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Advances in Generalized Disjunctive and Mixed-Integer Nonlinear Programming Algorithms and Software for Superstructure Optimization

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Motivation

Goal

Present recent advances in optimization algorithms and software to solve process superstructure problems in a way that is easily accessible to users and extensible to advances modeling systems.

State-of the-art

- Process units implemented in programming languages with interface to optimization solvers.
- Modeling of superstructure done through Mixed-integer nonlinear programming (MINLP).

Challenges

Challenging Optimization problems

- Requirement for **versatile modeling framework** combining **discrete and continuous variables**, with **nonlinear constraints**.

Diverse and incompatible solutions tools

- Requirement for specialized solution methods

Modeling needs to be **accessible to users** and allow for **advanced optimization** algorithmic capabilities.

Approach

Introduce MINLP and Generalized Disjunctive Programming (GDP) **open-source modeling tools** and **solvers** in Python to implement **process superstructure** and release examples in library GDPLib.

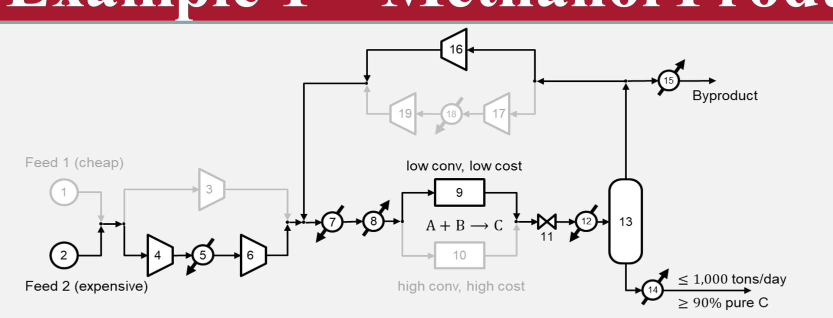
GDPLib – A Library of GDP Problems

Library of GDP problems ready to be solved

- More than **25 different GDP problems** relevant to **Process Systems Engineering** and **Superstructure Optimization**
  - **Methanol production process**
  - **Hydrodealkylation (HDA) process to produce Toluene**
  - Biofuel processing network
  - Heat exchanger network evaluating modular process design
  - Plant capacity expansion model
  - Synthesis gas production plant from methane
  - Kaibel distillation column
  - Tray distillation column design
- Problem ranging from 6 to 31968 continuous variables, 2 to 516 disjunctions, 0 to 5040 integer variables, and 30 to 14927 constraints

```
pip install gdplib
```

Example 1 – Methanol Production Process



- 285 variables
- 277 constraints
- 4 disjunctions

- Problem with 2 reactor types, two feed choices, and single- or two-stage compressor in feed in reactor = 2^4 **process alternatives**
- Solved in **only 2 iterations using LOA** of GDPOpt

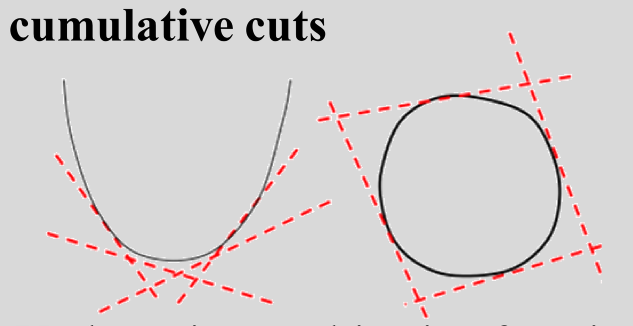
Mixed-Integer Nonlinear Programming

Formulation

$\min_{x,y} f(x,y)$	Objective function
$s.t.\ g(x,y) \le 0$	Nonlinear constraints
$x \in X \subseteq \mathbb{R}^{n_x}$	Continuous vars.
$y \in Y \subseteq \mathbb{Z}^{n_y}$	Discrete vars.

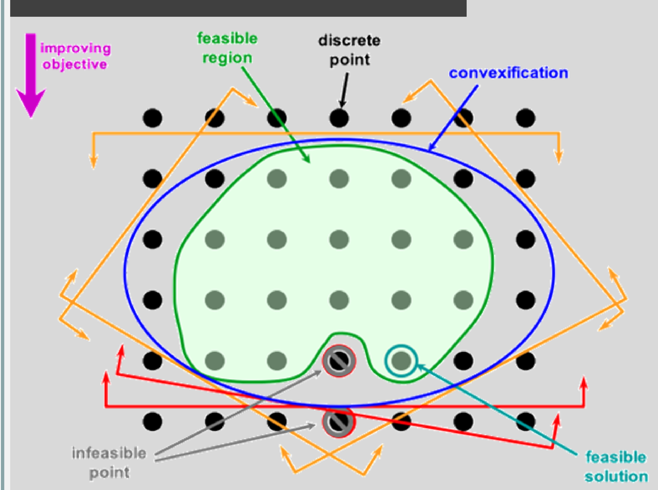
Convex MINLP

Guaranteed to converge by **cumulative cuts**



- Underestimate objective function
- Overestimate feasible region

Nonconvex MINLP



Requires convexification ($g \to \hat{g}$) to converge

Overview and solution approach

- **Optimization** problems with algebraic **nonlinear constraints** in terms of **discrete and continuous variables.**
- **Solution methods** rely on solving **easier subproblems** leading to **bounds** of optimal solution:
  - **Relaxations**: on larger feasible spaces give optimistic or **Lower bound** on the optimum
  - **Restrictions**: evaluating only a subset of the possible solutions provide a feasible or **Upper bound** on optimum

Branch-and-bound

- Start from **continuous relaxation**
- Systematically **enforce integer constraints**
- **Strengthened** with **inequalities** or **cuts**
  - **Really** successful for the linear case

Decomposition-methods

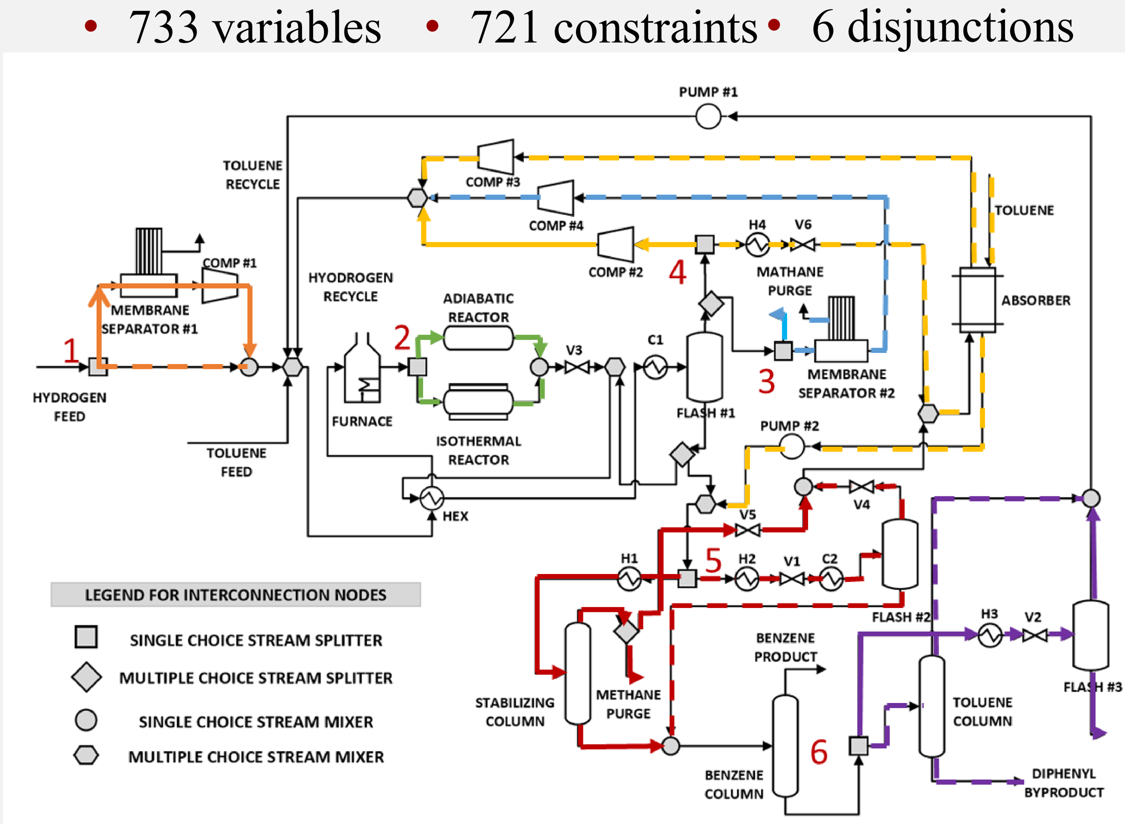
- Iterative solution of restrictions and approximations to find feasible solutions.
- If approximations are valid relaxations, and subproblems are solved globally, global optimality for MINLP can be guaranteed.
- Examples:
  - Outer-Approximation
  - Extended-Cutting Planes
  - Generalized Benders Decomposition

Example 2 – HDA Process

Problem with 6 different disjunctions: **Hydrogen feed pretreatment**, **adiabatic or isothermal reactor**, **methane stream purge or recycle**, **absorber installation or vapor stream recycle**, **stabilizing column or a flash to remove extra methane**, and **Dyphenyl flash separation or Toluene distillation**

- 2^6=64 different process alternatives

- 733 variables
- 721 constraints
- 6 disjunctions



- Commercial global solvers fail to solve MINLP reformulation
- Complete and stable process alternatives enumeration using superstructure model
- LOA from GDPOpt is able to find global optimal solution in less than a minute in a normal desktop using free-access solvers

Generalized Disjunctive Programming

Modeling framework

- Alternative to traditional MINLP modeling
- Preserves logical structure and ability to decompose problem
- Extends mathematical programming with logical correlations

Formulation

$\min_{x,Y,z} f(x,z)$	Objective function
$s.t.\ g(x,z) \le 0$	Global constraints
$\bigvee_{i \in D_k} \begin{bmatrix} Y_{ik} \\ r_{ik}(x,z) \le 0 \end{bmatrix} \quad \forall k \in K$	Disjunctions
$\Omega(Y) = True$	Logic correlations
$x \in X \subseteq \mathbb{R}^{n_x}$	Continuous vars.
$Y \in \{True, False\}^{n_y}$	Logic variables
$z \in Z \subseteq \mathbb{Z}^{n_z}$	Discrete vars.

Solution methods

MINLP Reformulation

- Assign a **binary variable y** for each **logic variable Y**
- Ensure that **feasible regions** are **equivalent**
  - Big-M and Hull

Logic-based methods

- Logic Branch-and-Bound (LBB)
- Logic Outer-Approximation (LOA)
- **Activate** and **deactivate** terms in **disjunction**
- **Evaluate solutions** and generate **relaxations**

Proposed modeling and solution tools

Chosen Platform

python + PYOMO + GitHub

Tools

MindtPy - Mixed-Integer Decomposition Toolbox in Pyomo

- **Algorithms implementation**: (Global) Outer-Approximation, Extended Cutting Planes
- **Novel algorithmic enhancements**: Feasibility pumps, regularization techniques, generalized McCormick cuts, single-tree implementation

Pyomo.GDP

- **Native modeling** extension for **GDP**
- **Automatic reformulation** into **MINLP**

GDPOpt

- **Algorithms implementation** for GDP: LBB and (Global) LOA
- **Enhanced** with **satisfiability solvers** such as Z3

CORAMIN

- **Refinable relaxation generator** for nonlinear functions in MINLP and GDP
- Complementary with solvers in Pyomo, such as MindtPy and GDPOpt

References, QR, and Disclaimer

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