Handling Non-Linearities with Gurobi

Gurobi Live Barcelona

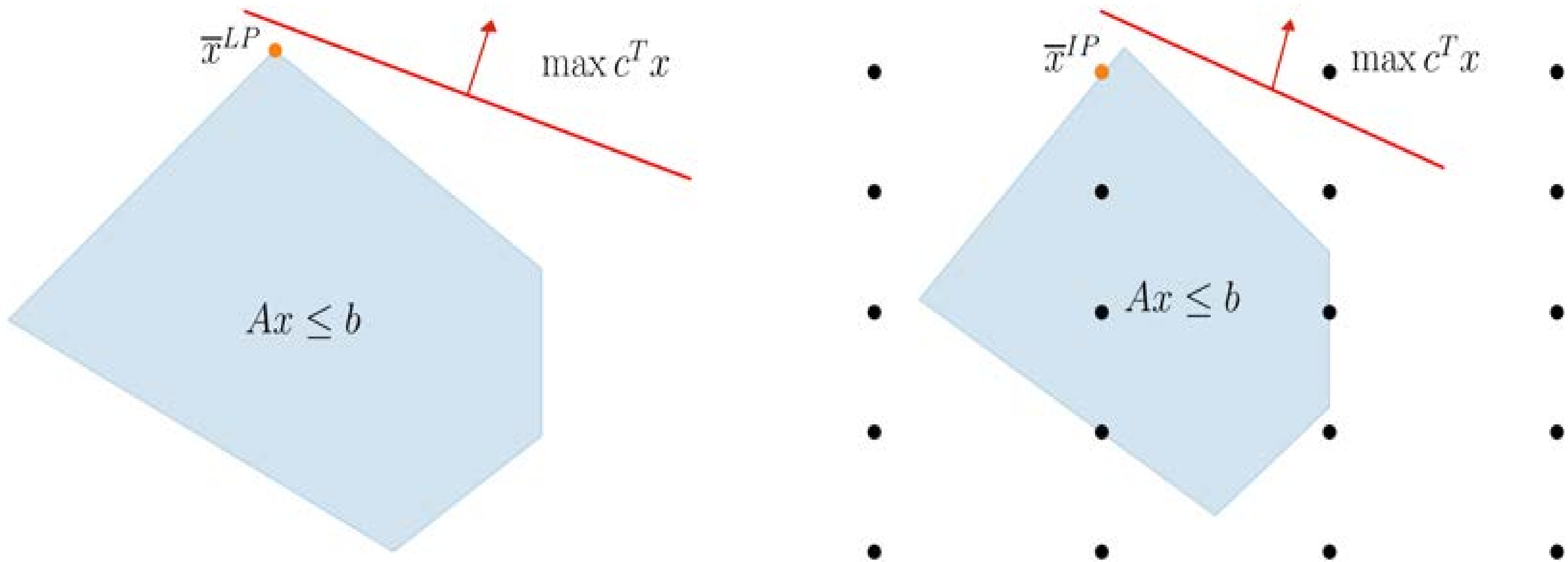
Pierre Bonami

Agenda

1. Introduction
2. Mixed-Integer Convex Quadratic Optimiziation
3. Non-Convex Quadratic Optimization
4. General Functions, piece-wise linear and beyond

GUROBI LiVE!

LP and MIP



- Base problems that Gurobi solves
- Simplex and Barrier algorithms for LP
- Branch-and-cut for MIP

Nonlinearities

Application	Phenomenon	Nonlinearity
Finance	risk	quadratic (convex)
Truss topology	physical forces	quadratic (convex)
Pooling (petrochemical, mining, agriculture)	mixing products	quadratic non-convex
electricity distribution (ACOPF)	Alternative Current	$\sin$ and $\cos$ (can be made quadratic)
machine learning	—	logistic function, $\tanh$
chemical engineering	chemical reactions	—

- many more…

The MINLP Goal

Ideally, we seek to solve

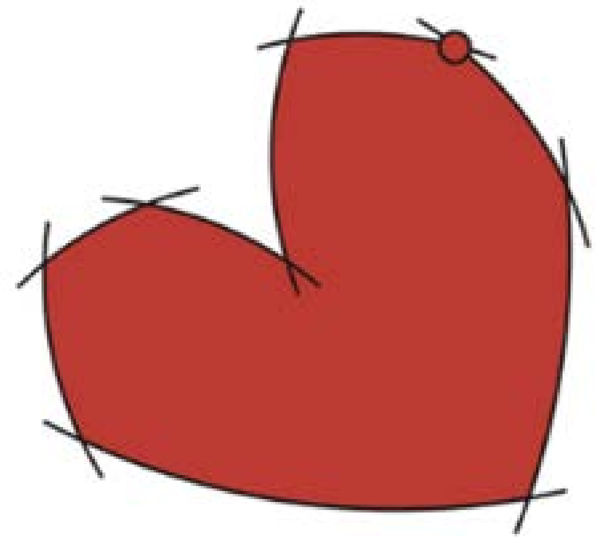
$$
\begin{aligned}
&\min f(x) \\
&\text{s.t:} \\
&g_i(x) \leq 0, i = 1, \ldots, m \\
&x_j \in \mathbb{Z}, j \in \square \\
&l \leq x \leq u
\end{aligned}
$$

- $f : \mathbb{R}^n \to \mathbb{R}$, $g_i : \mathbb{R}^n \to \mathbb{R}$, reasonably smooth
- If l or u is not finite: undecidable in general
- Even assuming finiteness it’s very difficult in theory and practice
- Note that integer variables are “not convex” and can be represented as a polynomial if bounded

Convex or not convex?

Convex Region

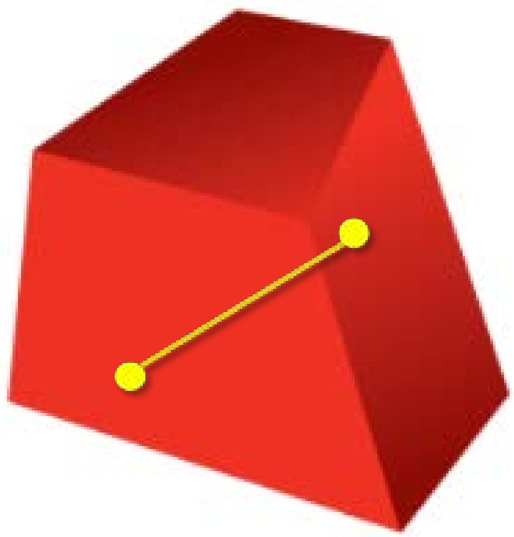
Any segment connecting two points inside the region is inside the region.



Non-Convex Region

There exists two points in the region the segment connecting them is not completely in the region.

Convex or not convex?



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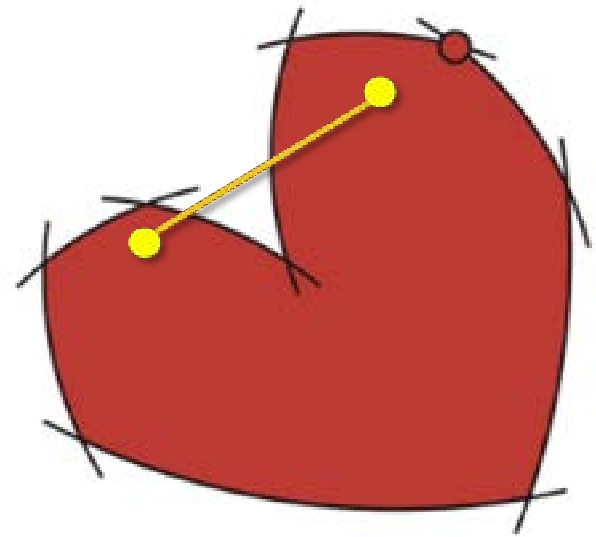

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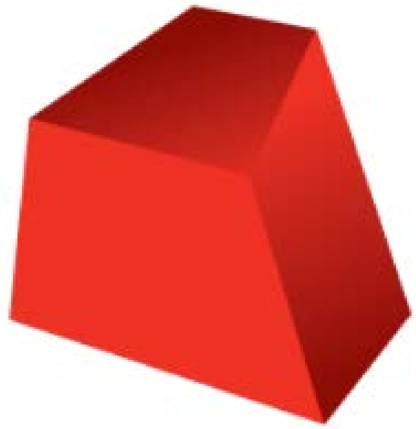
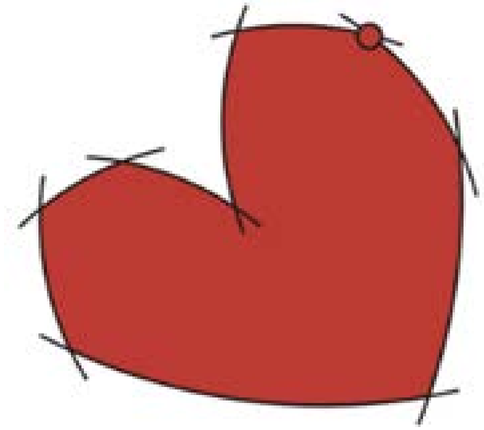
Why?





- Optimization "easy" (usually)
  - Start from any point in the region
  - Take steps inside the region improving objective
  - When there is no more step **global optimum**
- Interior point methods for any closed convex region
- Simplex algorithm for polyhedra

- Optimization "hard"
  - Start from any point in the region
  - Take steps inside the region improving objective
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- Need a divide-and-conquer algorithm to find a **global optimum**.

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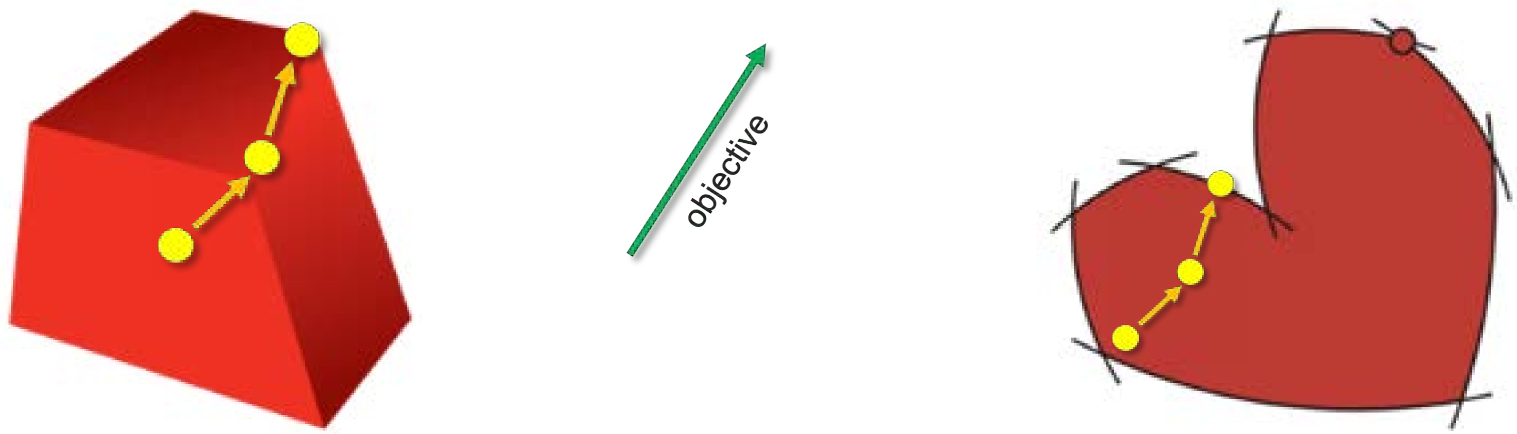

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Nonlinearities in Gurobi

Convex

- Quadratic objective: $\min c^T x + x^T Q x$ with $Q \succeq 0$
- Quadratic constraints: $a^T x + x^T Q x \leq b$ describing a convex region
  - $Q \succeq 0$ is a simple case, can be more complex

Non-Convex

- Discrete objects: integer variables, SOS constraints
- Bilinear terms: $z_{ij} = x_i x_j$
  - Non-Convex quadratic forms: $a^T x + x^T Q x \leq b$
- General functions: $\exp$, $\log$, $\cos$,
  - Reformulated as PWL in Gurobi 9 and 10
  - Treated directly

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New in Gurobi 11

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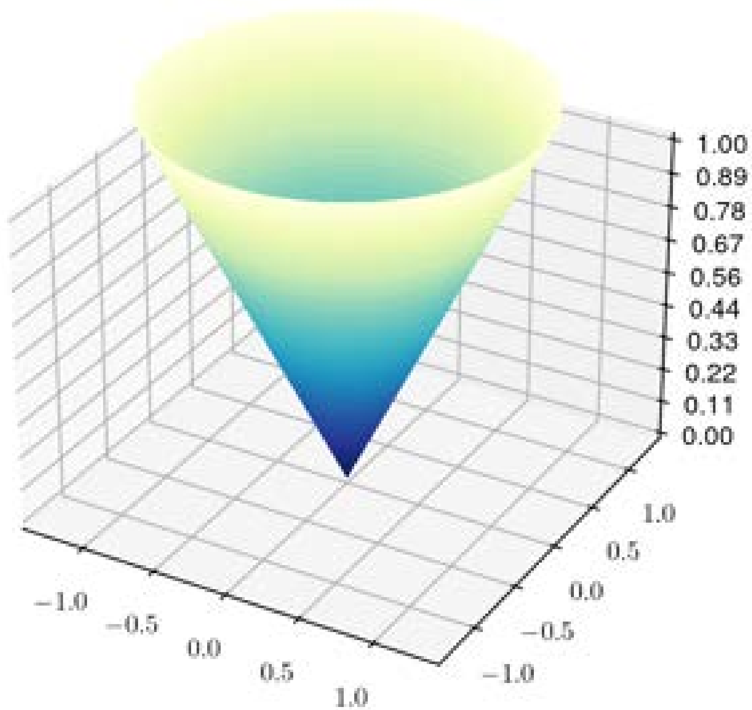
Problem definition

$$\min c^T x + x^T Q^0 x$$
$$\text{s.t:}$$
$$a_k{}^T x + x^T Q^k x \leq b_k, k = 1, \ldots, m$$
$$x_j \in \mathbb{Z}, j \in \square$$
$$l \leq x \leq u$$

- $Q^0, Q^1, \ldots, Q^m$ are assumed to be symmetric
  - Q^0 is positive semi definite
  - The quadratic forms $a_k^T + x^T Q^k x - b_k$ are *second order cone representable*.

The second order cone



$\square^n = \{x \in \mathbb{R}^{n+1} : \sum_{j=1}^{n} x_j^2 \leq x_0^2, x_0 \geq 0\}$

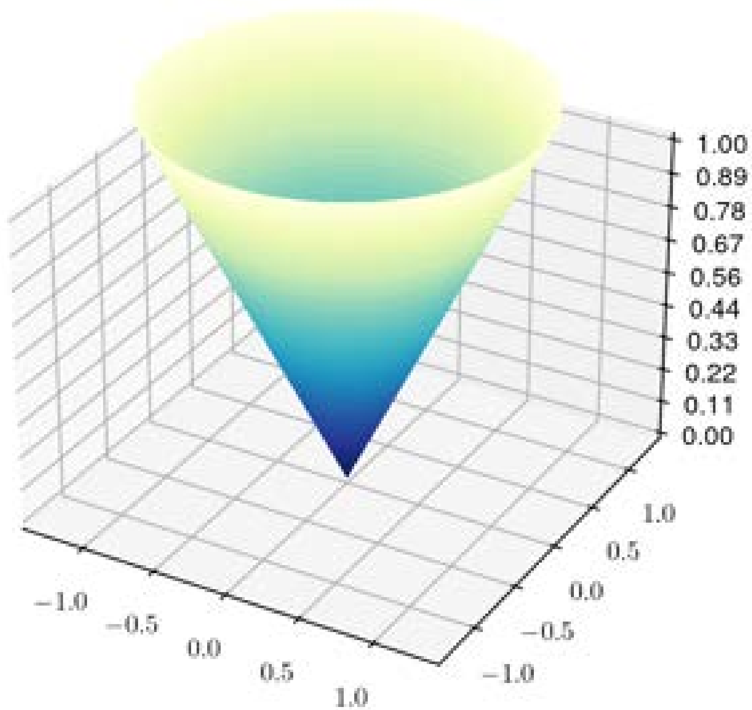
Through simple algebra, can be represented as SOC:

- $\sum_{i=1}^{n} x_i^2 \leq x_0^2$, with $x_0 \geq 0$
- $\sum_{i=2}^{n} x_i^2 \leq x_0 x_1$, with $x_0, x_1 \geq 0$ (rotated SOC)
- $a^T x + x^T Q x \leq b$, with $Q \geq 0$
- $x^T Q x \leq y^2$, with $Q \geq 0, y \geq 0$

Very powerful but modeling sometimes far from obvious.

Not all forms recognized by solvers

The second order cone



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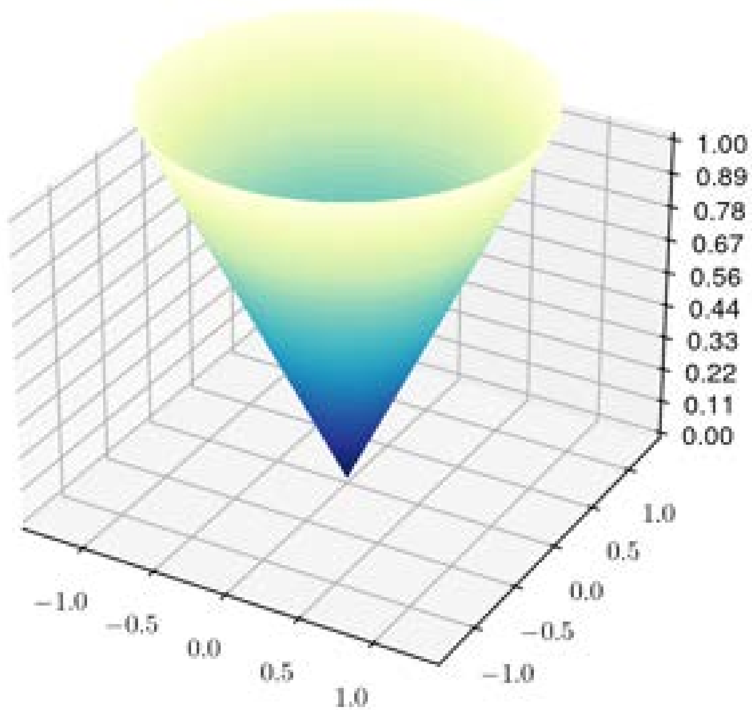

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Note

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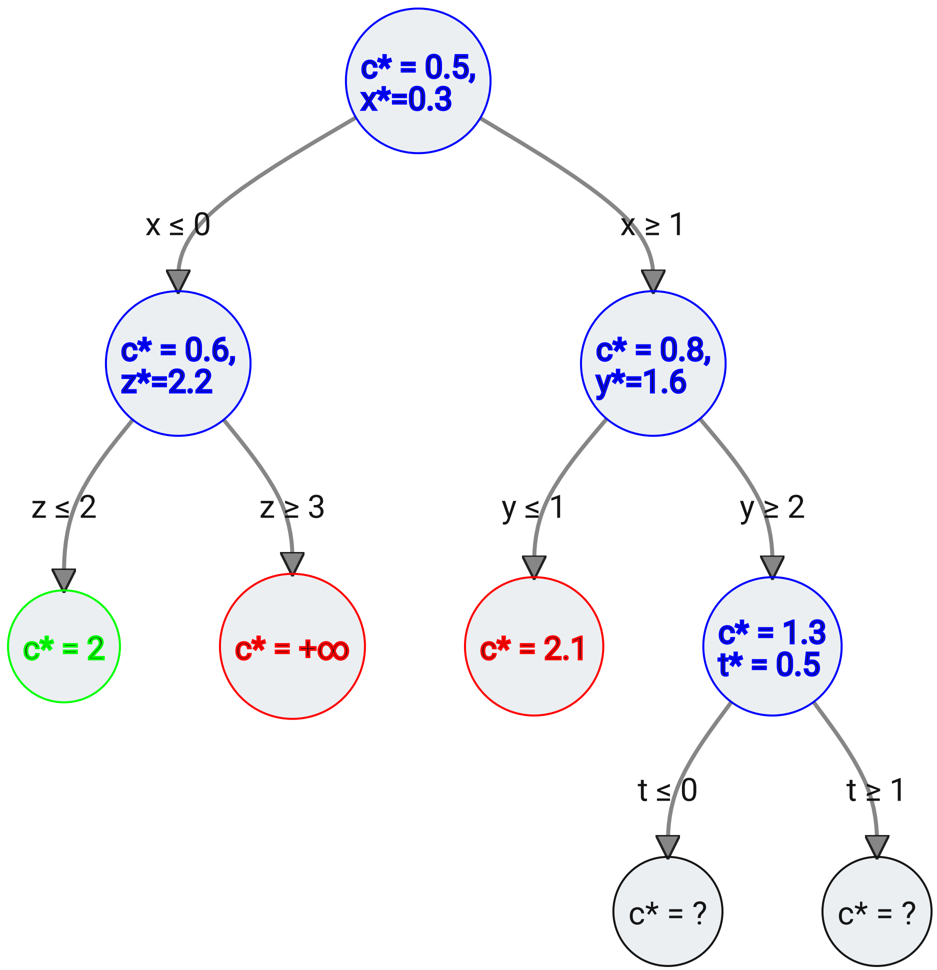
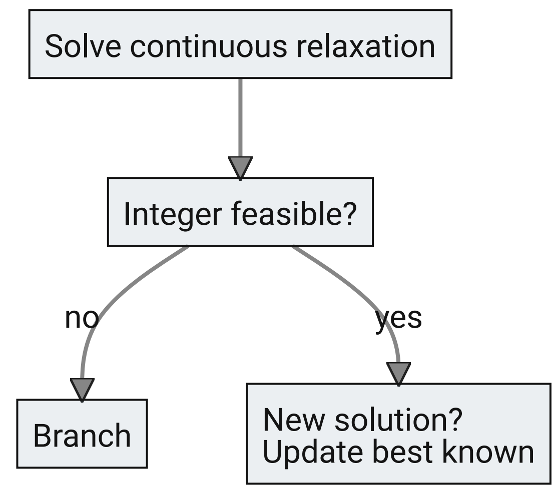
The basic branch-and-bound algorithm



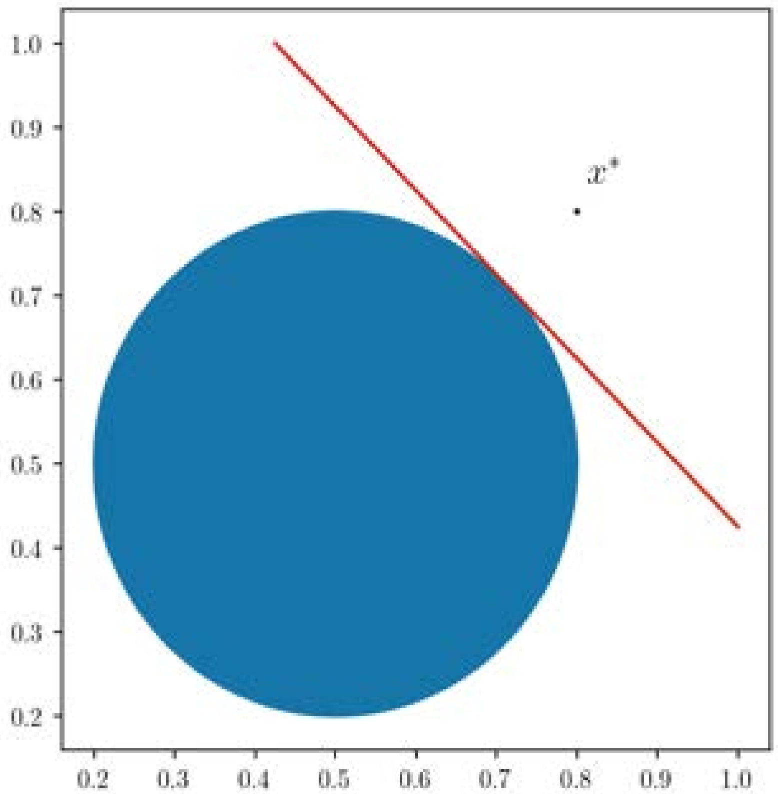
At each node of the tree:



In MILP and MIQP continuous relaxation usually solved by simplex.

In MISOCP/MIQCP, continuous relaxation solved by barrier.

The outer approximation cut



- Let $C = \{g(x) \leq b : x \in R^n\}$, with g a convex function
- For any $x^* \in \mathbb{R}^n$, the constraint:

$$\nabla g(x^*)(x - x^*) + g(x^*) \leq 0$$

  is valid
- If $x^* \notin C$, it cuts x^*:

$$\nabla g(x^*)(x^* - x^*) + g(x^*) > 0$$

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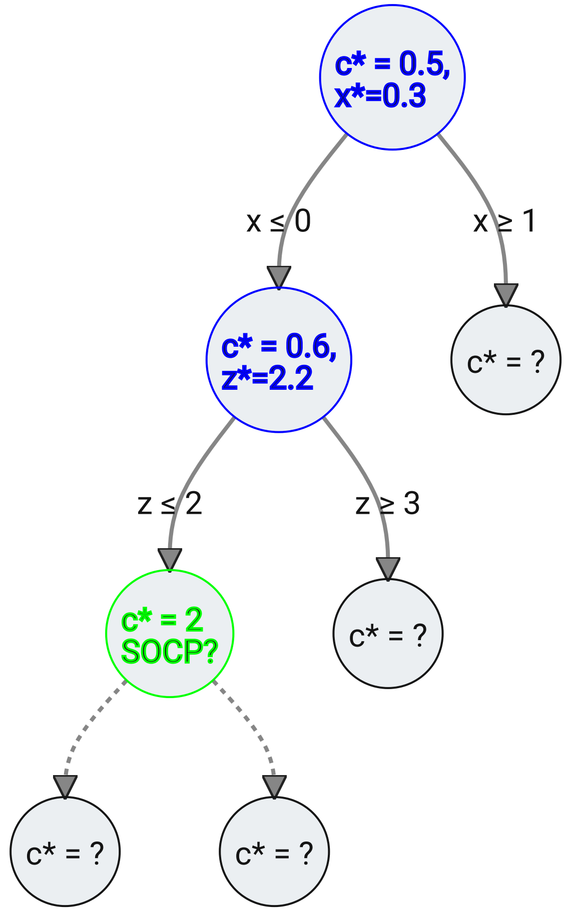
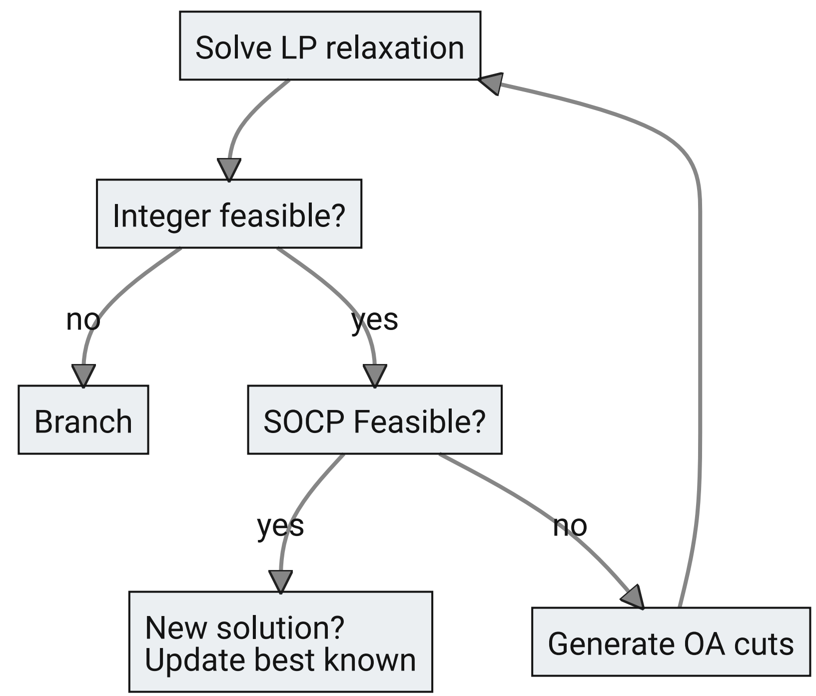
Outer approximation branch-and-cut



Drop quadratic constraints and solve an LP relaxation at each node.

Integer feasible nodes are not necessarily solutions.



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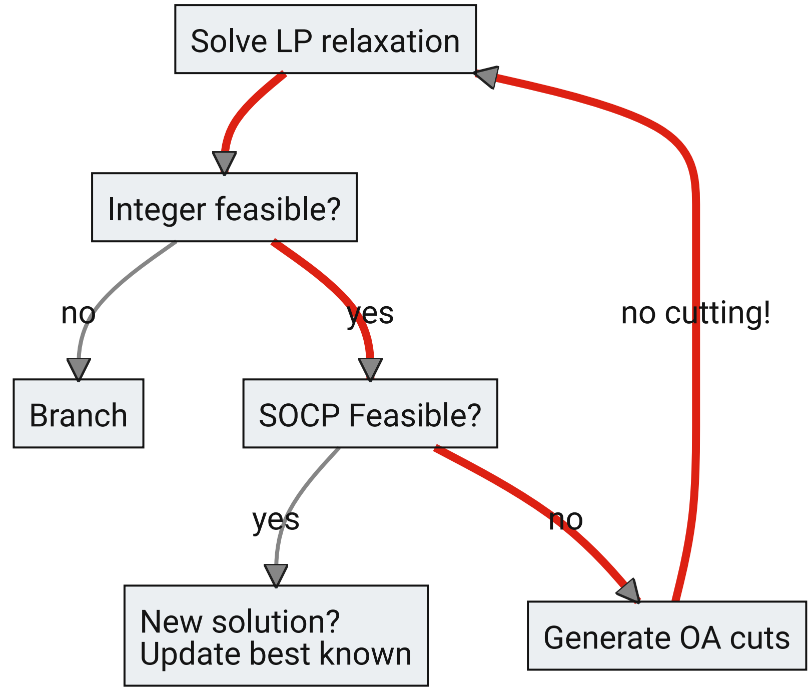
Numerical difficulties

- OA branch-and-cut builds a cutting plane approximation of smooth functions
- It can happen that node solution:
  - is integer feasible
  - is not SOC feasible
  - OA cuts are not cutting enough



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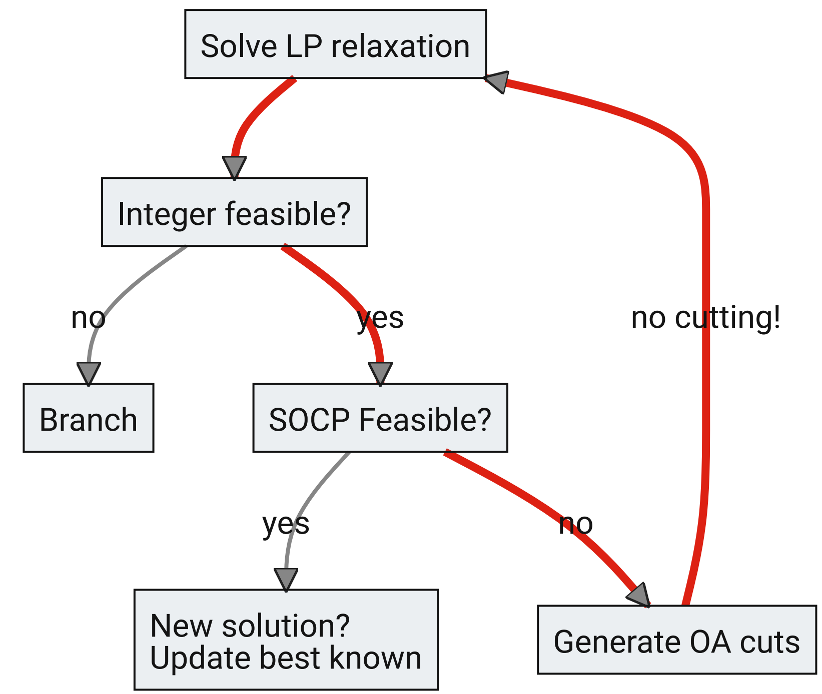

New in Gurobi 11

Rely on barrier algorithm for those nodes (usually very few).

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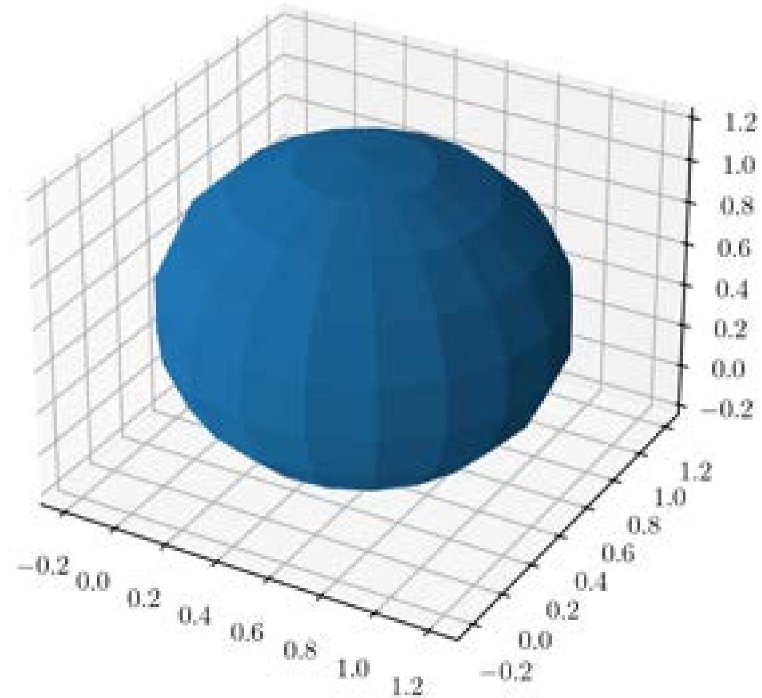
Cone disaggregation and outer approximation

An exponential number of cutting planes is needed to approximate a convex quadratic form.



Cone disaggregation

From

$$\sum_{i=1}^{n} x_i^2 \leq x_0^2, x_0 \geq 0$$

- Create variables $y_i \geq 0$, such that $x_i^2 \leq y_i x_0$ (rotated SOC)
- Replace initial constraint with $\sum_{i=1}^{n} y_i \leq x_0$

Pitfalls of disaggregation

$$(A)\begin{cases}\sum_{i=1}^{n} x_i^2 \le x_0^2, \\ x_0 \ge 0\end{cases} \qquad (B)\begin{cases}\sum_{i=1}^{n} y_i \le x_0 \\ x_i^2 \le y_i x_0 & i = 1, \dots, n \\ y \ge 0, x \ge 0\end{cases}$$

- The reformulation is correct: every solution of (B) translates to (A)
- But a solution of (B) with a small infeasibility can have a large one in (A):
- Suppose $x_0 = 1, y_i = \frac{1}{n}$ and $x_i = \sqrt{\frac{1}{n} + \epsilon}$:
  - Infeasibility in (B) is ϵ
  - Infeasibility in (A) is $n \cdot \epsilon$

Gurobi tries to deal with it but can be an issue.

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Options for MISOCP/MIQCQP

MIQCPMethod

- -1 Automatic choice (default)
- 0 Use QCP branch-and-bound
- 1 Use Outer Approximation

PreMIQCPForm

- -1 Automatic choice (default)
- 0 Leave the model as is (for B&B)
- 1 Reformulate to SOC
- 2 Reformulate to SOC and disaggregate

Example

Portfolio Optimization

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Stepping into a non-convex world

Non-Convex MIQCQP

$$\min c^T x + x^T Q^0 x$$

$$\text{s.t:}$$

$$a_k{}^T x + x^T Q^k x \leq b_k, \qquad k = 1, \ldots, m$$

$$x_j \in \mathbb{Z}, j \in \square$$

$$l \leq x \leq u$$

- $Q^0, Q^1, \ldots, Q^m$ are assumed to be symmetric
- Continuous relaxation is NP-hard!
- Solution strategy:
  - Build a convex relaxation
  - Refine it through branching.

Non-Convex MIQCQP

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Note

NonConvex parameter in Gurobi

NonConvex

- -1 automatic (default)
- 0 Return error if original model has non-convex Q objective or constraints
- 1 Return error if presolved model has non-convex Q that cannot be linearized
- 2 Accept non-convex Q by building a bilinear formulation

New in Gurobi 11

Default behavior change: New default 2 (was 1)).

Bilinear formulation

- For each product $x_i x_j$ in the model
  - Introduce a new variable z_{ij}
  - Add the **bilinear** constraint $z_{ij} = x_i x_j$
  - Replace product with z_{ij}

$$\min c^T x + \langle Q^0, Z \rangle$$

s.t:

$$a_k{}^T x + \langle Q^k, Z \rangle \leq b_k, \qquad k = 1, \ldots, m$$

$$Z = xx^T$$

$$l \leq x \leq u$$

$$(\langle Q, Z \rangle = \sum_i \sum_j q_{ij} z_{ij})$$

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More details on bilinear formulation

- Try as much as possible to avoid creating bilinear terms:
  - if one variable is fixed
  - if one variable is binary (can be reformulated)
  - square of binary $x^2 = x$
  - square term $q_{ii}x^2$ with $q_i i > 0$ is convex
- If $x_i x_j$ always appears in inequalities with q_{ij} of same sign relax to:
  - $z_{ij} \geq x_i x_j$, if $q_{ij} > 0$
  - $z_{ij} \leq x_i x_j$, if $q_{ij} < 0$

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⚠ **Warning**

Bilinear relaxation

- Relax non-convex constraint $Z = xx^T$ using convex enveloppes.

$$\min c^T x + \langle Q^0, Z \rangle$$

s.t:

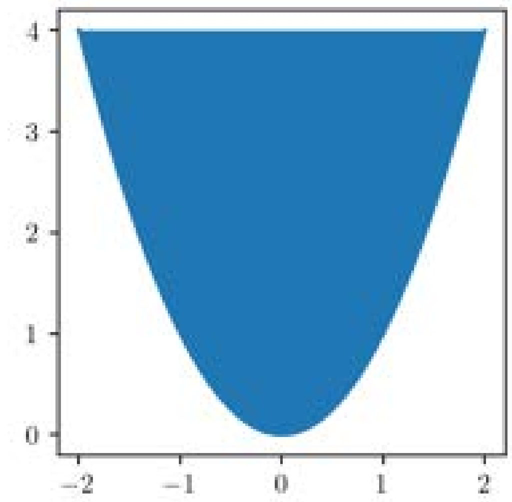
$$a_k^T x + \langle Q^k, Z \rangle \leq b_k, \qquad k = 1, \ldots, m$$

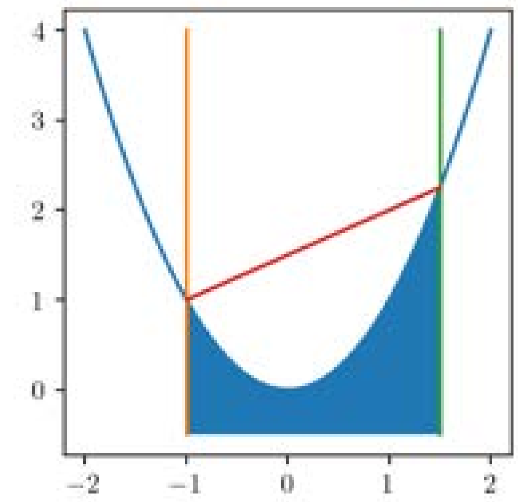
$$z^-(x_i, x_j) \leq z_{ij} \leq z^+(x_i, x_j)$$

$$l \leq x \leq u$$

Convex envelopes: parabola

Consider the square case: $z = x^2$





$z \geq x^2$

It is convex:

$$z^-(x_i, x_i) = x_i^2$$

Can be dealt with by OA.

$z \leq x^2, -1 \leq x \leq 1.5$

$z^+(x_i, x_i)$ is given by the secant:

$$z_{ii}^+ = (u+1)x_i - 1 \cdot u$$

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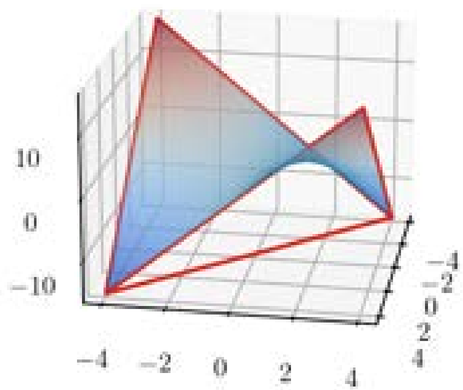
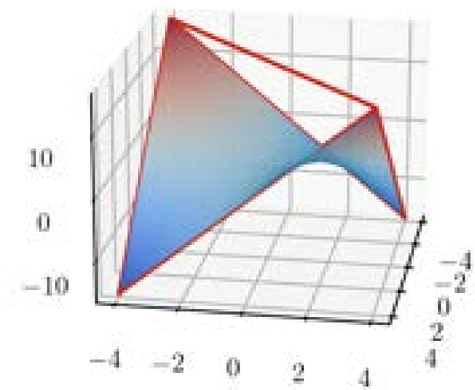
Convex envelopes: products (McCormick)



Lower enveloppe z_{ij}^-

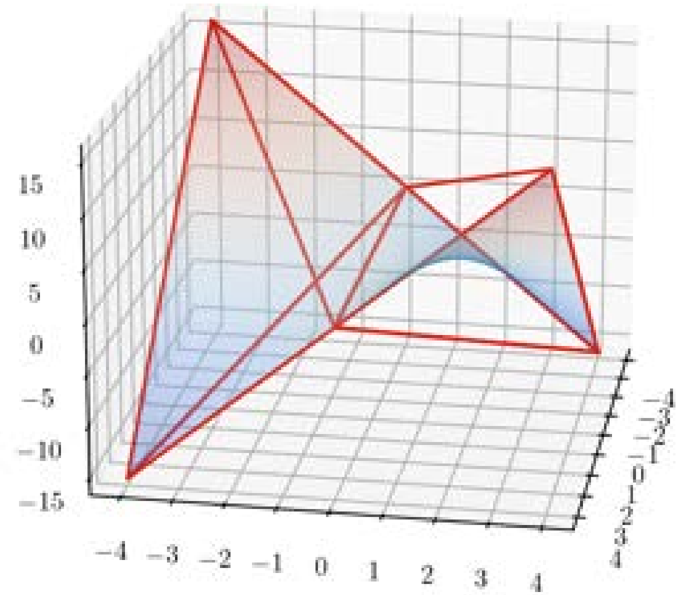


Upper enveloppe z_{ij}^+

$$z_{ij}^- = \max\left\{\begin{array}{l} l_j x_i + l_i x_j - l_i l_j \\ u_j x_i + u_i x_j - u_i u_j \end{array}\right\} \leq z_{ij} \leq z_{ij}^+ = \min\left\{\begin{array}{l} l_j x_i + u_i x_j - u_i l_j \\ u_j x_i + l_i x_j - l_i u_j \end{array}\right\}$$

Spatial branching

- Let (x^*, z^*) be the solution of the bilinear relaxation
- If not integer feasible, can branch on an integer variable
- Otherwise:
  - If $z_{ij}^* = x_i^* x_j^*$, for all bilinear term, we have a solution
  - Otherwise refine our bilinear relaxation:
    - Pick x_i or x_j s.t. $z_{ij}^* \neq x_i^* x_j^*$
    - Create two child nodes with $x_i \leq x_i^*$ and $x_i \geq x_i^*$
    - Refine bilinear relaxation in the two nodes



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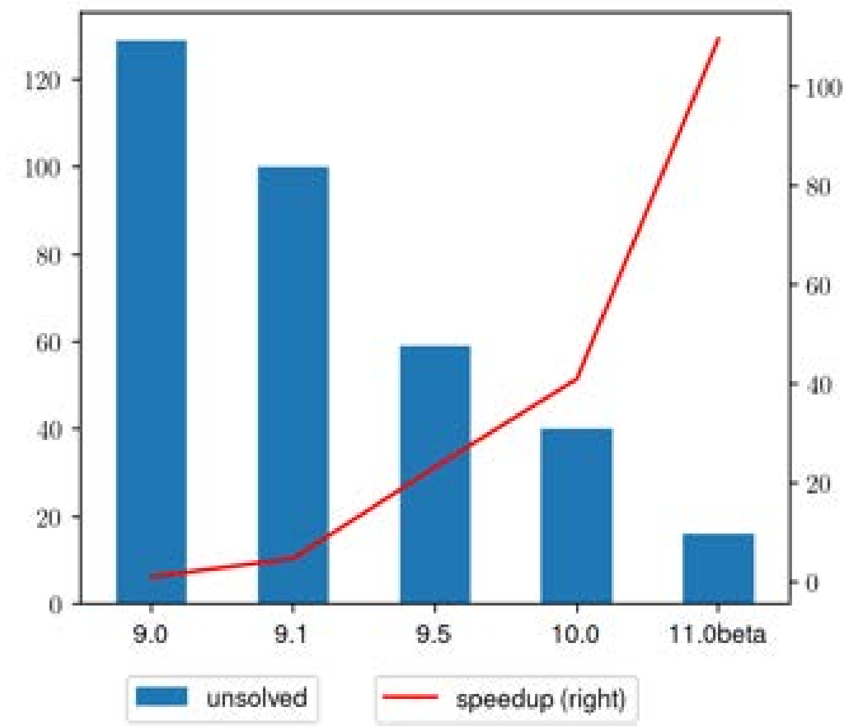
Other techniques targeted at non-convex MIQCQP

- `RLTCuts`
  - Reformulation Linearization Technique (Sherali and Adams, 1990)
  - Multiply linear constraint by a variable, linearize resulting products
- `BQPCuts`
  - Facets of the *Binary Quadratic Polytope* (Padberg 1989)
  - Clique cuts from the paper
- `SDPCuts`
  - Relax $Z = xx^T$ to $Z \succeq xx^T$, and outer approximate resulting cone
- `OBBT`:
  - Optimization based bound tightening
  - Infer tighter bound on variables involved in products by LP.

Non-convex MIQCQP performance history

New in Gurobi 11

- Improved recognition of convexity
- Branching improvements
  - Strong branching for bilinear terms
  - Better choice for deciding to branch on an integer or bilinear



874 models – discarded: 40 due to inconsistent answers, 278 that none of the versions can solve

Example solve

Pooling problem from MINLPLIB

```
m.optimize()
```

```
Gurobi Optimizer version 11.0.0 build v11.0.0beta2 (mac64[x86] - macOS
13.6 22G120)

CPU model: Intel(R) Core(TM) i5-1038NG7 CPU @ 2.00GHz
Thread count: 4 physical cores, 8 logical processors, using up to 8
threads

Optimize a model with 662 rows, 403 columns and 2229 nonzeros
Model fingerprint: 0x883de6ff
Model has 70 quadratic constraints
Variable types: 295 continuous, 108 integer (108 binary)
Coefficient statistics:
  Matrix range     [2e-03, 1e+03]
  QMatrix range    [1e+00, 1e+00]
  QLMatrix range   [1e+00, 1e+00]
```

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Function constraints in Gurobi

Since Gurobi 9.0. Allow to state $y = f(x)$

- f is a predefined function
- y and x are one-dimensional variables

Library of predefined functions include:

- e^x, a^x, $\ln(x)$, $\log_a(x)$, logistic
- $\sin(x)$, $\cos(x)$, $\tan(x)$,
- monomials x^a, polynomials of one variable $a_0 + a_1 x^1 + a_2 x^2 + \ldots$

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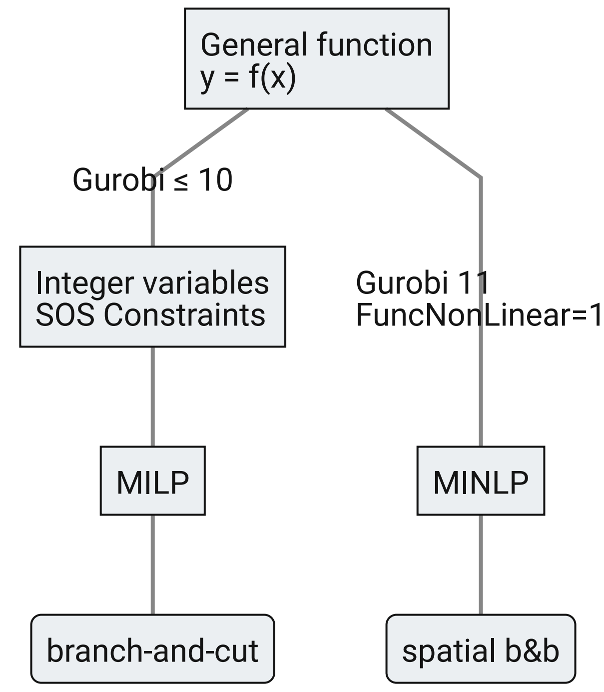
Example:

```
m = gp.Model()
x = m.addVar()
y = m.addVar()
m.addGenConstrLog(x, y)
```

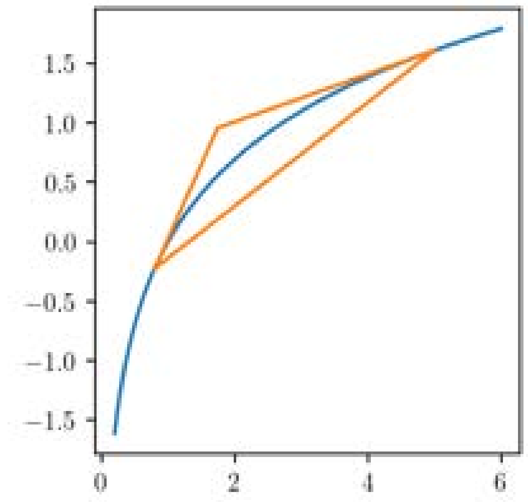
New treatment in Gurobi 11

- Gurobi 9.0-10.0: nonlinear functions replaced during presolve by a piece-wise linear approximation.
- Gurobi 11, can treat nonlinear functions directly:
  - Set `FuncNonLinear=1`
  - No other changes to users' code



Algorithmic approach

- Similar to bilinear formulation/relaxation
- For each function, compute lower/upper envelope
- Spatial branching to refine them
- Additional difficulties:
  - detect when functions are convex/concave
  - functions can be locally convex



$y = \log(x), 0.8 \le x \le 5$

Great powers and great responsabilities

- Gurobi 11.0 handles select univariate nonlinear functions
- But, those can be composed

E.g.: Consider for $x \geq 0$:

$$f(x) = \sqrt{1 + x^2} + \ln(x + \sqrt{1 + x^2}) \leq 2$$

We can formulate it:

- introduce auxiliary variables $u, v, w, z \geq 0$
- add constraints $u = 1 + x^2, v = \sqrt{u}, w = x + v, z = \ln(w)$
- $f(x) = v + z$

Caution

Feasibility tolerances!

Decomposition leading to large infeasibility

$$y = f(x) = \frac{x}{\sin(x)}$$

a solution is $x = 0.0001, y = 1.0000000016666666.$

Now decompose $f(x)$: $u = \sin(x), v = \frac{1}{u}, y = x \cdot v.$

And consider:

- $\overline{x} = 0.0001$
- $\overline{u} = 0.00009899999983333343$ $(\sin(\overline{x}) - 10^{-6})$
- $\overline{v} = 10101.010118015167$
- $\overline{y} = 1.0101010118015167$

⚠ 😱

We have $\overline{y} - f(\overline{x}) \approxeq 10^{-2}$

Example

Logistic Regression

Thank You!

For more information: www.gurobi.com

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