weak** but **cheap**
- Optimality-based bound tightening
... optimize over convex relaxations: **expensive** but **strong**



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