Computational practicum
Lecture 5
Numerical Optimization - Linear & Mixed-Integer Linear Programming

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Wednesday, 10 December 2025

Recap

- In the previous lecture, we covered:
  - Fundamentals of mathematical optimization – definitions
  - Optimality conditions (1st order sufficient and 2nd order sufficient/necessary conditions)
  - Methods to solve unconstrained optimization (steepest descent & Newton method)

Learning goals of this lecture

- After successfully completing this lecture, you are able to. . . .
  - formulate a linear and mixed-integer linear programming model from an engineering problem statement
  - explain at a high-level different algorithms used to solve linear and mixed-integer linear programming models
  - analyze optimal solutions obtained on solving these models

- Note: No need to be able to implement corresponding solution algorithms from scratch.

Outline

- **Anatomy of an optimization problem**
- **Linear Programming (LP)**
  - Fundamentals
  - Solving LPs – conceptual overview of simplex and interior point algorithms
  - Formulating linear programming models given an engineering problem statement
  - Analyzing optimal solutions
- **Mixed-Integer Linear Programming (MILP)**
  - Fundamentals
  - Formulating a MILP from an engineering problem statement

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Nonlinear unconstraint optimization problem (as discussed in Q2 Lecture 4)

$$\min_{\boldsymbol{x}} f\,(\boldsymbol{x})$$

Objective function

Number of variables: n

Degrees of freedom: n

Chemical engineering challenges often come with constraints - our task is to optimize within these boundaries.

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Enter the session ID: **191-696-711**

Or scan the QR code

What constraints exist in chemical engineering applications?

What constraints exist in chemical engineering applications?

Anatomy of a mathematical optimization problem

Typically, mathematical optimization problem consists of:

$$\min_{\boldsymbol{x},\boldsymbol{y}} f(\boldsymbol{x},\boldsymbol{y})$$

Objective function

$$\text{s.t. } \boldsymbol{h}(\boldsymbol{x},\boldsymbol{y}) = 0$$

Equality constraints

$$\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) \leq 0$$

Inequality constraints

$$\boldsymbol{x} \in [\boldsymbol{x}^{\mathrm{L}}, \boldsymbol{x}^{\mathrm{U}}], \boldsymbol{y} \in \{\boldsymbol{y}^{\mathrm{L}}, \ldots, \boldsymbol{y}^{\mathrm{U}}\}$$

Variable bounds

$$\boldsymbol{x} \in \mathbb{R}^{n}, \boldsymbol{y} \in \mathbb{Z}^{k}$$

$$f\colon \mathbb{R}^{n+k} \to \mathbb{R},$$

$$\boldsymbol{h}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_h},$$

$$\boldsymbol{g}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_g},$$

Number of variables: $n + k$

Number of equality constraints: n_h

Number of inequality constraints: n_g

Degrees of freedom: $n + k - n_h$

Equality constraints, $\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{y}) = 0$

- A set or a vector of n_h equality constraints → typically defines the mathematical model
- The model equations can be:
  - Linear or nonlinear
  - Algebraic or differential (ordinary or partial) or integral equations
- Determines the degrees of freedom (DOF) of a mathematical optimization model

$$\text{DOF} = n + k - n_h$$

- For all optimization models, degrees of freedom must always be greater than zero.
- Examples:
  - Mass and energy balances
  - Kinetic models determining the rate of a reaction
  - Thermodynamic models providing values of properties of interest

Inequality constraints, $g(x, y) \leq 0$

- Inequality constraints constraint the values that variables can possibly take
- Generally, it is a vector of n_g equations
- **Feasible region** defines the region where all constraints to the optimization problem are satisfied
- Equivalence: $\mathbf{g(x, y) \leq 0 \equiv -g(x, y) \geq 0}$

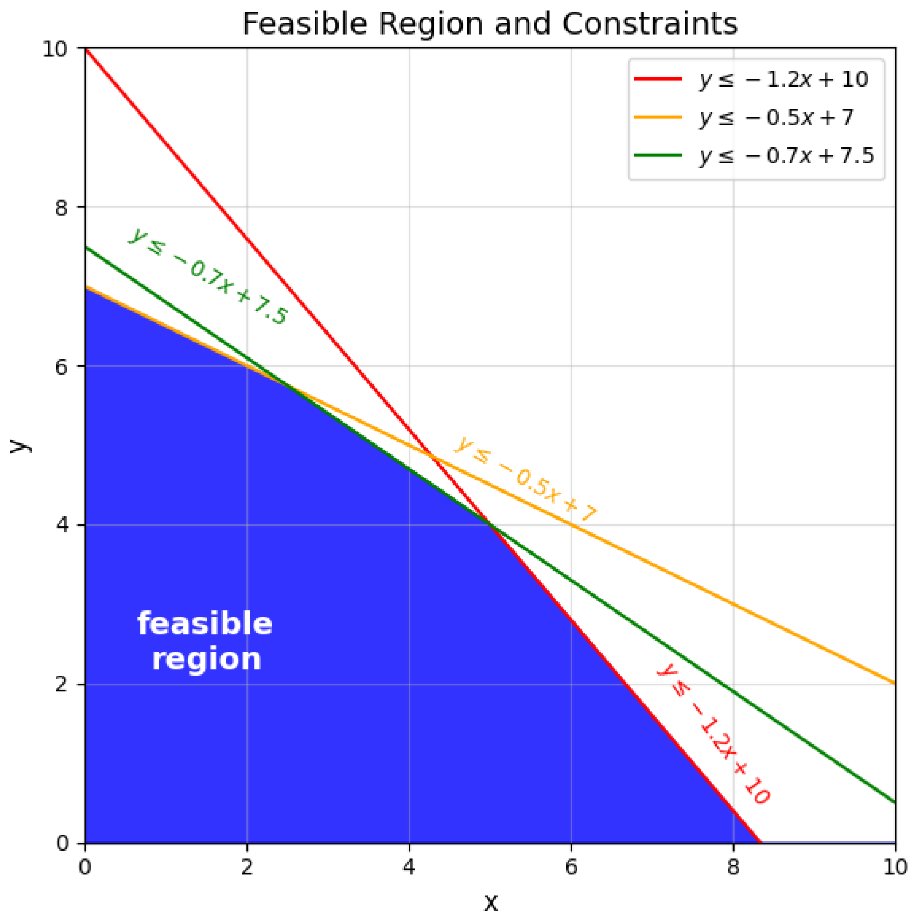

Figure: https://en.wikipedia.org/wiki/Feasible_region#/media/File:Linear_Programming_Feasible_Region.svg

Convexity of a set

The definition of convexity of a function (c.f. Q2 Lecture 4) is different from the definition of convexity for a set

- For a set of constraints defining the feasible set $\Omega = \{\boldsymbol{x} \in D \mid \boldsymbol{g}(\boldsymbol{x}) \leq 0, \boldsymbol{h}(\boldsymbol{x}) = 0\}$
- The set Ω is convex if $\forall\, \boldsymbol{x_1}, \boldsymbol{x_2} \in \Omega$ and $\forall\, \alpha \in [0,1]$ $\alpha \boldsymbol{x_1} + (1-\alpha)\boldsymbol{x_2} \in \Omega$
- Convexity of sets is challenging to establish
- **Sufficient condition for convexity**:
  If equality constraints $\boldsymbol{h}(\boldsymbol{x})$ are linear and $\boldsymbol{g}(\boldsymbol{x})$ are convex functions then Ω is convex
  → a limited case

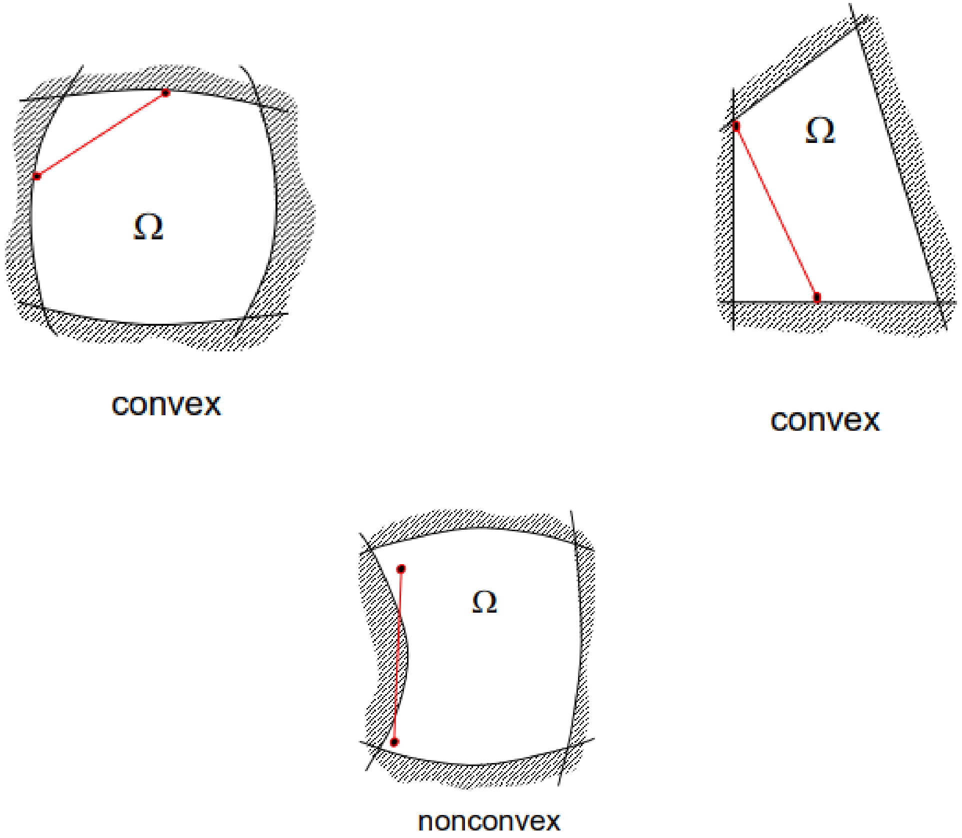

Figure taken from slides by Prof. Alexander Mitsos for his course on Applied Numerical Optimization (RWTH Aachen)

Types of optimization problems

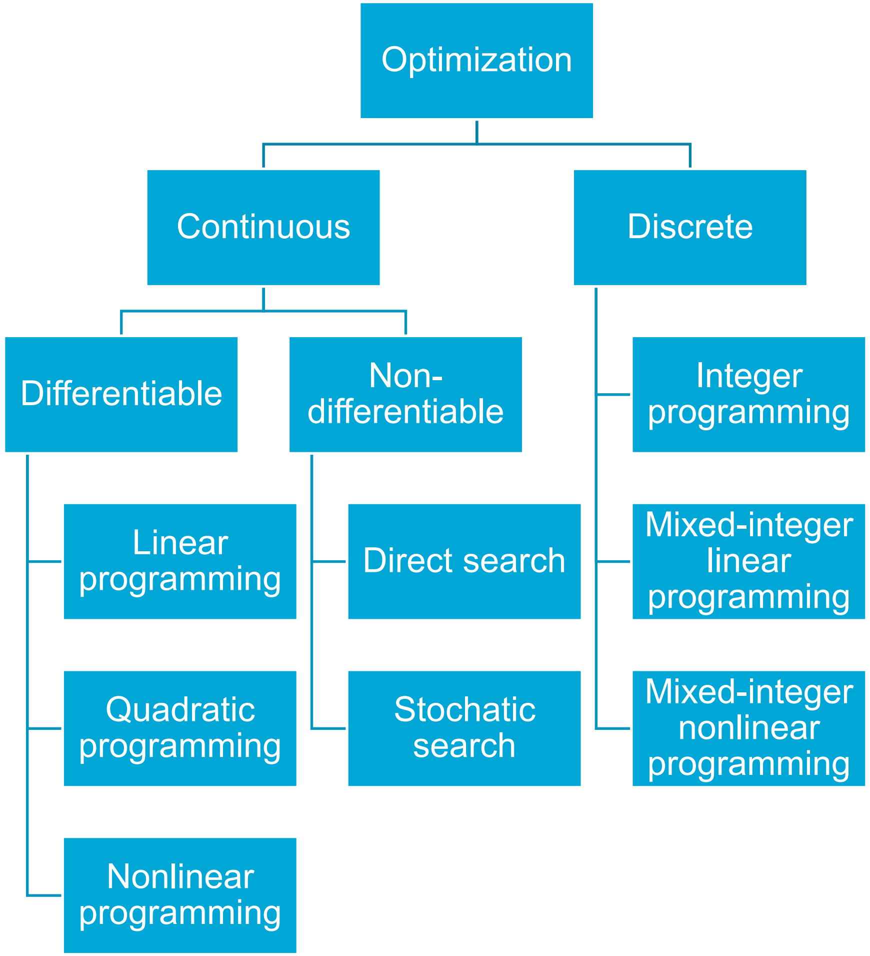

Figure adapted and simplified from https://neos-guide.org/guide/types/

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- Anatomy of an optimization problem
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  - **Fundamentals**
  - Solving LPs – conceptual overview of simplex and interior point algorithms
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- Mixed-Integer Linear Programming (MILP)
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What is linear programming (LP)

$$
\begin{aligned}
&\min_{\boldsymbol{x},\boldsymbol{y}} f\left(\boldsymbol{x},\boldsymbol{y}\right)\\
&\text{s.t. } \boldsymbol{h}\left(\boldsymbol{x},\boldsymbol{y}\right) = 0\\
&\quad \boldsymbol{g}\left(\boldsymbol{x},\boldsymbol{y}\right) \leq 0\\
&\quad \boldsymbol{x} \in \left[\boldsymbol{x}^{\mathrm{L}},\boldsymbol{x}^{\mathrm{U}}\right], \boldsymbol{y} \in \left\{\boldsymbol{y}^{\mathrm{L}},\ldots,\boldsymbol{y}^{\mathrm{U}}\right\}\\
&\quad \boldsymbol{x} \in \mathbb{R}^{n}, \boldsymbol{y} \in \mathbb{Z}^{k}\\
&\quad f\colon \mathbb{R}^{n+k} \to \mathbb{R},\\
&\quad \boldsymbol{h}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_h},\\
&\quad \boldsymbol{g}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_g},
\end{aligned}
$$

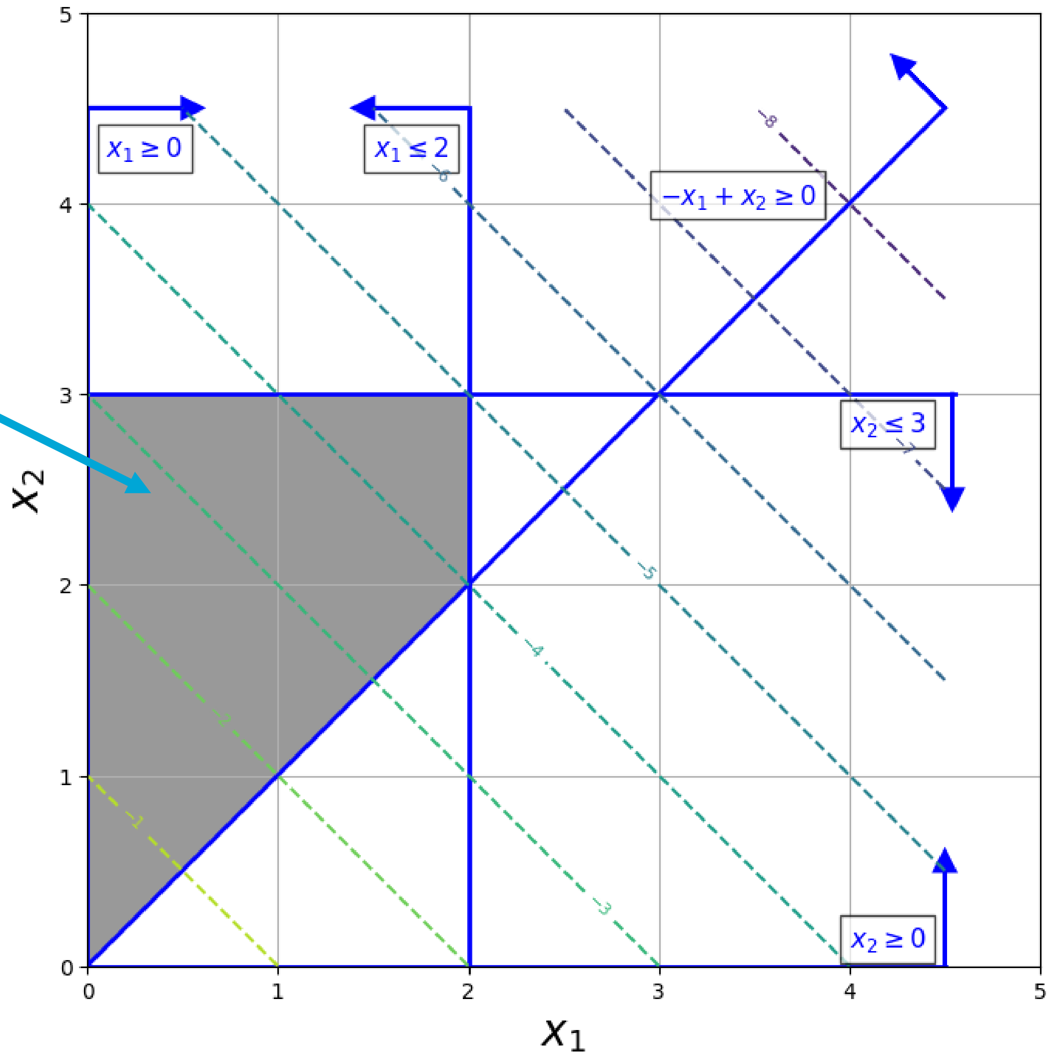
$$
\begin{aligned}
\min_{\mathbf{x}} \quad & f(\mathbf{x}) = \mathbf{c}^{\mathsf{T}}\mathbf{x}\\
\text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{b}\\
& \mathbf{x} \geq 0\\
& \mathbf{x} \in \mathbb{R}^{n}, \mathbf{c} \in \mathbb{R}^{n},\\
& \mathbf{b} \in \mathbb{R}^{n_g+n_h},\\
& \mathbf{A} \in \mathbb{R}^{(n_g+n_h)\times n}
\end{aligned}
$$

- Formulation above represents the standard form of LP
- All inequalities reformulated to equalities by introducing slack variables: $\mathbf{g}(\mathbf{x}) + \mathbf{s} = 0, \mathbf{s} \geq 0$

What does a feasible region look like?

$$\begin{aligned} \min \quad & -x_1 - x_2 \\ \text{s.t.} \quad & -x_1 + x_2 \geq 0 \\ & x_1 \leq 2 \\ & x_2 \leq 3 \\ & x_1, x_2 \geq 0 \end{aligned}$$

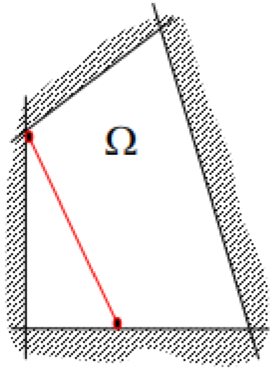
Feasible region



For LP problems, the feasible region is always a *polyhedron*

Fundamental properties of LPs

- Recall *sufficient condition* for a convex set:
  Given $\Omega = \{\boldsymbol{x} \in D \mid \boldsymbol{g}(\boldsymbol{x}) \leq 0, \boldsymbol{h}(\boldsymbol{x}) = 0\}$
- If equality constraints $\boldsymbol{h}(\boldsymbol{x})$ are linear and $\boldsymbol{g}(\boldsymbol{x})$ are convex functions then Ω is convex
- All linear functions are convex
- **→ all LPs are convex optimization problems**

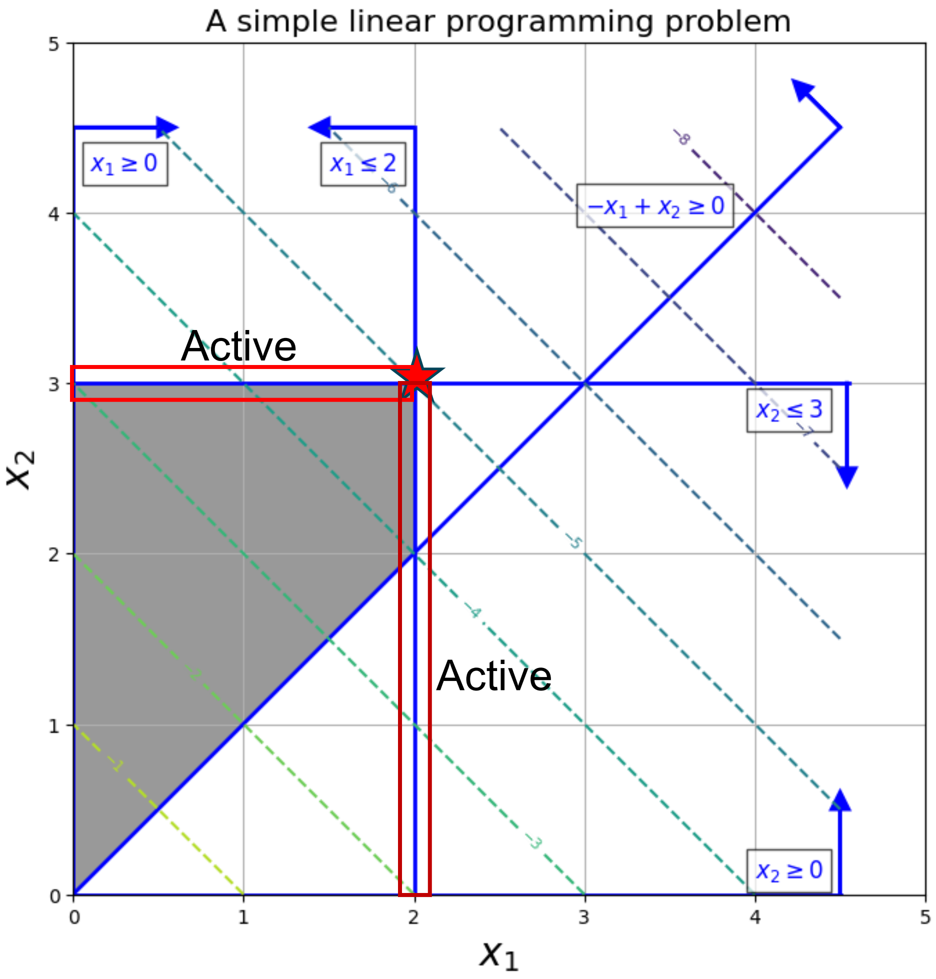


Convex feasible region

Figure taken from slides by Prof. Alexander Mitsos for his course on Applied Numerical Optimization (RWTH Aachen)

Where does the optimum lie?

- Since LPs are convex:
  - Every local optimum for an LP is a *global optimum*
  - If an LP has a non-constant objective function, then an optimal solution of an LP **cannot** lie in the interior of the feasible region
  - If an LP has a unique optimal solution, then the optimal **must** lie at an *extreme* point of the feasible region
  - If an LP has multiple optimal solutions, then one of them **must** occur at an *extreme* point of the feasible region



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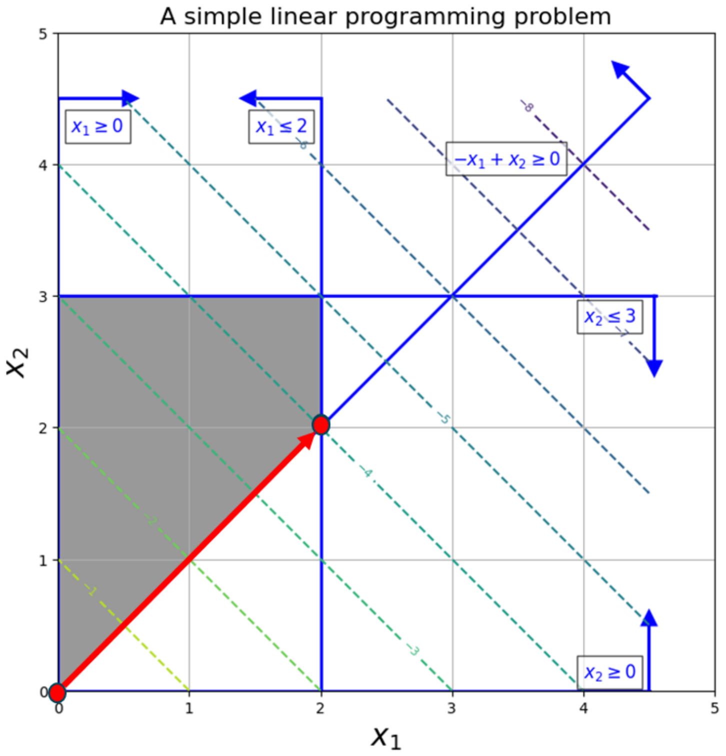
Solving LPs – general concept

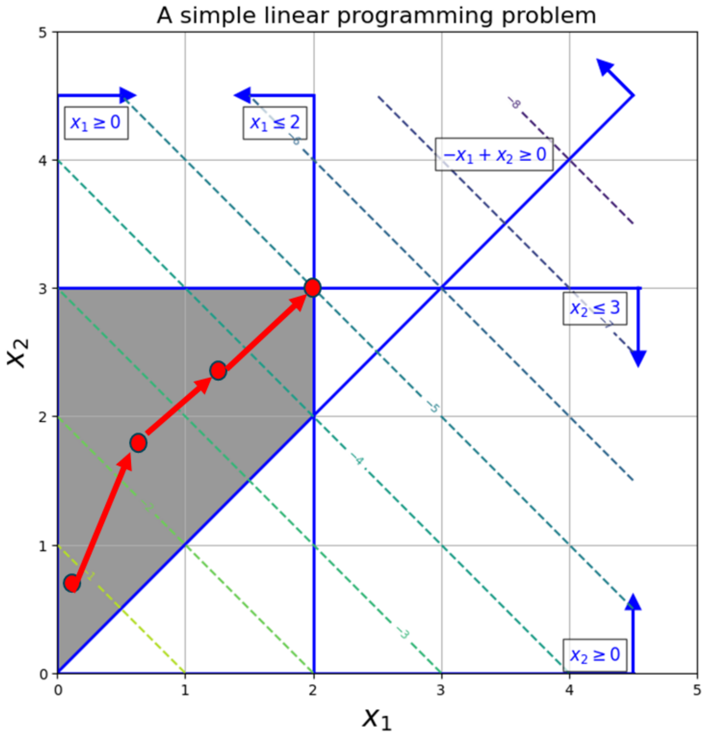
- Typically, the procedure to obtain the optimal solution of a linear programming problem involves:
  - Determining a feasible points in an iterative fashion such that the objective improves at every iteration
  - Terminating the search if no further improvement is possible
- This is popularly referred to as the *improving search principle*

Solving LPs – algorithms overview

- Simplex algorithm

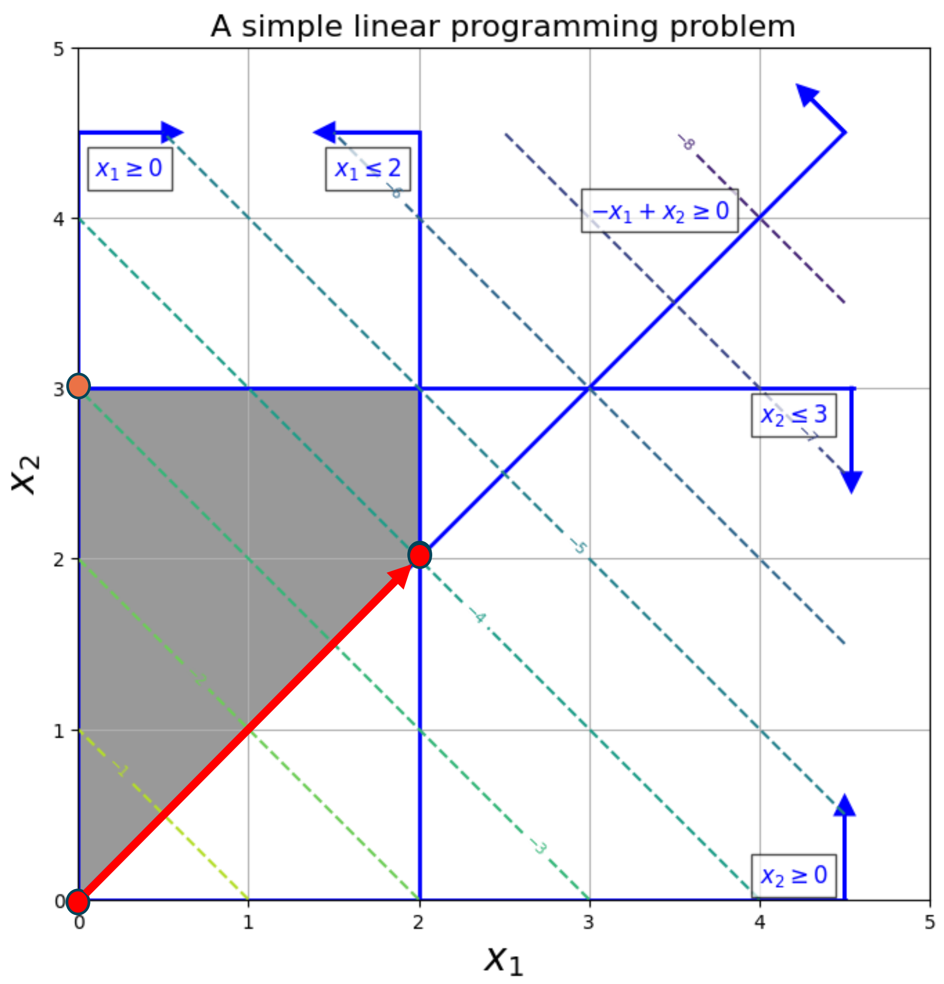


- Interior point algorihtm



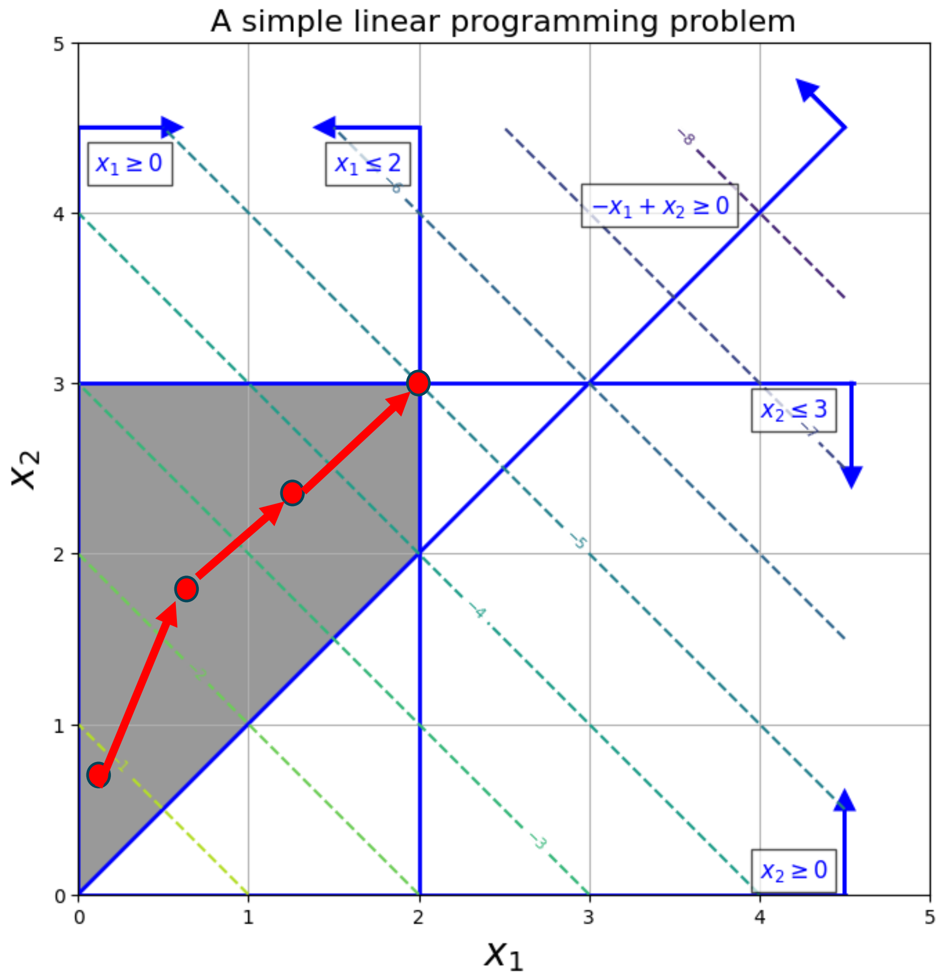
Simplex algorithm

- Only consider adjacent extreme points for improving direction
- Move along the edge that yield largest rate of improvement
- Move until another extreme point has been reached
- Check if further improvement is possible: if 'yes' *continue*; else *terminate*
- Can potentially struggle if there are a high number of extreme points
- High number of extreme points occur when there are many variables and constraints but few degrees of freedom



Interior point algorithm

- Determine an *improving* direction
- Move along that direction, but the feasible point in should *strictly* remain in the interior of the feasible region
- Check of significant change has been made: if ‘yes’ *continue*; else *terminate*
- Works well when degrees of freedom n is large
- For smaller problems simplex algorithm may be more efficient.



Linear programming in SciPy

- Function: Use `scipy.optimize.linprog` for Linear Programming (LP).
- Objective: Minimize $\boldsymbol{c}^T\boldsymbol{x}$ by passing the coefficient vector $\boldsymbol{c}$. For maximization, use - $\boldsymbol{c}$.
- Constraints:
  - Inequalities - ($\boldsymbol{A}_{ub}\boldsymbol{x} \leq \boldsymbol{b}_{ub}$): $\boldsymbol{A}_{ub}$ and $\boldsymbol{b}_{ub}$ represent coefficients of inequality constraints
  - Equalities - ($\boldsymbol{A}_{eq}\boldsymbol{x} = \boldsymbol{b}_{eq}$): $\boldsymbol{A}_{eq}$ and $\boldsymbol{b}_{eq}$ represent coefficients of equality constraints.
- Bounds: Define variable ranges with bounds using. Defaults to non-negative variables.
- Solvers: Default is '**highs**', with alternatives for specific needs.
- Result: Check `result.success`, and retrieve `result.x` (solution) and `result.fun` (optimal value).

$$
\begin{aligned}
\min_{\mathbf{x}} \ & \mathbf{c}^\mathsf{T}\mathbf{x} \\
\text{s.t.} \ & \mathbf{A}_{ub}\mathbf{x} \leq \mathbf{b_{ub}} \\
& \mathbf{A}_{eq}\mathbf{x} = \mathbf{b}_{eq} \\
& \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}
\end{aligned}
$$

https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.linprog.html

Implementing a LP in SciPy

$$\begin{aligned} \min \quad & -x_1 - x_2 \\ \text{s.t.} \quad & -x_1 + x_2 \geq 0 \\ & x_1 \leq 2 \\ & x_2 \leq 3 \\ & x_1, x_2 \geq 0 \end{aligned}$$

Order used is $[x_1, x_2]$

$$\boldsymbol{c}^T := [-1, -1]$$

$$\boldsymbol{A}_{ub} := \begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}; \ \boldsymbol{b}_{ub} := [0, 2, 3]$$

```python
from scipy.optimize import linprog

# Minimize: c^T x
c = [-1, -1]  # Coefficients for the objective function
A = [[1, -1], [1, 0], [0,1]]  # Coefficients for inequality constraints
b = [0, 2, 3]  # Bounds for inequality constraints
x_bounds = [(0, None), (0, None)]  # Variable bounds

# Solve the LP
result = linprog(c, A_ub=A, b_ub=b, bounds=x_bounds, method='highs')
```

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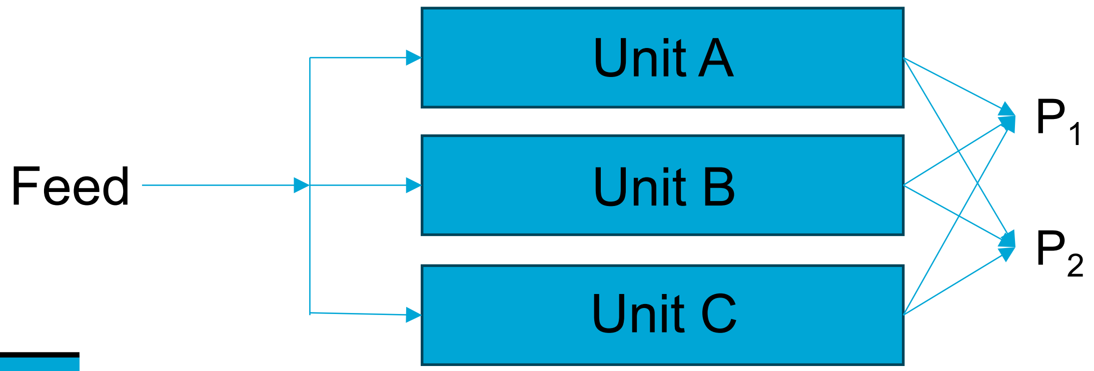
Multi-product problem (1/2) – General problem setup

- Feed to three units is split into three streams: F_A, F_B and F_C.
- Two products are produced: P_1 and P_2,
- Each unit has individual product yields



Yield (wt %)	Unit A	Unit B	Unit C
P_1	40	30	50
P_2	60	70	50

Multi-product problem (2/2) - Additional constraints

- We have some capacity limitations:
  - The plant can handle a maximum feed F of 10,000 kg/day
  - Each unit (A, B and C) cannot handle more than 5,000 kg/day
  - The maximum demand of P_1 and P_2 are 4,000 kg/day and 5,000 kg/day

Costs of feed and product streams

Stream	Value ($/kg)
F	0.40
P_1	0.60
P_2	0.30

Determine the optimal values of F_A, F_B and F_C that maximize the daily profit of the plant?

Formulating the objective function

- Objective function: maximize the profit by selling the products P_1 and P_2
- The profit of the plant is the difference between the amount we earn by selling the products and the amount spent in buying the feed F
- Amount earned by selling the products: unit cost of the product × amount of product produced
- Similarly, amount spent in buying feed: unit cost of the feed × amount of feed bought
- Mathematically,

$$\text{Profit} = C_{P1}P_1 + C_{P2}P_2 - C_F F$$

- P_1, P_2 and F represent the amounts of the products and the feed respectively in kg.
- We know $C_{P1} = 0.6$, $C_{P2} = 0.3$, and $F = 0.4$
- Recall the equivalence of objective function (c.f. Q2 Lecture 4): maximizing profit is equivalent to minimizing negative profit
- Objective function: $-\text{Profit}$

Modeling the material balances

- Feed F is split and sent to three units as $F_A,\ F_B,$ and F_C. Hence,

$$F = F_A + F_B + F_c$$

- Given the yield of each unit, we model the conversion of feed to the products in each unit A, B and C and sum up over all reactors

Yield (wt %)	Unit A	Unit B	Unit C
P_1	40	30	50
P_2	60	70	50

$$P_1 = 0.4F_A + 0.3F_B + 0.5F_C$$

$$P_2 = 0.6F_A + 0.7F_B + 0.5F_C$$

Accounting for capacity and demand

- The maximum capacity of each unit is 5000 kg/day. Hence,

$$F_A, F_B, F_C \leq 5000$$

- Overall, the plant can handle a maximum of 10000 kg/day of feed.

$$F \leq 10000$$

- Due to known demand, we have a maximum limit of the products we can produce giving us an upper bound

$$P_1 \leq 4000 \text{ and } P_2 \leq 5000$$

- All material flows are non-negative,

$$F, F_A, F_B, F_C, P_1, P_2 \geq 0$$

The linear programming formulation

$$
\begin{aligned}
\min\ & 0.4F - 0.6P_1 + -0.3P_2 \\
\text{s.t. } & \left.\begin{aligned}
F &= F_A + F_B + F_C \\
P_1 &= 0.4F_A + 0.3F_B + 0.5F_C \\
P_2 &= 0.6F_A + 0.7F_B + 0.5F_C
\end{aligned}\right\} \text{Equality constraints} \\
& \left.\begin{aligned}
F &\leq 10000 \\
F_A &\leq 5000 \\
F_B &\leq 5000 \\
F_C &\leq 5000 \\
P_1 &\leq 4000 \\
P_2 &\leq 5000 \\
F, F_A, F_B, F_C, P_1, P_2 &\geq 0
\end{aligned}\right\} \text{Inequality constraints}
\end{aligned}
$$

Live coding: Solving the LP in SciPy

- Open Colab: Solving the formulated LP using SciPy

- Find more in the Github repository of the course: https://github.com/process-intelligence-research/computational_practicum_lecture_coding/tree/main

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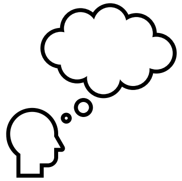
  - Fundamentals
  - Modelling using discrete variables
  - Branch and bound algorithms for solving MILPs
- Introduction to genetic algorithms

Analyzing the optimal solution obtained

- The optimal values are:

Variable	Value
Profit ($/day)	325.0
F (kg/day)	8750.0
F_A (kg/day)	3750.0
F_B (kg/day)	0.0
F_C (kg/day)	5000.0
P_1 (kg/day)	4750.0
P_2 (kg/day)	5000.0



Understanding the output generated (1/5)

```
       message: Optimization terminated successfully. (HiGHS Status 7: Optimal)
       success: True
        status: 0
           fun: -325.0
             x: [ 8.750e+03  3.750e+03  0.000e+00  5.000e+03  4.000e+03
                  4.750e+03]
           nit: 2
         lower:  residual: [ 8.750e+03  3.750e+03  0.000e+00  5.000e+03
                             4.000e+03  4.750e+03]
                marginals: [ 0.000e+00  0.000e+00  2.500e-02  0.000e+00
                             0.000e+00  0.000e+00]
         upper:  residual: [       inf        inf        inf        inf
                                   inf        inf]
                marginals: [ 0.000e+00  0.000e+00  0.000e+00  0.000e+00
                             0.000e+00  0.000e+00]
         eqlin:  residual: [ 0.000e+00  0.000e+00  0.000e+00]
                marginals: [ 4.000e-01 -5.500e-01 -3.000e-01]
       ineqlin:  residual: [ 1.250e+03  1.250e+03  5.000e+03  0.000e+00
                             0.000e+00  2.500e+02]
                marginals: [-0.000e+00 -0.000e+00 -0.000e+00 -2.500e-02
                            -5.000e-02 -0.000e+00]
mip_node_count: 0
mip_dual_bound: 0.0
       mip_gap: 0.0
```

Understanding the output generated (2/5)

- Printing the result object gives a more detailed insight into the solution
- First part of the log shows whether the solver terminated successfully or not.
- **Always** check first if the solver terminated successfully or not before analyzing the solution reported

```
message: Optimization terminated
successfully. (HiGHS Status 7:
Optimal)

success: True

status: 0
```

Understanding the output generated (3/5)

- `fun` reports the value of the objective function of your problem
- x is a vector of the decision variables in your problem and SciPy reports their values in the order you defined
- In the live coding, we defined them in the order:

  ```
  x := [F, F_A, F_B, F_C, P1, P2]
  ```

- nit represents the number of iterations the solver required to optimize the problem

```
fun: -325.0


x: [ 8.750e+03  3.750e+03  0.000e+00
5.000e+03  4.000e+03 4.750e+03]

nit: 2
```

Understanding the output generated (4/5)

- Here, the information about the lower and upper bounds of the variables is reported
- Residual refers to the difference between the value at the optimal solution and the value of the respective bound
- Marginal refers to the dual cost or shadow price and is only non-zero if the value is at the bound → constraint is active
- Marginals tells us how will the value of the objective change on changing the limit of the bound (beyond the scope of this lecture)

```
lower:  residual: [ 8.750e+03
3.750e+03  0.000e+00  5.000e+03
4.000e+03  4.750e+03]

        marginals: [ 0.000e+00
0.000e+00  2.500e-02  0.000e+00
0.000e+00  0.000e+00]

upper:  residual: [       inf
inf        inf        inf inf
inf]

        marginals: [ 0.000e+00
0.000e+00  0.000e+00  0.000e+00
0.000e+00  0.000e+00]
```

Understanding the output generated (5/5)

- Here, marginals and residuals for the constraints are reported
- Equality constraints always have a zero residual
- Inequality constraint only have a zero residual if the constraint is active
- Marginal is non-zero if the residual is zero → constraint is active

```
eqlin:    residual: [ 0.000e+00
0.000e+00  0.000e+00]

          marginals: [ 4.000e-01 -
5.500e-01 -3.000e-01]

ineqlin:  residual: [ 1.250e+03
1.250e+03  5.000e+03  0.000e+00
0.000e+00  2.500e+02]

          marginals: [-0.000e+00 -
0.000e+00 -0.000e+00 -2.500e-02
-5.000e-02 -0.000e+00]
```

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Mixed-Integer Linear Programming (MILP)

- Building on from linear programming, a mixed-integer linear program also comprises a set of integer (or discrete) variables
- Similar to linear programming, $f(\mathbf{x},\mathbf{y}), \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}), \boldsymbol{h}(\boldsymbol{x},\boldsymbol{y})$ are all linear
- For the case when set of continuous variables $\boldsymbol{x}$ is not present → pure integer linear programming (ILP) problem

$$\min_{\boldsymbol{x},\boldsymbol{y}} f(\boldsymbol{x},\boldsymbol{y})$$

$$\text{s.t. } \boldsymbol{h}(\boldsymbol{x},\boldsymbol{y}) = 0$$

$$\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) \leq 0$$

$$\boldsymbol{x} \in [\boldsymbol{x}^{\mathrm{L}},\boldsymbol{x}^{\mathrm{U}}], \boldsymbol{y} \in \{\boldsymbol{y}^{\mathrm{L}},\ldots,\boldsymbol{y}^{\mathrm{U}}\}$$

$$\boldsymbol{x} \in \mathbb{R}^{n}, \boldsymbol{y} \in \mathbb{Z}^{k}$$

$$f\colon \mathbb{R}^{n+k} \to \mathbb{R},$$

$$\boldsymbol{h}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_h},$$

$$\boldsymbol{g}\colon \mathbb{R}^{n+k} \to \mathbb{R}^{n_g},$$

The feasible region of mixed-integer problems

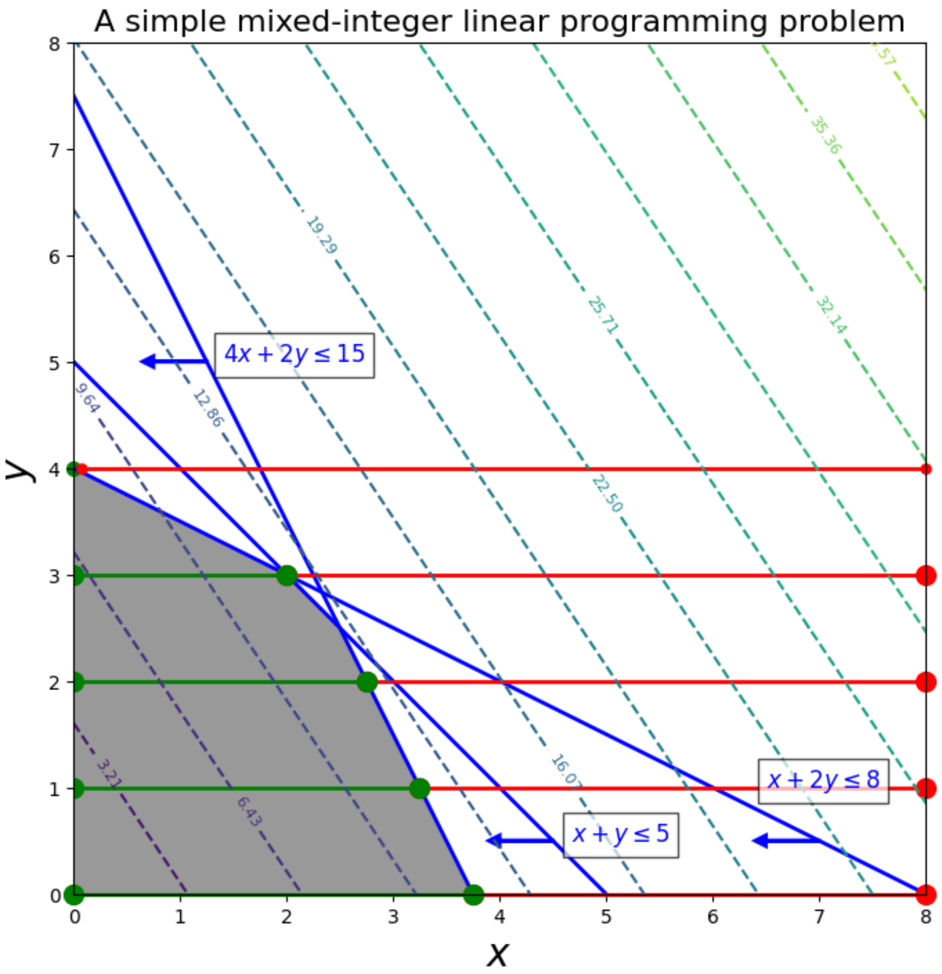
$$\max_{x,y} 3x + 2y$$

$$\text{s.t. } 4x + 2y \leq 15$$

$$x + 2y \leq 8$$

$$x + y \leq 5$$

$$x \in [0, 9], y \in \{0, 1, \ldots, 8, 9\}$$



The feasible region is discontinuous → *non-convex*

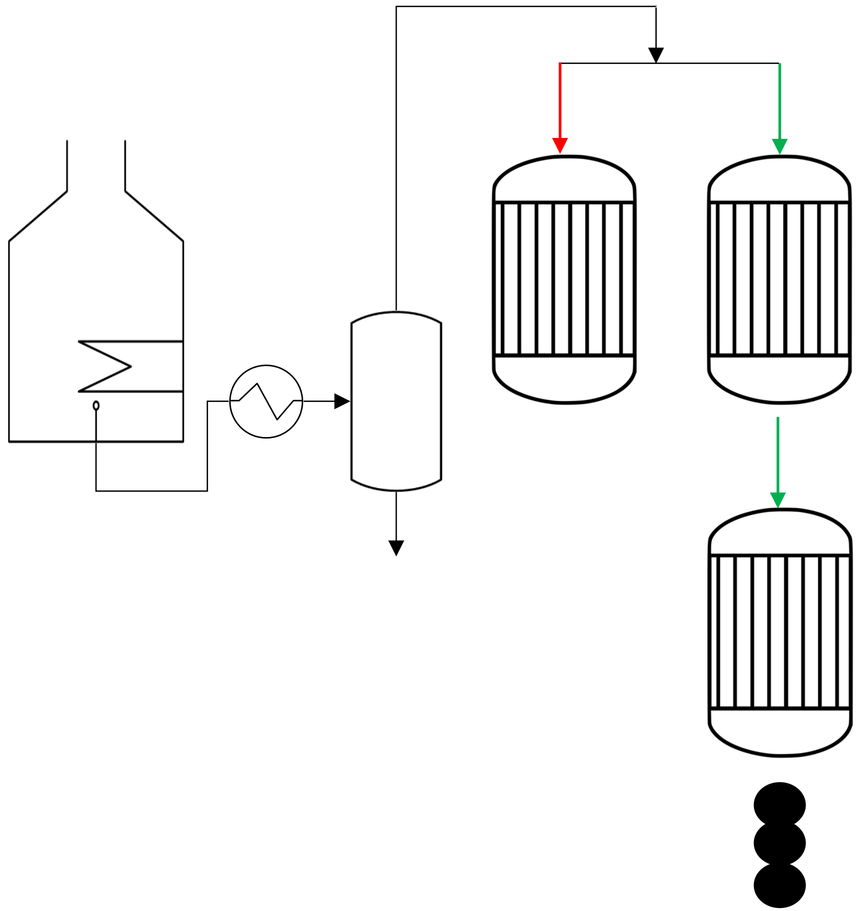
Since MILPs are inherently non-convex, they are more difficult to solve

Discrete variables

- Discrete variables are of two types:
  - **Binary variables** – Can only take values 0 or 1.

    Example: Should feed be sent to the reactor?
  - **Integer variables** – Can take any integer value (e.g., 0,1,2,3,4,5, . . .).

    Example: How many reactors are in series?
- **In this lecture, we will focus on binary decisions (without loss of generality)**



Modelling the logical proposition: OR

- We can model common logical propositions using binary variables
- Assuming J is a set representing multiple options, generally.
- We can model:
  - Selecting at least one component (logically equivalent to inclusive OR) → $\sum_{j \in J} y_j \geq 1$
  - Select exactly one component (logically equivalent to exclusive OR) → $\sum_{j \in J} y_j = 1$
  - Selecting at most one component → $\sum_{j \in J} y_j \leq 1$

Model the logical proposition: For separation you can either pick distillation (y_D) or absorption (y_A), not both

Model the logical proposition: For separation you can either pick distillation (y_D) or absorption (y_A), not both

Correct answers will be shown here

Modeling the logical proposition OR – truth table

Selecting at most one component $\sum_{j \in J} y_j \leq 1$

Pick absorption (y_A)	Pick distillation (y_D)	$y_A + y_D$
0	0	0
0	1	1
1	0	1
1	1	2

Equivalent to inclusive OR ($\sum_{j \in J} y_j \geq 1$)

Equivalent to exclusive OR ($\sum_{j \in J} y_j = 1$)

Modeling the logical propositions – AND & NOT

- Example of AND:
  - [Reactor (y_R)]AND [Separator (y_S)]→ $y_R \geq 1$, $y_s \geq 1$

- Example of NOT:
  - If y_A represents that absorption is selected, $1 - y_A$ represents absorption is not selected

Activating specific constraints only if needed

- Sometimes, we may want to activate certain constraint if a logical condition is met.
- This is particularly useful when values of continuous variables are linked to discrete variables
- Example:

You have two different reactor designs to consider. You can only choose one.

If reactor one is chosen, then pressure P must be between 5 and 10 atm.

If reactor two is chosen, then pressure P must be between 20 and 30 atm.

- How can we mathematically model this?

$$5 - M_1(1-y_1) \leq P \leq 10 + M_1(1-y_1)$$
$$20 - M_2(1-y_2) \leq P \leq 30 + M_2(1-y_2)$$
$$y_1 + y_2 = 1$$

Assuming $M_1 = 100$, $M_2 = 100$

$y_1 = 1$

$$5 - 0 \leq P \leq 10 + 0$$
$$20 - 100 \leq P \leq 30 + 100$$

P is bounded between 5 and 10

$y_1 = 0$

$$5 - 100 \leq P \leq 10 + 100$$
$$20 - 0 \leq P \leq 30 + 0$$

P is bounded between 20 and 30

This approach is called Big-M formulation

Example taken from the book - Biegler, L. T., Grossmann, I. E., & Westerberg, A. W. (1997). Systematic methods for chemical process design.

Choosing appropriate big-M values

- Big-M values should be sufficiently high
- If the Big-M value is too low, *feasible* solution becomes *infeasible*
- Consider the example on previous slide:

Assuming $M_1 = 5$, $M_2 = 5$

$$5 - M_1(1 - y_1) \leq P \leq 10 + M_1(1 - y_1)$$
$$20 - M_2(1 - y_2) \leq P \leq 30 + M_2(1 - y_2)$$
$$y_1 + y_2 = 1$$

$y_1 = 1$

$$5 - 0 \leq P \leq 10 + 0$$
$$20 - 5 \leq P \leq 30 + 5$$

$y_1 = 0$

$$5 - 5 \leq P \leq 10 + 5$$
$$20 - 0 \leq P \leq 30 + 0$$

P has inconsistent bounds → infeasible

- If Big-M value is too large → solve times become slower

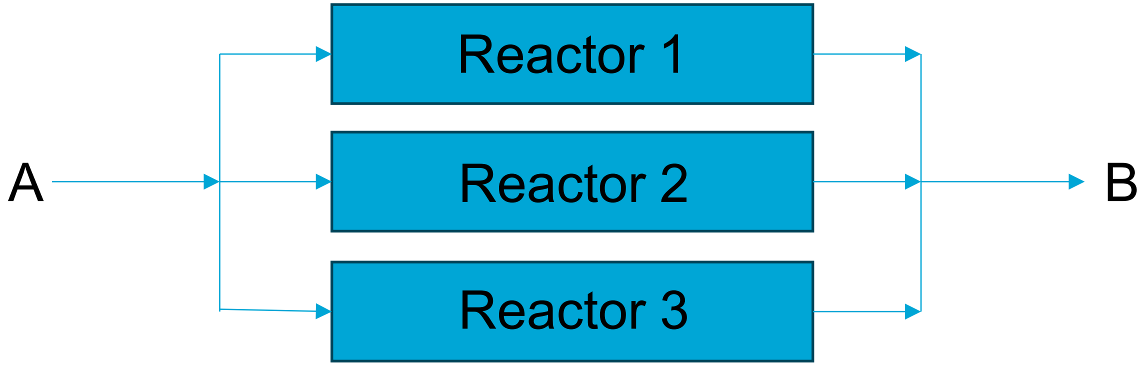
Outline

- **Anatomy of an optimization problem**
- **Linear Programming (LP)**
  - Fundamentals
  - Solving LPs – conceptual overview of simplex and interior point algorithms
  - Formulating linear programming models given an engineering problem statement
  - Analyzing solutions
- **Mixed-Integer Linear Programming (MILP)**
  - Fundamentals
  - **Formulating a MILP from an engineering problem statement**

Reactor selection problem

- Design a process with minimum cost to produce 10 kg/h of B from feedstock A (maximum availability = 15 kg/h). There are three reactors available each with different yields and costs. The details are:

	Yield	Fixed cost ($/h)	Variable cost($/kg)
Reactor 1	0.80	80	35
Reactor 2	0.667	54	30
Reactor 3	0.555	27	25



Formulating the objective function

- Objective function – minimize the cost of the plant by choosing appropriate reactors
- The reactor has a fixed cost and a variable cost
- Fixed cost should only be included if a reactor is selected:

$$80y_1 + 54y_2 + 27y_3$$

- Variable cost is dependent on the amount of feed ($\boldsymbol{x}$) to the reactor:

$$35x_1 + 30x_2 + 25x_3$$

- Thus, total cost representing the objective:

$$80y_1 + 35x_1 + 54y_2 + 30x_2 + 27y_3 + 25x_3$$

- Later we will ensure that $\boldsymbol{x} = 0$ if the reactor is not chosen

Modeling the material balances

- We consider the yield of each reactors when fed A to produce B

	Yield
Reactor 1	0.80
Reactor 2	0.667
Reactor 3	0.555

- Summing up over all reactors to get the total amount of B produced:

$$0.8x_1 + 0.667x_2 + 0.555x_3 = 10$$

- The coefficient on the right-hand side is 10 because we want to produce exactly 10 kg/h of B

Constraint on feed availability

- We have a constraint on maximum amount of feed available to us
- Over all three reactors this is expressed as

$$x_1 + x_2 + x_3 \leq 15$$

- All material flows are non-negative,

$$x_1, x_2, x_3 \geq 0$$

Feed flowrate should be zero if a reactor is not chosen

- We have the option to select among the reactors available.
- The feed to a reactor should only be non-zero only if the reactor is chosen
- We use the Big-M approach to model this:

$$x_i - 15\, y_i \leq 0, i \in \{1,2,3\}$$

- Here, M is 15 → maximum feed availability is 15
- When $y_i = 0$, we get $x_i \leq 0$. Recall we also have a constraint $x_i \geq 0$ to ensure non-negative flow of x_i → enforces $x_i = 0$
- When $y_i = 1$, we get $x_i - 15 \leq 0$, x_i can take any value between 0 and 15

Mixed-integer linear formulation for the problem

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{y}} \quad & 80y_1 + 35x_1 + 54y_2 + 30x_2 + 27y_3 + 25x_3 \\
\text{s.t.} \quad & 0.8x_1 + 0.667x_2 + 0.555x_3 = 10 \\
& \sum_{i=1}^{3} x_i \leq 15 \\
& x_i - 15y_i \leq 0, \ \forall\, i \in \{1,2,3\} \\
& \mathbf{x} \geq 0, \mathbf{y} \in \{0,1\}
\end{aligned}
$$

Live coding: Solving the MILP in SciPy

- Open Colab: Solving the formulated MILP using SciPy

- Find more in the Github repository of the course: https://github.com/process-intelligence-research/computational_practicum_lecture_coding/tree/main

Analyzing the solution obtained

- The optimal values are:

Variable	Value
Cost ($/h)	503.78
y_1	0
y_2	1
y_3	0
x_1	0
x_2	14.992
x_3	0

```
        message: Optimization terminated successfully. (HiGHS Status 7: Optimal)
        success: True
         status: 0
            fun: 503.7751124437781
              x: [ 0.000e+00  1.499e+01  0.000e+00 -0.000e+00  1.000e+00
                  -0.000e+00]
 mip_node_count: 1
 mip_dual_bound: 503.7751124437781
        mip_gap: 0.0
```

Do these results make sense to you?

Superstructure optimization – a brief discussion

- Modeling of such logical propositions widely carried out in Chemical Engineering
- Superstructure optimization is where we systematically chose among many alternatives during conceptual design of chemical processes[1]
- Superstructure optimization offers an alternative to hierarchical design of chemical processes
- Example: Optimal defossilization pathways for industrial cluster at the port of Rotterdam obtained by solving MILPs[2]

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Chemical Engineering Science

Volume 321, Part A, 1 February 2026, 122783

CHEMICAL ENGINEERING SCIENCE

Superstructure-based optimization framework to assess defossilization pathways in petrochemical clusters ☆

Michael Tan [a], Igor Nikolic [b], Andrea Ramírez Ramírez [c]

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1. Mencarelli, L., Chen, Q., Pagot, A., & Grossmann, I. E. (2020). A review on superstructure optimization approaches in process system engineering. *Computers & Chemical Engineering*, *136*, 106808.
2. Tan, M., Nikolic, I., & Ramírez, A. R. (2025). Superstructure-based optimization framework to assess defossilization pathways in petrochemical clusters. *Chemical Engineering Science*, 122783.

What if I have larger problems?

- Real-world problems often contain millions of variables and constraints
- Current state-of-the-art MIP solvers are capable of efficiently solving such large problems using branch-and-bound methods
- SciPy is not particularly amenable to model such large problems
- Specialised optimization modelling environments exist

AMPL

GAMS

AIMMS

PYOMO

JUMP

Learning goals of this lecture

- After successfully completing this lecture, you are able to. . . .
  - formulate a linear and mixed-integer linear programming model from an engineering problem statement
  - analyze optimal solutions obtained on solving these models
  - explain at a high-level different algorithms used to solve linear programming models

Thank you very much for your attention!