Mixed-Integer Nonlinear Programming

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Introduction

Introduction

- About this lecture
- What is mixed-integer nonlinear programming
- Solving a mixed-integer optimisation problem
- What is special about nonlinear problems

About This Lecture

Goals of the lecture:

- Introduce the viewers to the key concepts of mixed-integer nonlinear programming
- Explain the basics of MINLP solution methods
- Share some practical tips

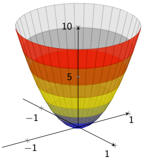
It is assumed that the viewers are familiar with the following:

- Basic notions of optimisation: optimisation problem, feasible set, objective function, feasible and optimal solutions
- Basic notions of mixed-integer linear programming: mixed-integer linear program, integer variables, continuous relaxation
- MILP branch-and-bound: branching and bounding, primal and dual bounds, optimality gap, pruning, cutting planes

Mixed-Integer Nonlinear Programs

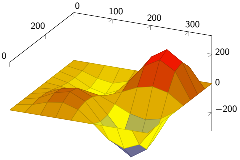
$$\begin{aligned} \min\ & c^{\mathsf{T}} x \\ \text{s.t. } & g_k(x) \leq 0 & \forall k \in [m] \\ & x_i \in [\ell_i, u_i] & \forall i \in [n] \\ & x_i \in \mathbb{Z} & \forall i \in \mathcal{I} \subseteq [n] \end{aligned}$$

The nonlinear part: functions $g_k \in C^1([\ell, u], \mathbb{R})$:



convex

or



nonconvex

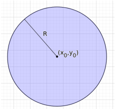
Examples of Nonlinearities

- Variable fraction $p \in [0, 1]$ of variable quantity q: qp. Example: water treatment unit

- AC power flow - nonlinear function of voltage magnitudes and angles

$$p_{ij} = g_{ij} v_i^2 - g_{ij} v_i v_j \cos(\theta_{ij}) + b_{ij} v_i v_j \sin(\theta_{ij})$$

- Distance constraints



$$(x - x_0)^2 + (y - y_0)^2 \leq R$$

- etc.

Solving a Mixed-Integer Optimisation Problem

Two major tasks:

1. Finding and improving feasible solutions (primal side)
    - Ensure feasibility, sacrifice optimality
    - Important for practical applications
2. Proving optimality (dual side)
    - Ensure optimality, sacrifice feasibility
    - Necessary in order to actually solve the problem

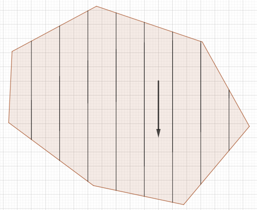
Connected by:

3. Strategy
    - Ensure convergence
    - Divide: branching, decompositions, ...
    - Put together all components

Nonlinearity Brings New Challenges

- More numerical issues
- NLP solvers are less efficient and reliable than LP solvers

1. Finding feasible solutions
   - Feasible solutions must also satisfy nonlinear constraints
   - If nonconvex: fixing integer variables and solving the NLP can produce local optima
2. Proving optimality
   - NLP or LP relaxations?
   - If nonconvex: continuous relaxation no longer provides a lower bound
   - "Convenient" descriptions of the feasible set are important
3. Strategy
   - Need to account for all of the above
   - Warmstart for NLP is much less efficient than for LP



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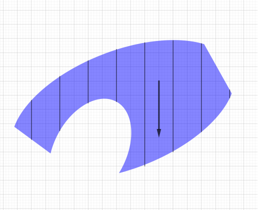


Introduction: Recap

- What is an MINLP problem? What do constraints, variables, objective look like?
- Solving an MINLP can be roughly divided into two major tasks. What are they and how are they connected?
- Adding "nonlinear" to "mixed-integer" makes the problem even more difficult. How does this affect different parts of the solution process?

Finding Feasible Solutions

Primal Heuristics

The goal of primal heuristics is to find solutions that are:

- feasible (satisfying all constraints) and
- good quality (solutions with lower objective value are preferable).

The best of solutions found so far is referred to as best feasible or incumbent. It provides an upper bound on the optimal value.

Common theme in primal heuristics: restrict the problem to obtain a subproblem for which a feasible solution can be found.

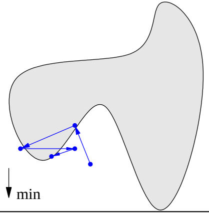
Nonconvex: NLP subproblems are usually solved to local optimality.

- Local optima are still feasible solutions
- Not finding the global optimum affects the quality of upper bounds

Primal Heuristics for MINLPs

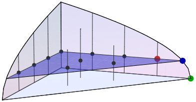
NLP local search

- Fix integer variables to values at reference point; solve the NLP.
- Reference point: integer feasible solution of the LP relaxation.



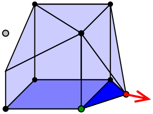
Undercover

- Fix some variables so that the subproblem is linear and solve the MIP.



Sub-MINLP

- Search around promising solutions.
- The region is restricted by additional constraints and/or fixing variables.



Proving Optimality

Proving Optimality

- Using relaxations for finding lower bounds
- Relaxations for convex MINLPs
- Managing cuts: initial cuts and dynamically added cuts
- Relaxations for nonconvex MINLPs
- How to strengthen the relaxations

Finding Lower Bounds: Relaxations

Key task: describe the feasible set in a convenient way.
Requirement: the relaxed problem should be efficiently solvable to global optimality.

It is preferable to have relaxations that are:

- Convex: NLP solutions are globally optimal, infeasibility detection is reliable
- Linear: solving is more efficient, good for warmstarting

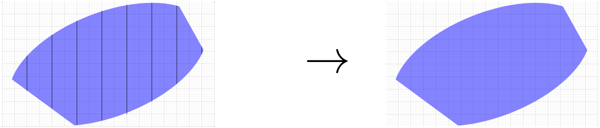
and to avoid:

- Very large numbers of constraints and variables
- Bad numerics

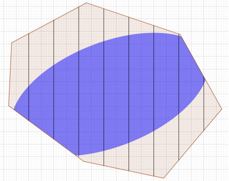
Let F be the feasible set. We look for a relaxation: a set R such that $F \subseteq R$ which satisfies some of the above.

Relaxations for Convex MINLPs

- Relax integrality



- Replace the nonlinear set with a linear outer approximation



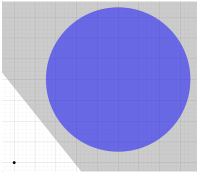
- Linear outer approximation + relax integrality $\rightarrow$ LP relaxation

Outer Approximating Convex Constraints

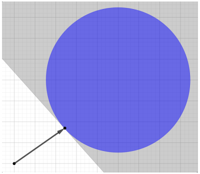
A linear inequality $ax \leq b$ is valid if $x \in F \Rightarrow ax \leq b$ (such inequalities are called cutting planes, or cuts)

Given constraint $g(x) \leq 0$ (g convex, differentiable) and a reference point $\hat{x}$, one can build:

Gradient cuts (Kelley):
$g(\hat{x}) + \nabla g(\hat{x})(x - \hat{x}) \leq 0$

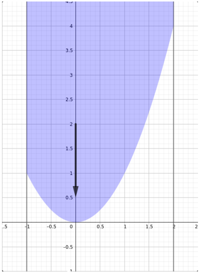


Projected cuts: same, but move $\hat{x}$ to the boundary of F



Which Cuts to Add?

There are infinitely many possible cuts, how to choose them?



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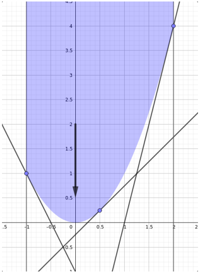

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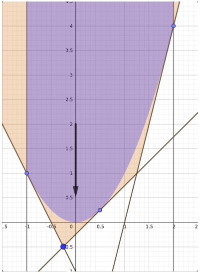

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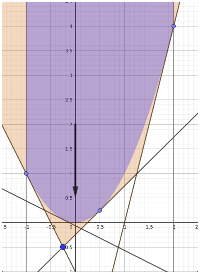

Separation

- Reference point is a relaxation solution $\hat{x} \notin F$
- Valid inequalities $ax \leq b$ violated by $\hat{x}$: $a\hat{x} > b$
- Thus $\hat{x}$ is separated from F

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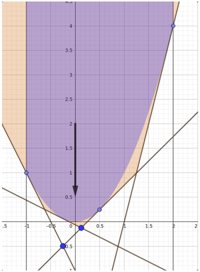

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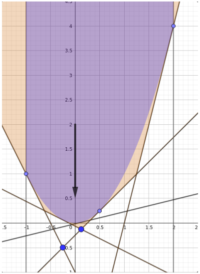

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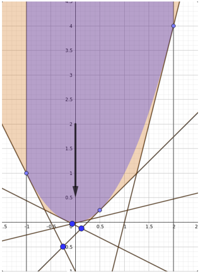

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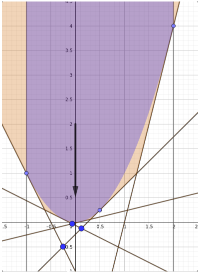

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Cut selection: choose from violated cuts using various criteria for cut "usefulness".

Convex Relaxations for Nonconvex MINLPs

Only relaxing integrality no longer provides a lower bound, and gradient cuts might no longer be valid $\Rightarrow$ construct a convex relaxation.

The best relaxation is $conv(F)$: convex hull of F, i.e. the smallest convex set containing F. In general, cannot be constructed explicitly.

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  $\uparrow$

- Find convex underestimators g_k^{cv} of functions g_k:
  $g_k^{cv}(x) \leq g_k(x) \; \forall x \in [l, u]$

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  $\uparrow$

- Find and combine relaxations of simple functions

Examples of simple functions: x^2, x^k, $\sqrt{x}$, xy, etc.
Exercise: write the tightest possible convex underestimators for $-x^2$ and x^3, given $x \in [-1, 1]$ (hint: for x^3, you need more than one function for each estimator).

Combining Relaxations

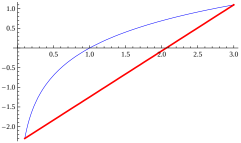
Find underestimator for $g(x) = \phi(\psi_1(x), \ldots, \psi_p(x))$, where functions ϕ and ψ_j are "simple", i.e. can be convexified directly.

- McCormick relaxations for factorable functions: piecewise continuous relaxations utilising convex and concave envelopes of ϕ and ψ_j.
- Auxiliary variable method: introduce variables $y_j = \psi_j(x)$. Then $g(x) = \phi(y_1, \ldots, y_p)$. Enables individual handling of each function.

Linear Relaxations for Nonconvex MINLPs

Gradient cuts might no longer be valid!

- If possible, directly construct linear underestimators for nonconvex functions
  - Secants for concave functions
  - McCormick envelopes for bilinear products
  - etc.



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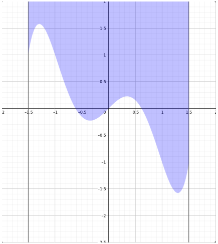

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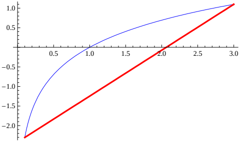

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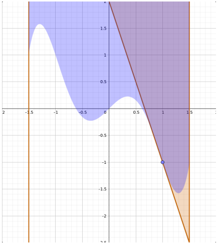

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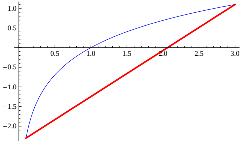

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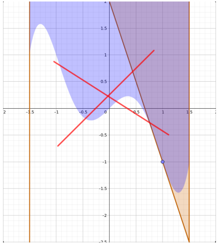

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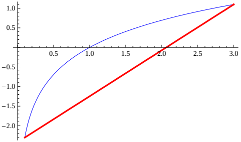

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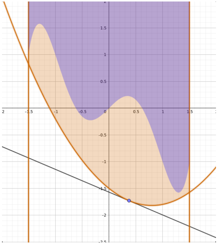

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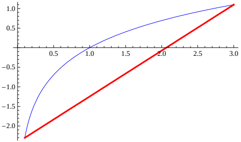

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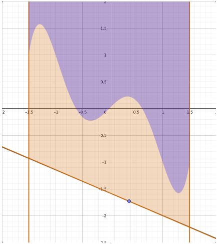
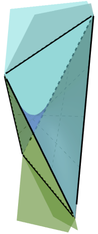


Impact of Variable Bounds

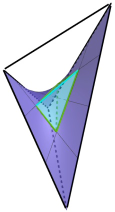
Tighter bounds ⇒ tighter relaxations.

Example: McCormick relaxation of a bilinear product relation $z = xy$:

$$z \le x^u y + x y^l - x^u y^l$$
$$z \le x^l y + x y^u - x^l y^u$$
$$z \ge x^l y + x y^l - x^l y^l$$
$$z \ge x^u y + x y^u - x^u y^u$$



$(x, y) \in [-1, 2] \times [-2, 2]$



$(x, y) \in [0, 1] \times [-1, 1]$

Tighter bounds obtained from:

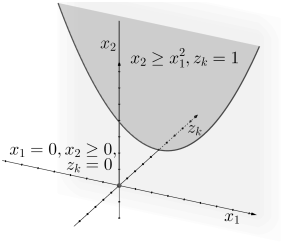
- Branching
- Specialised bound tightening techniques (see linked materials)

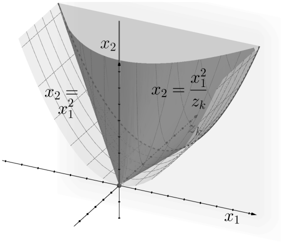
Strengthening Relaxations: Using More Constraints

More constraints ⇒ tighter relaxations.

Example: perspective cuts. Use an additional constraint that requires x to be semicontinuous.

$$g(x) \leq 0, \; lz \leq x \leq uz$$





Proving Optimality: Recap

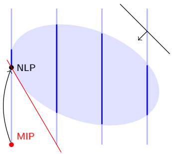
- What are relaxations used for? What are some common types of relaxations?
- What are gradient cuts and when can they be applied?
- What is a convex hull and what is its practical significance?
- Auxiliary variable method: how does it reformulate a function $g(x) = \phi(\psi_1(x), \ldots, \psi_p(x))$ and what it is used for.
- How can relaxations of nonconvex problems be strengthened?

Strategy

Strategy

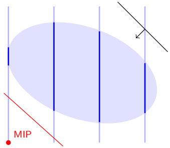
- Goal: bring together the primal and dual side, i.e. find the optimal solution and prove that it is optimal
- A brief overview of algorithms for convex MINLPs
- A closer look at spatial branch and bound

Algorithms for Convex MINLP: Overview



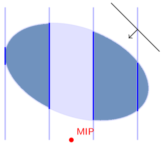
Outer Approximation:

- Solve MIP relaxations and NLP subproblems
- Add cuts at solutions of NLP subproblems
- Uses the equivalence of MINLP to MILP (see notes)



Extended Cutting Planes:

- Solve MIP relaxations
- Add cuts at solutions of MIP relaxations



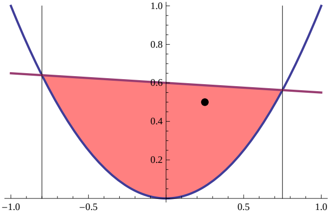
Branch and Bound:

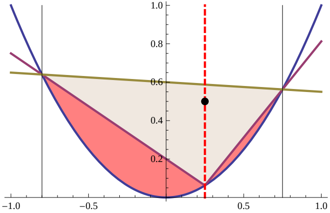
- Generalisation of MILP B&B
- The continuous relaxation is nonlinear (but convex)
- Different choices between LP and NLP relaxations

Algorithms for Nonconvex MINLP: Spatial Branching

Branching on variables in violated nonconvex constraints, because variable bounds determine the convex relaxation, e.g.,

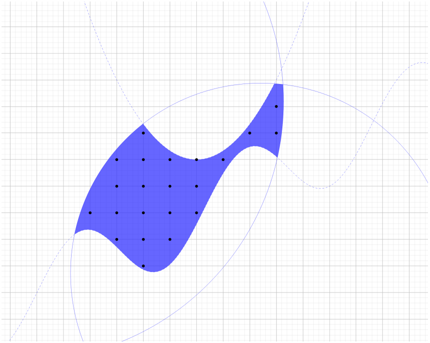
$$x^2 \leq \ell^2 + \frac{u^2 - \ell^2}{u - \ell}(x - \ell) \quad \forall x \in [\ell, u].$$





Spatial Branch and Bound

- Solve a relaxation → lower bound
- Run heuristics to look for feasible solutions → upper bound
- Branch on a suitable variable
- Discard parts of the tree that are infeasible or where lower bound > best known upper bound
- Repeat until gap is below given tolerance



Smaller domains → improved relaxations → improved bounds.

Spatial Branch and Bound

- Solve a relaxation → lower bound
- Run heuristics to look for feasible solutions → upper bound
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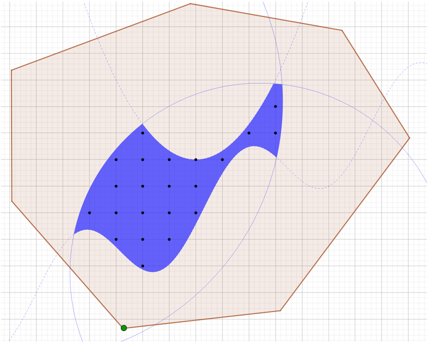

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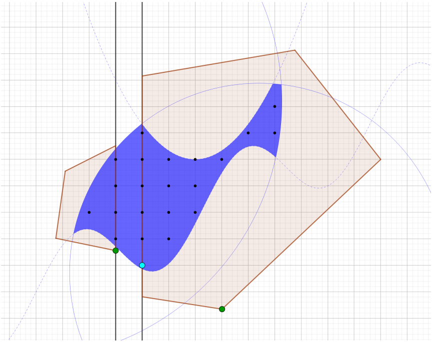

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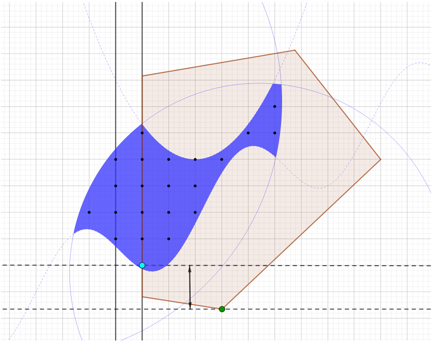

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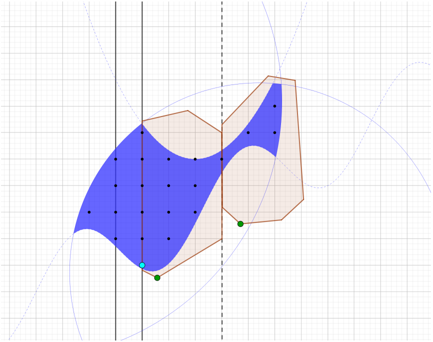

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Strategy: Recap

- There are several different approaches to solving convex MINLPs.
- In addition to branching to enforce integrality, what other type of branching does spatial B&B employ?
- Can you recall the main steps of the spatial B&B algorithm?

MINLP in SCIP

MINLP in SCIP

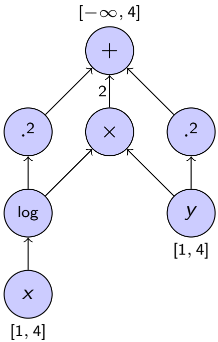
- SCIP implements LP-based spatial B&B
- Convex relaxations are constructed via the auxiliary variable method
- The handling of nonlinear constraints is based on expression graphs

Expression Trees

Algebraic structure of nonlinear constraints is stored in one directed acyclic graph:

- nodes: variables, operations, constraints
- arcs: flow of computation

$$\log(x)^2 + 2\log(x)y + y^2$$



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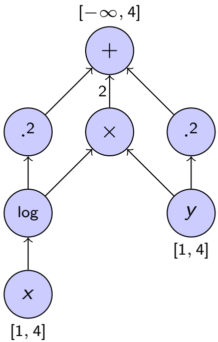
Operators:

- variable index, constant
- $+$, $-$, $*$, $\div$
- $\cdot^2$, $\sqrt{\cdot}$, $\cdot^p$ ($p \in \mathbb{R}$), $\cdot^n$ ($n \in \mathbb{Z}$), $x \mapsto x|x|^{p-1}$ ($p > 1$)
- exp, log
- min, max, abs
- $\sum$, $\prod$, affine-linear, quadratic, signomial
- (user)

$\log(x)^2 + 2\log(x)y + y^2$



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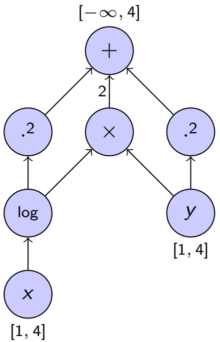
Additional constraint handlers: quadratic, abspower ($x \mapsto x|x|^{p-1}$, $p > 1$), SOC

$\log(x)^2 + 2\log(x)y + y^2$

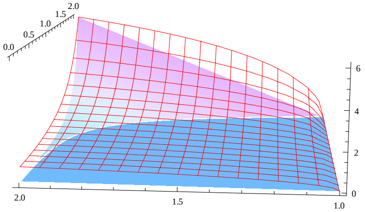


Reformulation (During Presolve)

Goal: reformulate constraints such that only elementary cases (convex, concave, odd power, quadratic) remain. Implements the auxiliary variable method.

Example:

$$g(x) = \sqrt{\exp(x_1^2)\ln(x_2)}$$



Introduces new variables and new constraints.

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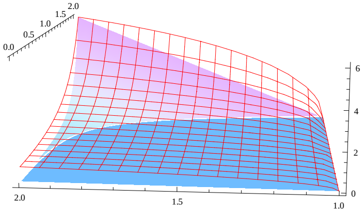


Reformulation:

$$g = \sqrt{y_1}$$
$$y_1 = y_2 y_3$$
$$y_2 = \exp(y_4)$$
$$y_3 = \ln(x_2)$$
$$y_4 = x_1^2$$

Introduces new variables and new constraints.

Practical Topics

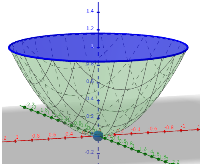
Impact of Modelling

If you know your problem structure - use it!

Example: x and y contained in circle of radius c if $z = 1$ and are both zero if $z = 0$.

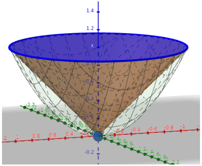
One could model this as:

$$x^2 + y^2 \leq cz$$
$$x, y \in \mathbb{R}, \ z \in \{0, 1\}$$



Or as:

$$x^2 + y^2 \leq cz^2$$
$$x, y \in \mathbb{R}, \ z \in \{0, 1\}$$



These describe the same feasible set ($z^2 = z$ if $z \in \{0, 1\}$). But the second formulation leads to a tighter continuous relaxation ($z^2 < z$ if $z \in (0, 1)$).

How to Experiment

- Performance variability
  - Significant changes in performance caused by small changes in model/algorithm
  - Occurs in MILP, but tends to be even more pronounced in MINLP
- Obtaining more reliable results
  - If possible and makes sense, use large and heterogeneous testsets
  - Take advantage of performance variability: model permutations (reordering variables and constraints) can help against random effects (in SCIP, this is controlled by a parameter)
- Using solver statistics
  - Information on tree nodes, primal and dual bounds, effects of solver components
  - Helpful for finding bottlenecks
- Isolating feature effects
  - Turn off some components to get rid of some random effects...
  - or to analyse interaction: some component might make the feature redundant, etc.