ETH zürich

EPSE Energy & Process Systems Engineering

Introduction to Modeling and Optimization of Sustainable Energy Systems:
Discrete Optimization

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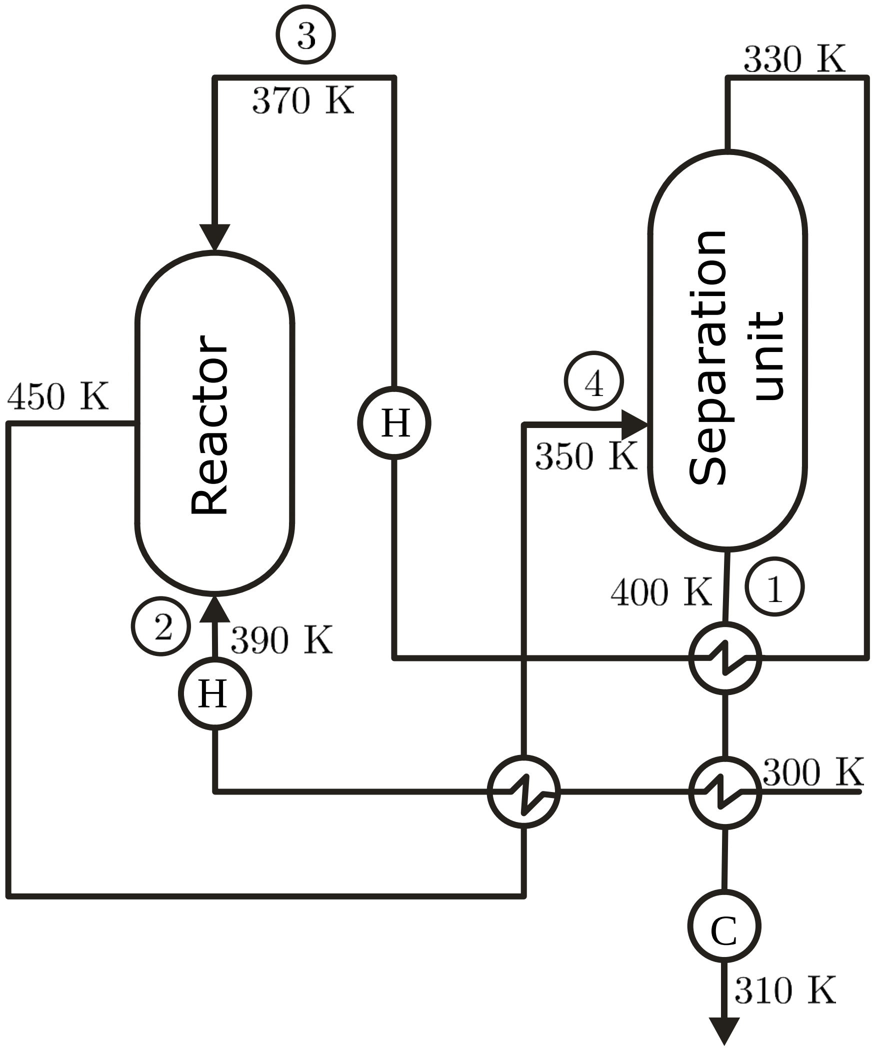
Energy and Process Systems Engineering

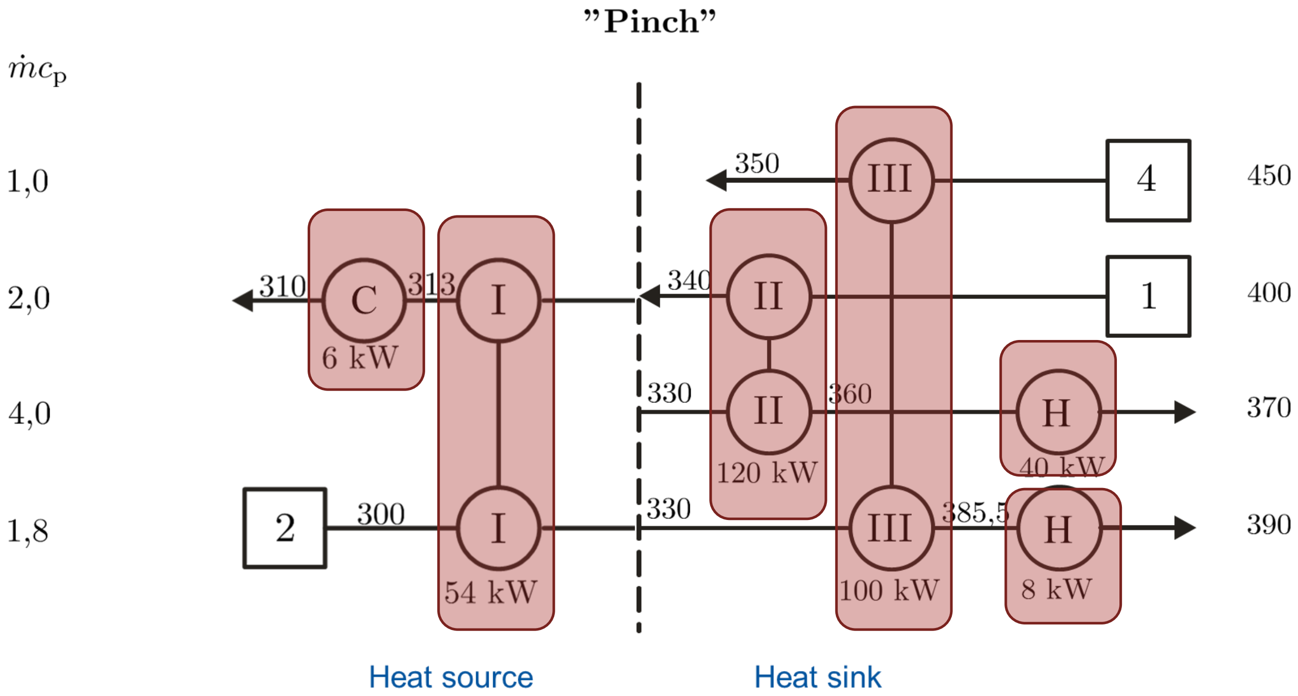
to end

Since the last lecture, you are able to…

- ✓ formulate **heat integration as optimization problem**
- ✓ **design networks** for heat integration of hot and cold streams **using pinch technology.**
- ✓ find a **feasible solution** for the heat exchanger design problem using **heuristics.**
- ✓ formulate the **modelling equations** for designing **heat exchanger networks.**

Heat exchanger network





6 heat exchanger

optimal network?

Optimization: Number of heat exchangers

$$\min_{\Delta\dot{Q}^*_z, \dot{Q}^{(z)}_{h,c}} \sum_h \sum_c \epsilon_{h,c}$$

Number of stream couplings
≤ Number of heat exchangers

$s.t.$ **Energy balances:**

$$\forall h, z \quad 0 = -\Delta\dot{Q}^*_{h,z} + \Delta\dot{Q}^*_{h,z-1} + \Delta\dot{H}^{(z)}_h - \sum_c \dot{Q}^{(z)}_{h,c},$$

$$0 = \Delta\dot{Q}^*_{h,1},$$

$$0 = \Delta\dot{Q}^*_{h,z_{max}},$$

$$\forall c, z \quad 0 = -\Delta\dot{H}^{(z)}_c + \sum_h \dot{Q}^{(z)}_{h,c}$$

Stream couplings:

$$\forall h, c \quad \sum_z \dot{Q}^{(z)}_{h,c} \leq \epsilon_{h,c} \cdot \Delta\dot{Q}^{max}_{h,c}$$

MILP

Papoulias, Grossmann. *A structural optimization approach in process synthesis II: Heat recovery networks.* Comput Chem Eng, *7*:707-721, 1983.

Lecture plan

No.	Date	Content	
1	29.09.	Introduction & Models	
2	06.10.	Heat integration	Applications
3	13.10.	Continuous Optimization	Methods
4	20.10.	Heat exchanger networks	Applications
5	27.10.	Discrete Optimization	Methods
6	03.11.	Life Cycle Assessment (LCA)	Metrics
7	10.11.	Thermoeconomics	Metrics
8	17.11.	Risk Key Performance Indicators for Security	Metrics
9	24.11.	Multi-energy dimension: introduction	Methods & Applications
10	01.12.	Design dimensions: technology modelling	
11	08.12.	Space dimensions: energy networks	
12	15.12.	Uncertainty in energy systems	
13	22.12.	Recap (online)	

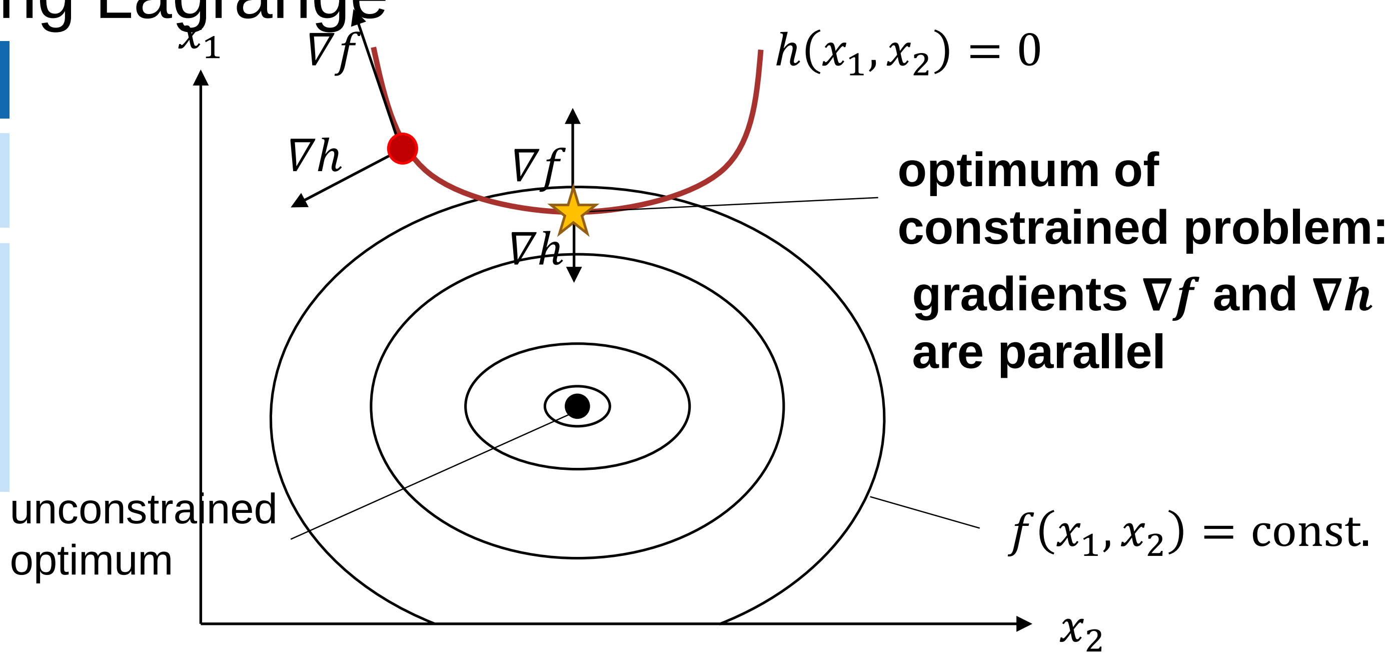
Lecture 3: Optimal conditions using Lagrange

Lagrange formulation

$$\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_j \lambda_j\, h_j(\boldsymbol{x})$$

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial f(\boldsymbol{x})}{\partial x_i} - \sum_j \lambda_j \frac{\partial h_j(\boldsymbol{x})}{\partial x_i} = 0, \qquad i = 0,\dots,m$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_j} = -h_j(\boldsymbol{x}) = 0, \qquad j = 0,\dots,o$$



Interpretation of Lagrange multipliers

Lagrange formulation

$$\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_j \lambda_j \, h_j(\boldsymbol{x})$$

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial f(\boldsymbol{x})}{\partial x_i} - \sum_j \lambda_j \frac{\partial h_j(\boldsymbol{x})}{\partial x_i} = 0, \qquad i = 0, \dots, m$$

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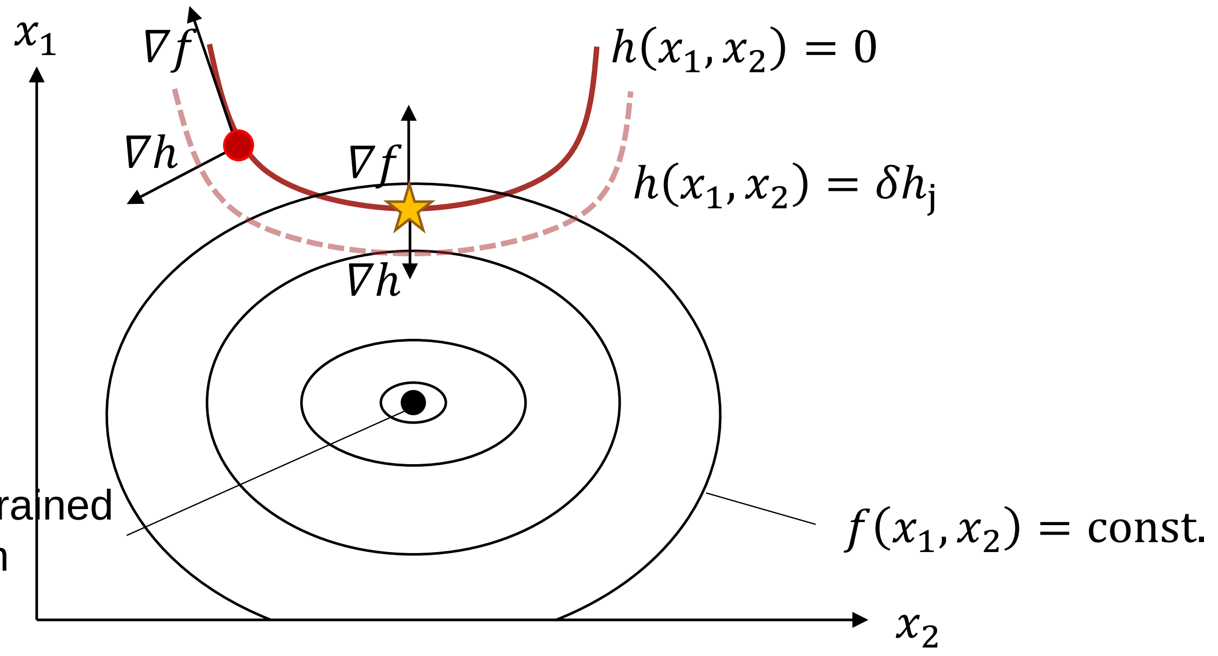


$\Rightarrow$ Small change δx of objective f and constraints h:

$$\delta f = \delta x^T \nabla f \qquad \delta h_j = \delta x^T \nabla h_j$$

$$\delta x^T \nabla f - \sum_j \lambda_j \delta x^T \nabla h_j = 0 \quad \Rightarrow \delta f - \sum_j \lambda_j \delta h_j = 0$$

Choosing $\delta h_j = 0, \forall j \neq i \qquad \Rightarrow \delta f - \lambda_i \delta h_i = 0$

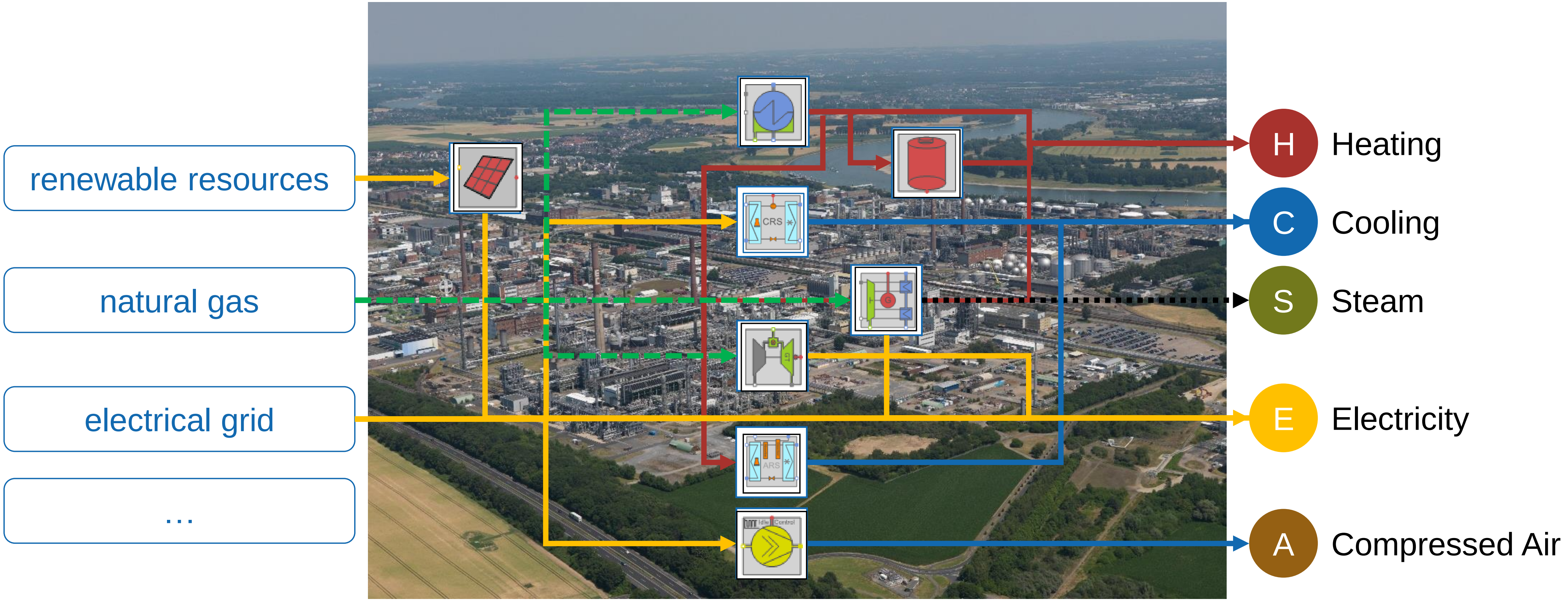
$$\Rightarrow \lambda_i = \left(\frac{\delta f}{\delta h_i}\right)_{\delta h_j = 0, \forall j \neq i}$$

Lagrange multiplier = change of objective function for small deviation from h_i @ optimum („shadow price“)

After this lecture, you will be able to…

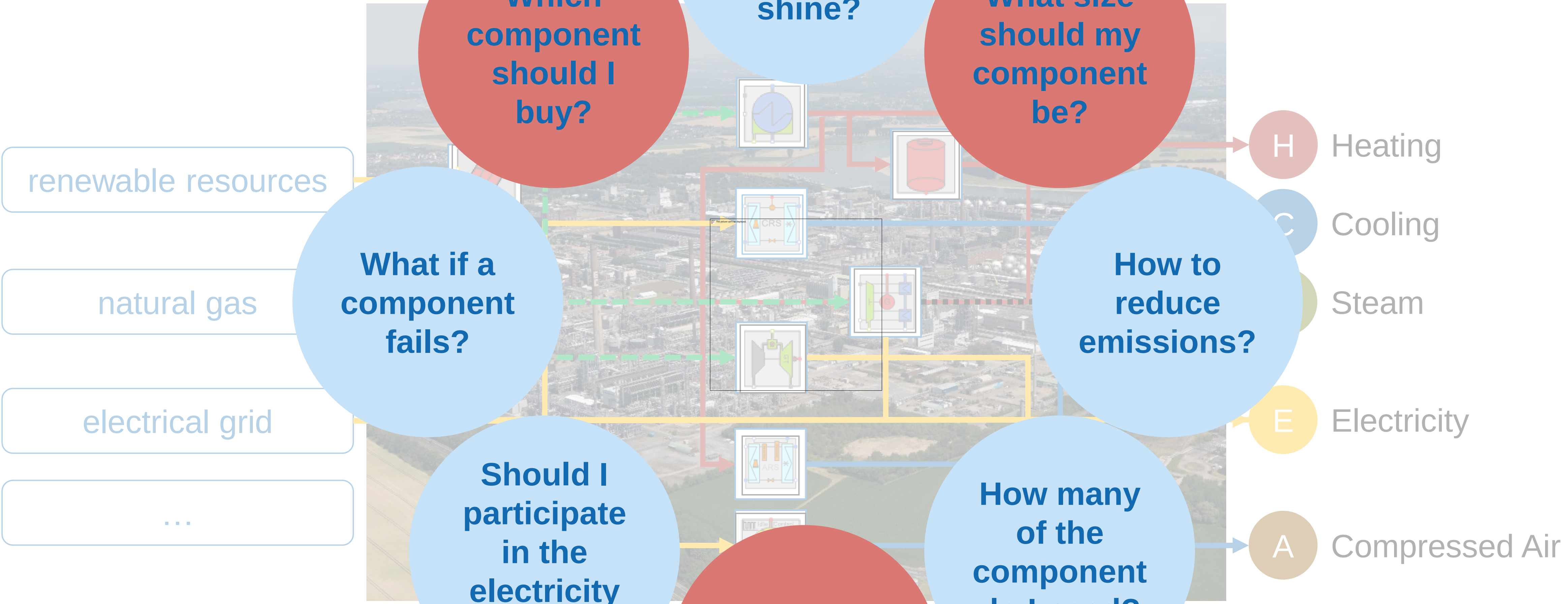
- employ basic **solution methods** for **mixed-integer linear** (MILP) & **nonlinear programming** (MINLP) problems.
- find optimal heat-exchanger networks and near-optimal solutions with **integer cuts**
- discuss **(dis)advantages** of optimization problem classes

Decision making in energy systems engineering



Source: INEOS Köln GmbH

Decision making in energy system … neering



Source: I

What to do if the sun does not shine?

Which component should I buy?

What size should my component be?

What if a component fails?

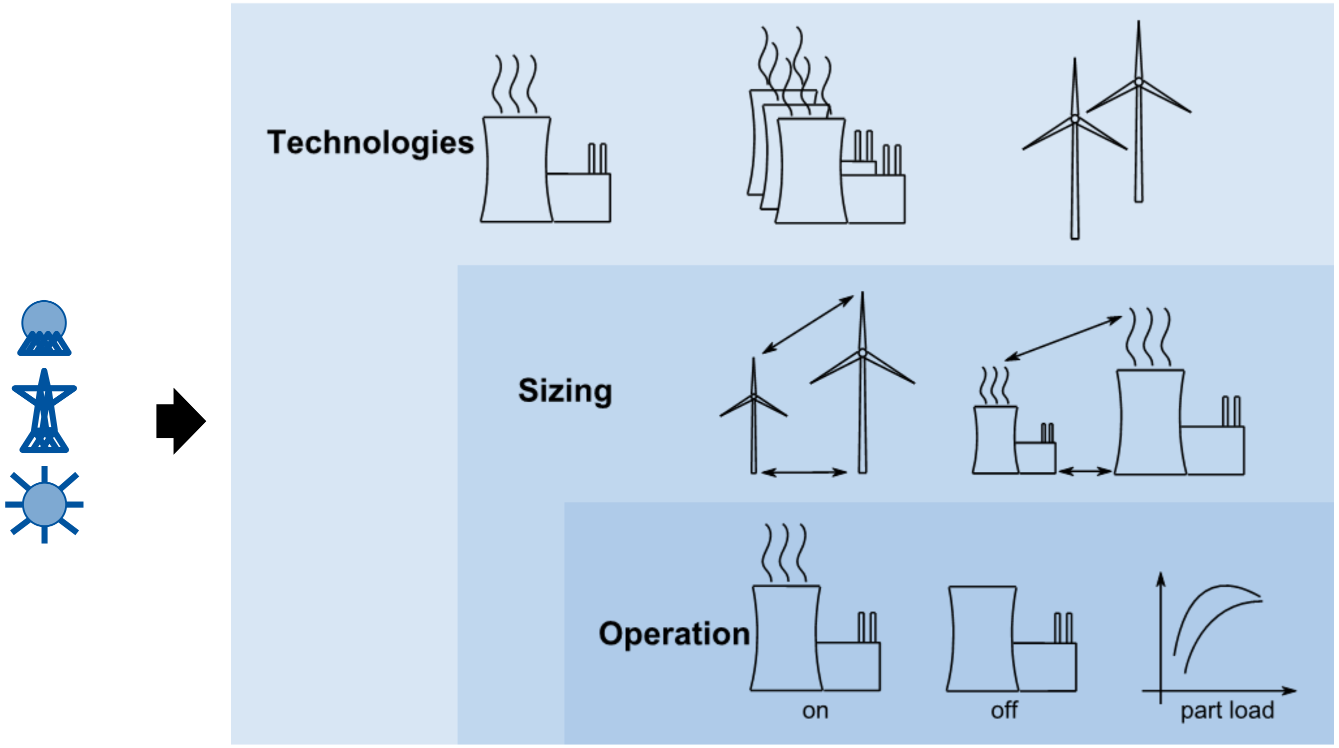
How to reduce emissions?

Should I participate in the electricity market?

How to operate the system?

How many of the component do I need?

Hierarchy of optimization problems for energy systems



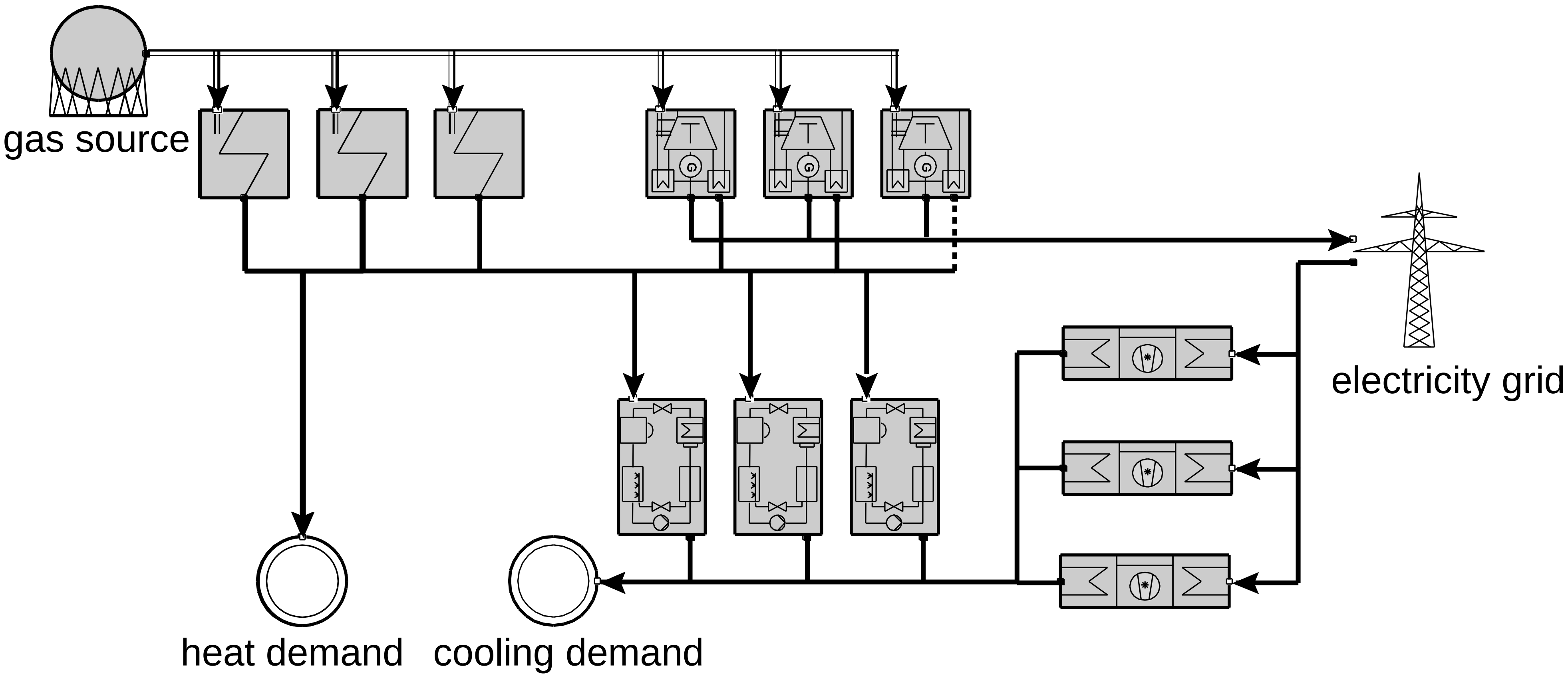
Which component should I buy?

What size should my component be?

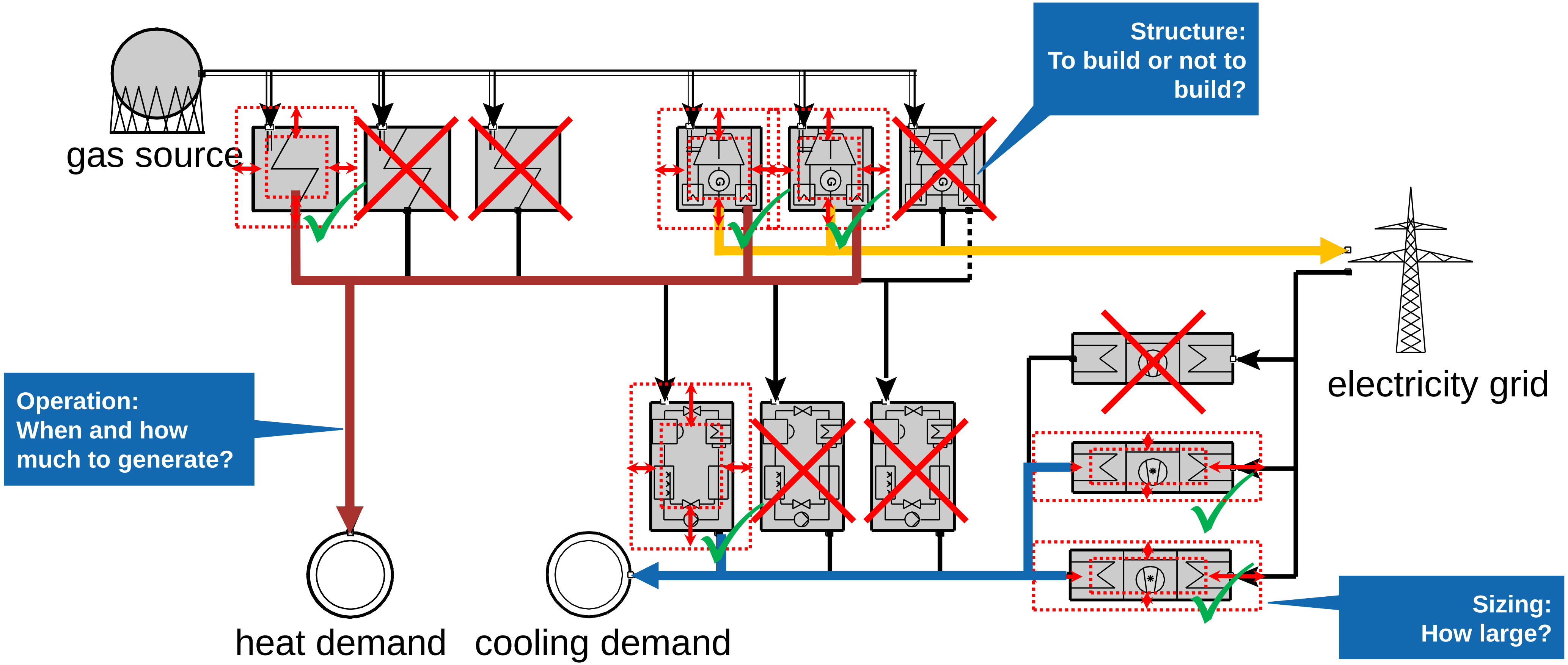
How to operate the system?

Frangopoulos et al., *Int J Appl Thermodyn* (2002)

Hierarchy of optimization problems for energy systems



Hierarchy of optimization problems for energy systems



Optimization problem classes

constraints \ variables	continuous	continuous & discrete
linear	linear program (LP)	mixed-integer linear program (MILP)
nonlinear	nonlinear program (NLP)	mixed-integer nonlinear program (MINLP)
	Lecture 3	today

Lecture 3: (Non)linear programming

Linear programming (LP)

Properties

✓ all variables continuous

✓ all functions affine:
$f(x) = a\,x + b$, where $a, b = \text{const.}$
= linear function + translation

$$\min_x \quad z = \boldsymbol{c}^T \boldsymbol{x}$$
$$\text{s.t.} \quad A\boldsymbol{x} \leq \boldsymbol{b}$$
$$E\boldsymbol{x} = \boldsymbol{f}$$
$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{c} \in \mathbb{R}^m,$$
$$A \in \mathbb{R}^{n\times m}, \boldsymbol{b} \in \mathbb{R}^n,$$
$$E \in \mathbb{R}^{o\times m}, \boldsymbol{f} \in \mathbb{R}^o$$

LP solution methods

- graphical solution method
- simplex method

Global optimum guaranteed!

Nonlinear programming (NLP)

Properties

✓ all variables continuous

✓ some functions $f(x)$ nonlinear
e.g.: $x_i^n, \prod_i x_i, \ln x, \sin(x), e^x$, ...

$$\min_x \quad z = f(x)$$
$$\text{s.t.} \quad g_j(\boldsymbol{x}) \leq 0, \quad j = 1, \dots, n$$
$$h_i(\boldsymbol{x}) = 0, \quad i = 1, \dots, o$$
$$\boldsymbol{x} \in \mathbb{R}^m$$

NLP solution methods

- Newton‘s method
- Lagrange multipliers

Local optimum possible.

This week: Mixed-integer (non)linear programming

Mixed-integer linear programming (MILP)

Properties

- ✓ variables discrete & continuous
- ✓ all functions affine:
  $f(x) = a\,x + b$, where $a, b = \text{const.}$
  = linear function + translation

$$\min_{x} \quad z = \boldsymbol{c}^T\boldsymbol{x} + \boldsymbol{a}^T\boldsymbol{y}$$

$$\text{s.t.} \quad A\boldsymbol{x} + B\boldsymbol{y} \leq \boldsymbol{b}$$

$$E\boldsymbol{x} + F\boldsymbol{y} = \boldsymbol{f}$$

$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{y} \in \mathbb{Z}^t, \boldsymbol{a} \in \mathbb{R}^t, \boldsymbol{c} \in \mathbb{R}^m,$$
$$A \in \mathbb{R}^{n\times m}, B \in \mathbb{R}^{n\times t}, \boldsymbol{b} \in \mathbb{R}^n,$$
$$E \in \mathbb{R}^{o\times m}, F \in \mathbb{R}^{o\times t}, \boldsymbol{f} \in \mathbb{R}^o$$

Mixed-integer nonlinear programming (MINLP)

Properties

- ✓ variables discrete & continuous
- ✓ some functions $f(x)$ nonlinear
  e.g.: $x_i^n, \prod_i x_i, \ln x, \sin(x), e^x$, ...

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

$$\text{s.t.} \quad g_j(\boldsymbol{x}, \boldsymbol{y}) \leq 0, \; j = 1, \dots, n$$
$$h_i(\boldsymbol{x}, \boldsymbol{y}) = 0, \; i = 1, \dots, o$$

$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{y} \in \mathbb{Z}^t$$

Mixed-integer solution methods

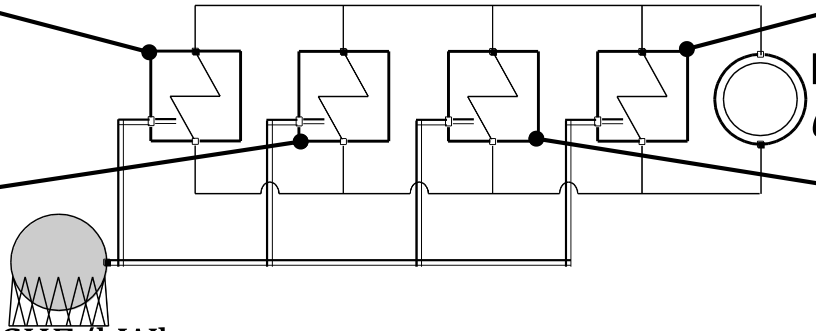
?

Example: Structural optimization of a heating system
Which boiler should we buy?

1
$\dot{Q}_{N,1} = 0.5\ \text{MW}$
$\eta_{N,1} = 0.9$
$I_1 = 43000\ \text{CHF}$

2
$\dot{Q}_{N,2} = 0.7\ \text{MW}$
$\eta_{N,2} = 0.8$
$I_2 = 42000\ \text{CHF}$

superstructure



heat demand
$\dot{Q}_d = 0.9\ \text{MW}$

gas supply
$c_{gas} = 0.06\ \text{CHF/kWh}$

4
$\dot{Q}_{N,4} = 0.4\ \text{MW}$
$\eta_{N,4} = 0.8$
$I_4 = 38000\ \text{CHF}$

3
$\dot{Q}_{N,3} = 0.6\ \text{MW}$
$\eta_{N,3} = 0.85$
$I_3 = 42500\ \text{CHF}$

$a \cdot y \quad + \quad c \cdot x$

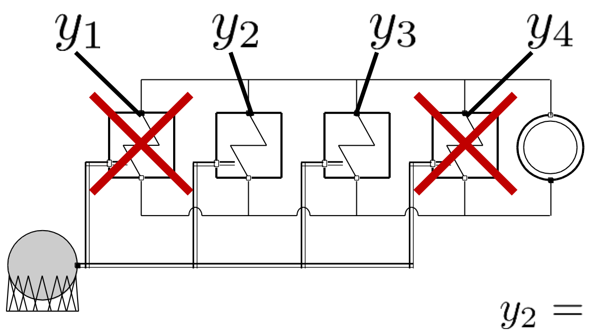
$$\underbrace{\min_{\substack{y_i, Q_i \\ i\in\{1,2,3,4\}}} \ \mathrm{TAC}(\dot{Q}_i, y_i)}_{\substack{\text{total annualized cost} \\ \text{(all details lecture 7)}}} = \underbrace{\sum_i y_i\, Invest/year}_{\text{investment}} + \underbrace{c_{gas} \int_{0\ \mathrm{h}}^{8760\ \mathrm{h}} \dot{Q}_{gas}\, dt}_{\text{cost of gas supply}}$$

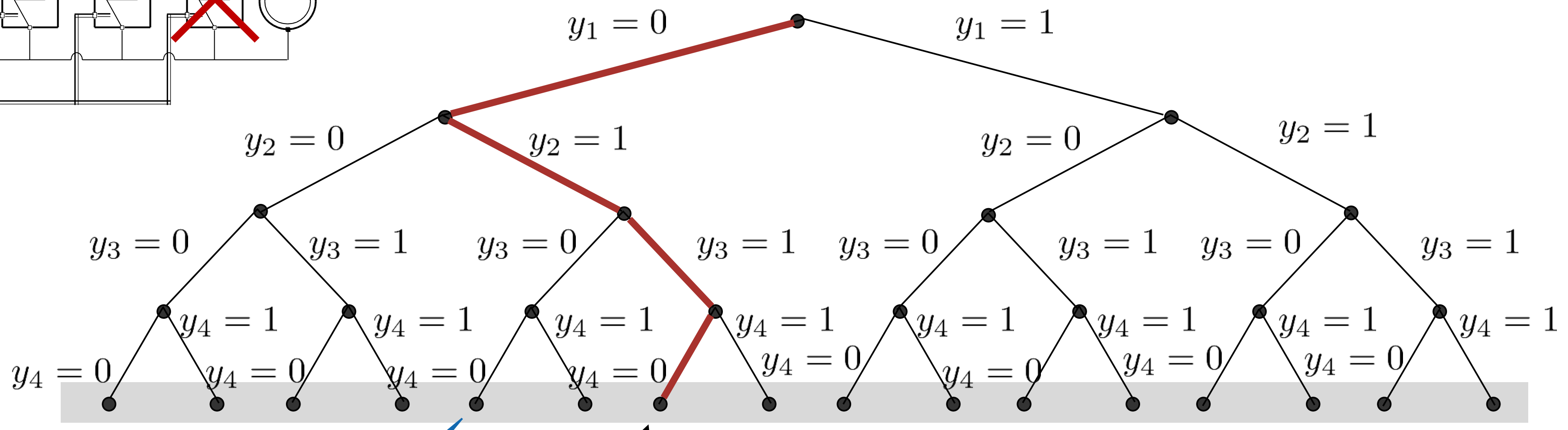
$$\begin{aligned} s.t. \quad & \textstyle\sum_i \dot{Q}_i = \dot{Q}_d, \\ & 0 \le \dot{Q}_i \le y_i \dot{Q}_{N,i}, \ \forall\, i \\ & \dot{Q}_i \in \mathbb{R}, \forall i \\ & y_i \in \mathbb{Z}, \forall i \end{aligned}$$

yes/no decision

Combinatorial complexity

$$2^m \text{ LP} \xrightarrow{m=4} 16 \text{ LP}$$





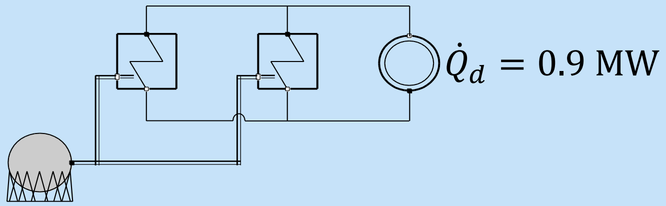
Solving every possible combination results in 16 LPs!

Can we get around solving all of them?

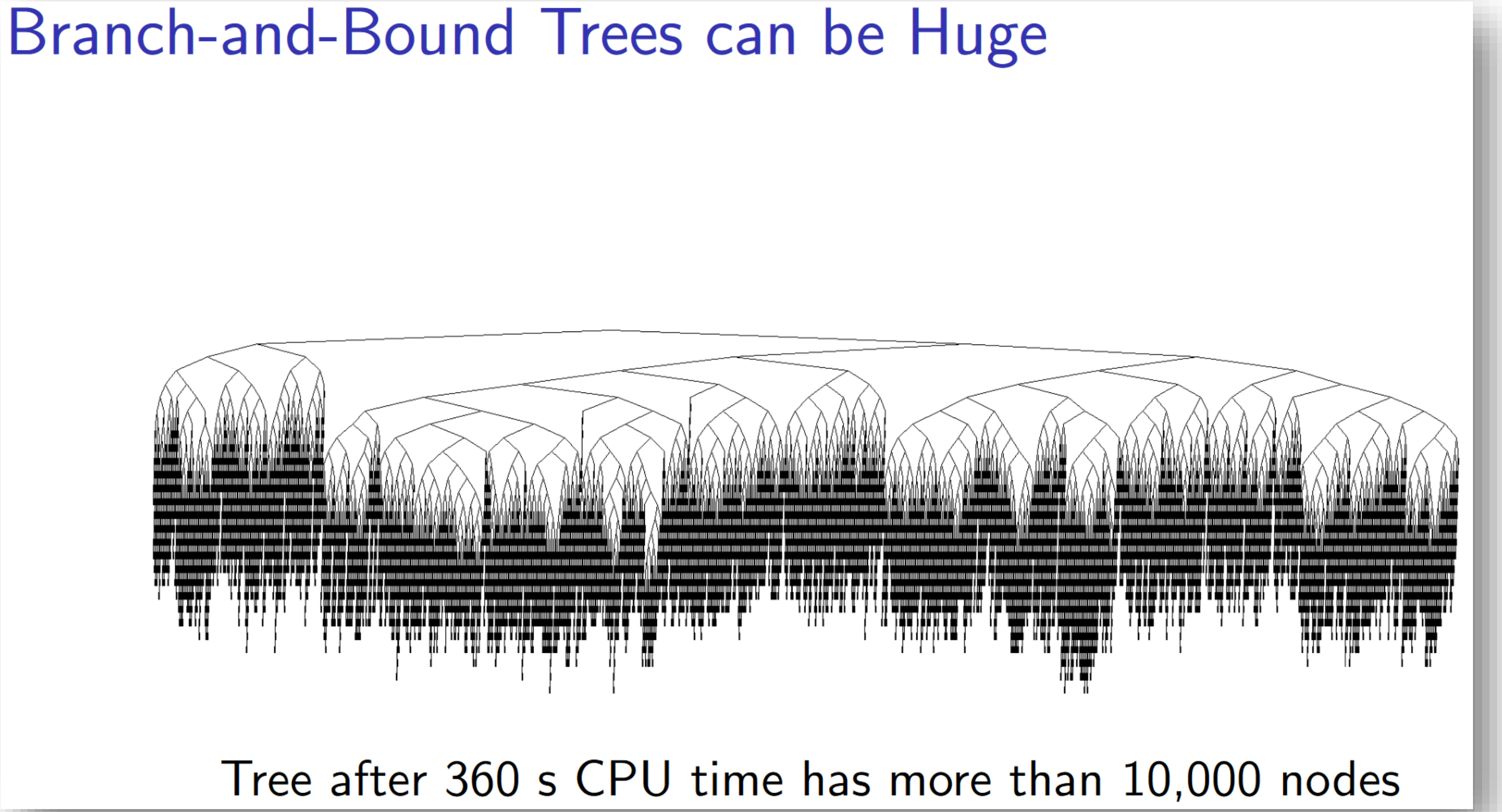
fix binary variables

$\Rightarrow$ LP problem = last week‘s operational optimization

$$\begin{aligned} \dot{Q}_{N,2} &= 0,7\,\text{MW} \\ \eta_{N,2} &= 0,8 \\ \dot{Q}_{N,3} &= 0,6\,\text{MW} \\ \eta_{N,3} &= 0,85 \end{aligned}$$



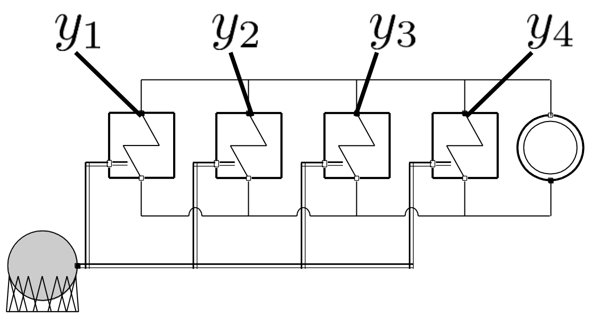
Combinatorial complexity



Argonne national laboratory: Sven Leyffer, Pietro Belotti, Ashutosh Mahajan, Christian Kirches, Jeff Linderoth, Jim Luedtke: Mixed-Integer Nonlinear Optimization: Applications, Algorithms, and Computation

Efficient solution of subproblems is decisive for performance of Branch-and-Bound algorithm.

Branch-&-Bound: Reducing the number of LPs to be solved



1 **LP-relaxation**: assume all integers are continuous

→ $y \in [0;1]$

LP

lower bound: the optimal solution cannot be cheaper than this!

TAC = 310000 CHF/a
$y = (1, 0, 0.667, 0)$

$$\left\{ \begin{array}{l} \dfrac{y_1 = 1,\ y_2 = 0,\ y_3 = \mathbf{0.667},\ y_4 = 0}{\dot{Q}_{N,1} = \mathbf{1} \cdot 0.5\ \text{MW},\ \dot{Q}_{N,3} = \mathbf{0.667} \cdot 0.6\ \text{MW}} \\ I_1 = \mathbf{1} \cdot 43.000\ \text{CHF},\quad I_3 = \mathbf{0.667} \cdot 42.500\ \text{CHF} \end{array} \right.$$

Illustration of linear relaxation

$$\min_{y_1,y_2} \quad z = -3y_1 - 2y_2$$

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

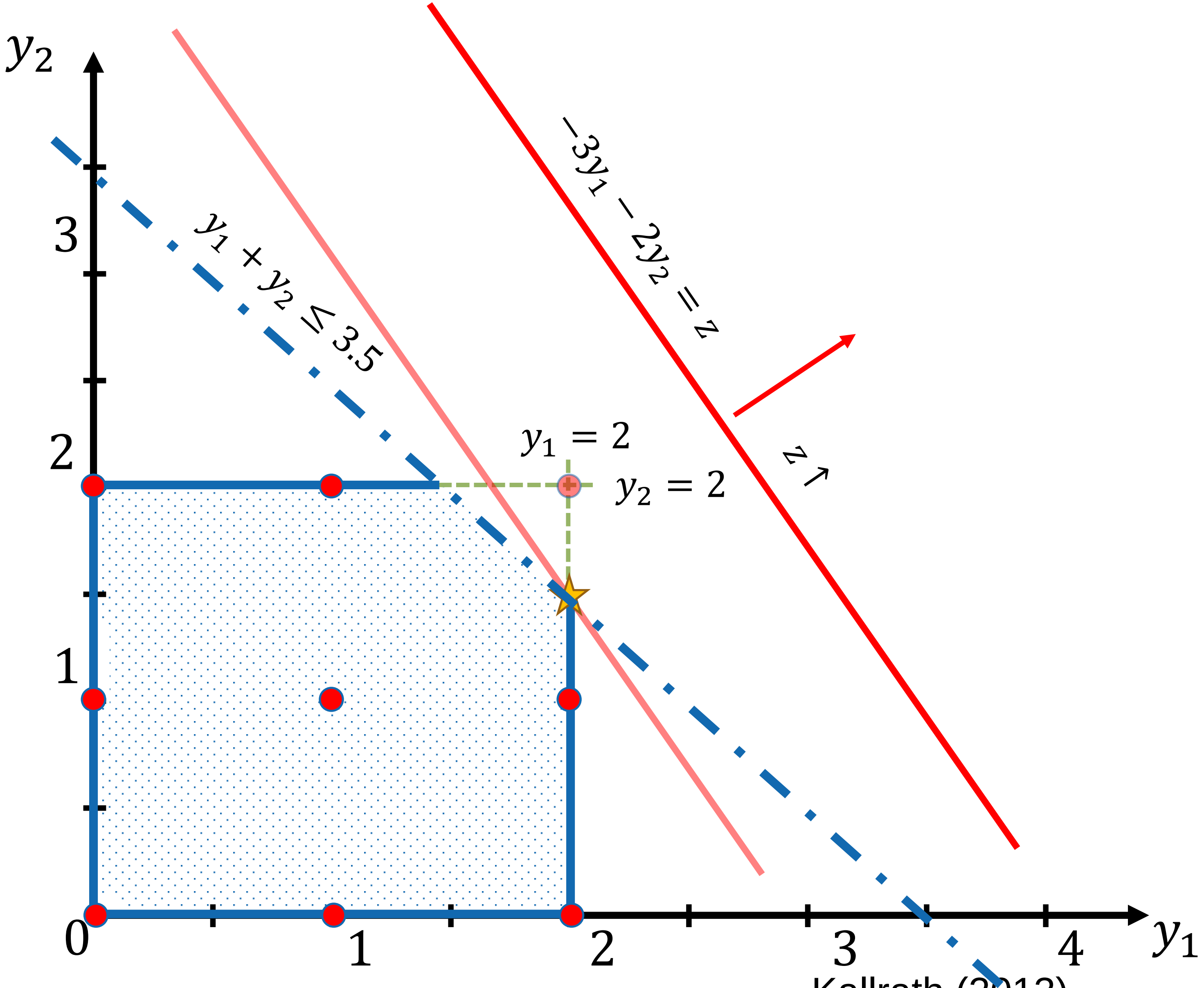
$$y_1 + y_2 \leq 3.5$$

$$0 \leq y_1 \leq 2$$

$$0 \leq y_2 \leq 2$$

$$y_1, y_2 \in \mathbb{Z}^t$$

LP relaxation: $y_1 = 2; y_2 = 1.5$; $z = -9$



Kallrath (2013)

Illustration of linear relaxation

$$\min_{y_1,y_2} \quad z = -3y_1 - 2y_2$$

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

$$y_1 + y_2 \leq 3.5$$

$$0 \leq y_1 \leq 2$$

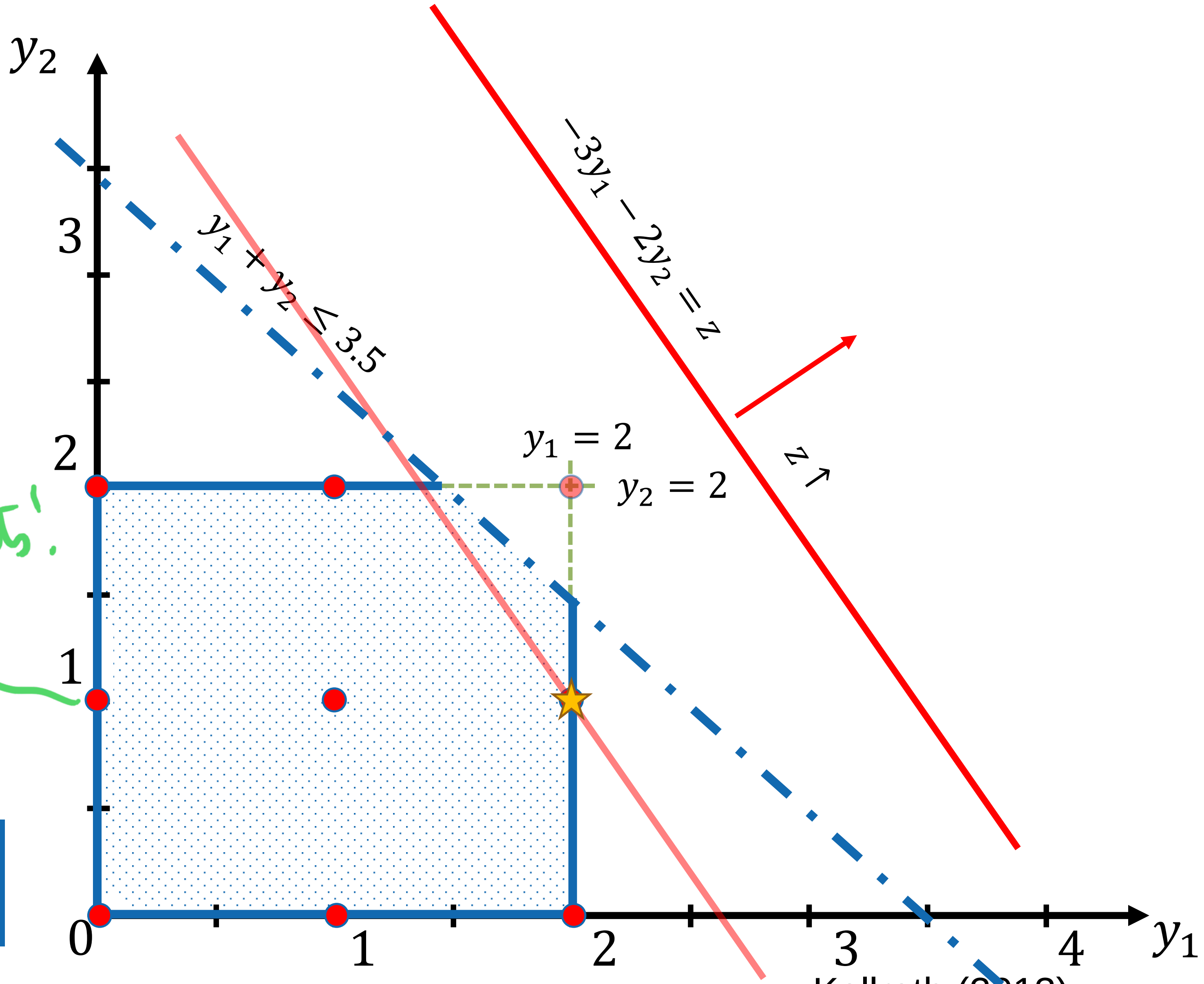
$$0 \leq y_2 \leq 2$$

$$y_1, y_2 \in \mathbb{Z}^t$$

LP relaxation: $y_1 = 2; y_2 = 1.5; z = -9$

$\Rightarrow$ Optimum : $y_1 = 2; y_2 = 1; z = -8$

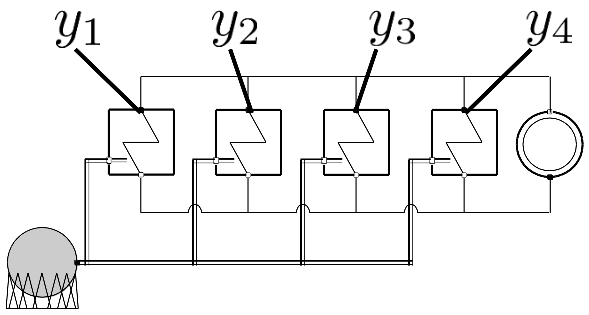
only allowed solution are points! (integers)



Kallrath (2013)

Linear relaxation provides lower bound on the minimization problem

Branch-&-Bound: Reducing the number of LPs to be solved



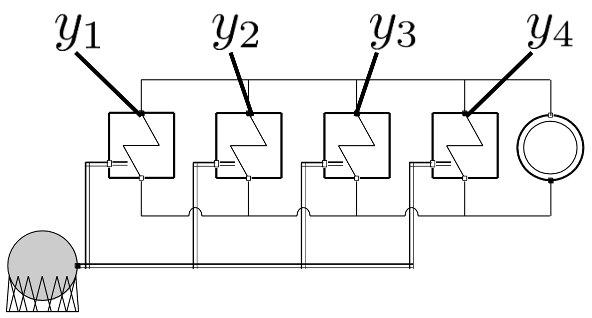
1 **LP-relaxation**: assume all integers are continuous

lower bound: the optimal solution cannot be cheaper than this!

$\text{TAC} = 310000\ \text{CHF/a}$
$y = (1, 0, 0.667, 0)$

$$\begin{cases} \dfrac{y_1 = 1,\ y_2 = 0,\ y_3 = \mathbf{0.667},\ y_4 = 0}{\dot{Q}_{N,1} = \mathbf{1} \cdot\ 0.5\ \text{MW},\ \dot{Q}_{N,3} = \mathbf{0.667} \cdot\ 0.6\ \text{MW}} \\ I_1 = \mathbf{1} \cdot 43.000\ \text{CHF},\quad I_3 = \mathbf{0.667} \cdot 42.500\ \text{CHF} \end{cases}$$

Branch-&-Bound: Reducing the number of LPs to be solved



1. **LP-relaxation**: assume all integers are continuous
2. **branching**: divide solution space into subspaces, excluding non-integer values

$\text{TAC} = 310000\ \text{CHF/a}$
$y = (1, 0, 0.667, 0)$

branching

$y_3 \leq 0$

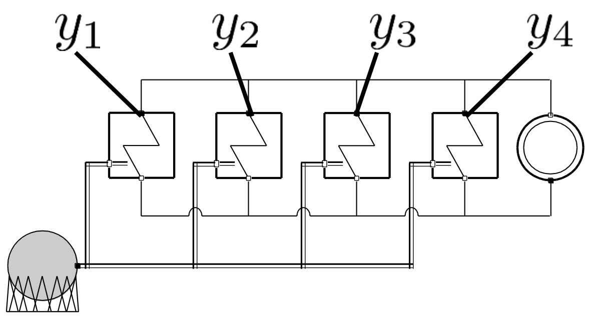
$\text{TAC} = 315000\ \text{CHF/a}$
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

$y_3 \geq 1$

$\text{TAC} = 311000\ \text{CHF/a}$
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

lower bound: the optimal solution cannot be cheaper than this!

Branch-&-Bound: Reducing the number of LPs to be solved



1 **LP-relaxation**: assume all integers are continuous

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$\mathrm{TAC} = 310000\ \mathrm{CHF/a}$
$y = (1, 0, 0.667, 0)$

lower bound: the optimal solution cannot be cheaper than this!

branching

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$y_3 \geq 1$

$\mathrm{TAC} = 311000\ \mathrm{CHF/a}$
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

branching

$y_1 \leq 0$

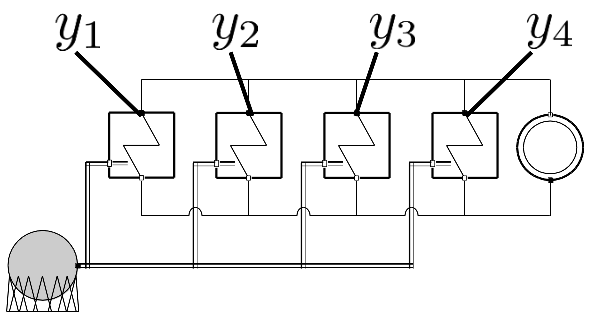
$\mathrm{TAC} = 318000\ \mathrm{CHF/a}$
$y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$

$y_1 \geq 1$

$\boxed{\mathrm{TAC} = 317000\ \mathrm{CHF/a} \quad y = (\mathbf{1}, 0, \mathbf{1}, 0)}$

upper bound: the optimal solution cannot be worse than this feasible solution!

Branch-&-Bound: Reducing the number of LPs to be solved



1 **LP-relaxation**: assume all integers are continuous

2 **branching**: divide solution space into subspaces, excluding non-integer values

3 **bounding**: do not explore subspaces that do not contain better solutions

TAC = 310000 CHF/a
$y = (1, 0, 0.667, 0)$

$y_3 \leq 0$ branching $y_3 \geq 1$

lower bound: the optimal solution cannot be cheaper than this!

TAC = 315000 CHF/a
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

TAC = 311000 CHF/a
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

$y_1 \leq 0$ branching $y_1 \geq 1$

feasible solutions in this subspace are worse than the upper bound

upper bound: the optimal solution cannot be worse than this feasible solution!

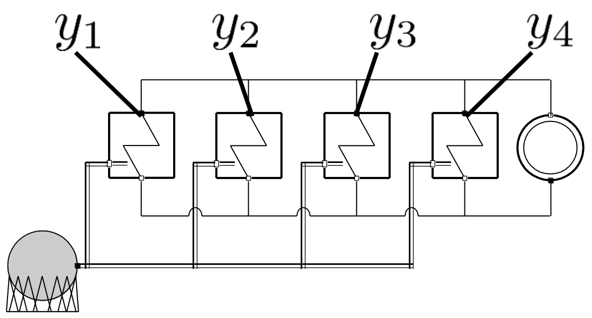
TAC = 318000 CHF/a
$y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$

TAC = 317000 CHF/a
$y = (\mathbf{1}, 0, \mathbf{1}, 0)$

bounding

vado prima quella
+ economica (penso però che anche prima e l'altro, vedi s. 31)

Branch-&-Bound: Reducing the number of LPs to be solved



1. **LP-relaxation**: assume all integers are continuous
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TAC = 310000 CHF/a
$y = (1, 0, 0.667, 0)$

branching

$y_3 \leq 0$:
TAC = 315000 CHF/a
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

$y_3 \geq 1$:
TAC = 311000 CHF/a
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

branching

$y_2 \leq 0$:
TAC = 323000 CHF/a
$y = (1, \mathbf{0}, \mathbf{0}, 1)$

$y_2 \geq 1$:
TAC = 322000 CHF/a
$y = (\mathbf{0.4}, \mathbf{1}, \mathbf{0}, 0)$

branching

$y_1 \leq 0$:
TAC = 318000 CHF/a
$y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$

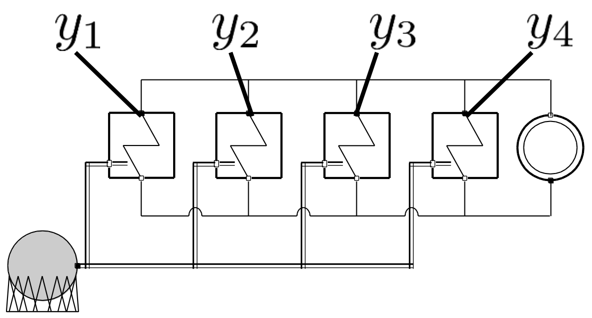
$y_1 \geq 1$:
TAC = 317000 CHF/a
$y = (\mathbf{1}, 0, \mathbf{1}, 0)$

bounding

upper bound: the optimal solution cannot be worse than this feasible solution!

Kombiniere branching + bounding Kriterien!
Stopkriterium!

Branch-&-Bound: Reducing the number of LPs to be solved



1 **LP-relaxation**: assume all integers are continuous

2 **branching**: divide solution space into subspaces, excluding non-integer values

3 **bounding**: do not explore subspaces that do not contain better solutions

1

TAC = 310000 CHF/a
$y = (1, 0, 0.667, 0)$

$y_3 \leq 0$ branching $y_3 \geq 1$

2 3

TAC = 315000 CHF/a
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

TAC = 311000 CHF/a
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

$y_2 \leq 0$ 4 branching $y_2 \geq 1$ 5

6 $y_1 \leq 0$ branching $y_1 \geq 1$ 7

TAC = 323000 CHF/a
$y = (1, \mathbf{0}, \mathbf{0}, 1)$

TAC = 322000 CHF/a
$y = (\mathbf{0.4}, \mathbf{1}, \mathbf{0}, 0)$
bounding

TAC = 318000 CHF/a
$y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$
bounding

TAC = 317000 CHF/a
$y = (\mathbf{1}, 0, \mathbf{1}, 0)$

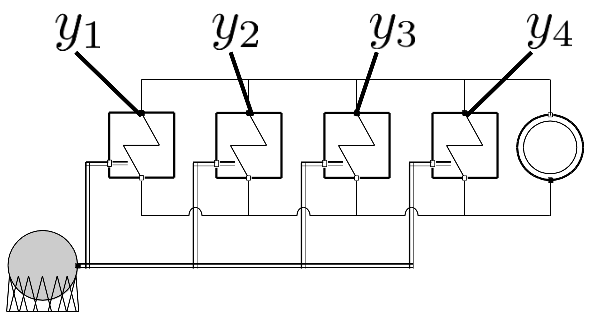
only 7 LPs!

#7 → solved

upper bound: the optimal solution cannot be worse than this feasible solution!

lower bound: the optimal solution cannot be cheaper than this!

Branch-&-Bound: Lower & upper bound to assess solution quality



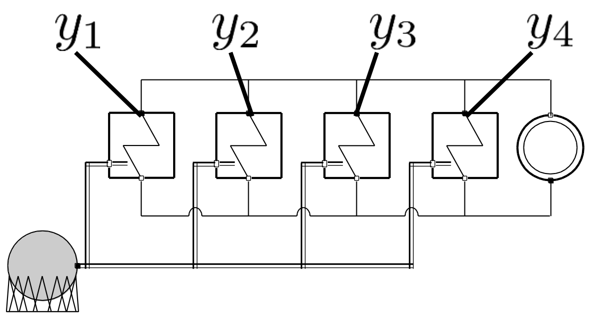
1

$\mathrm{TAC} = 310000\ \mathrm{CHF/a}$
$y = (1, 0, 0.667, 0)$

Root

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a						
upper bound	-						
gap	-						

Branch-&-Bound: Lower & upper bound to assess solution quality



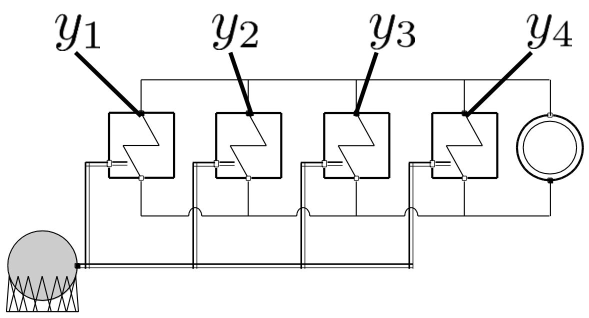
1 $\text{TAC} = 310000\ \text{CHF/a}$
$y = (1, 0, 0.667, 0)$

$y_3 \leq 0$ branching

2 $\text{TAC} = 315000\ \text{CHF/a}$
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a					
upper bound	-	-					
gap	-	-					

Branch-&-Bound: Lower & upper bound to assess solution quality



1
$\text{TAC} = 310000\ \text{CHF/a}$
$y = (1, 0, 0.667, 0)$

node is now inactive

a node is inactive, if
1) the node is branched,
2) the node is bounded,
3) the node is feasible, or
4) the node is infeasible.

branching

$y_3 \leq 0$

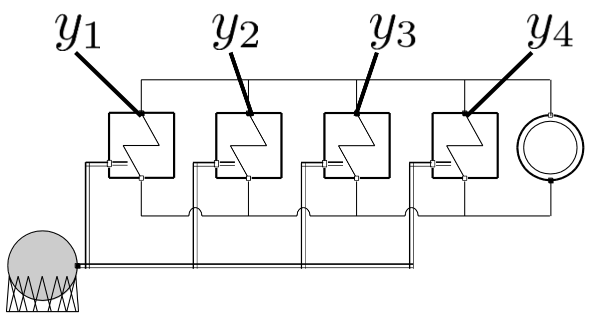
2
$\text{TAC} = 315000\ \text{CHF/a}$
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

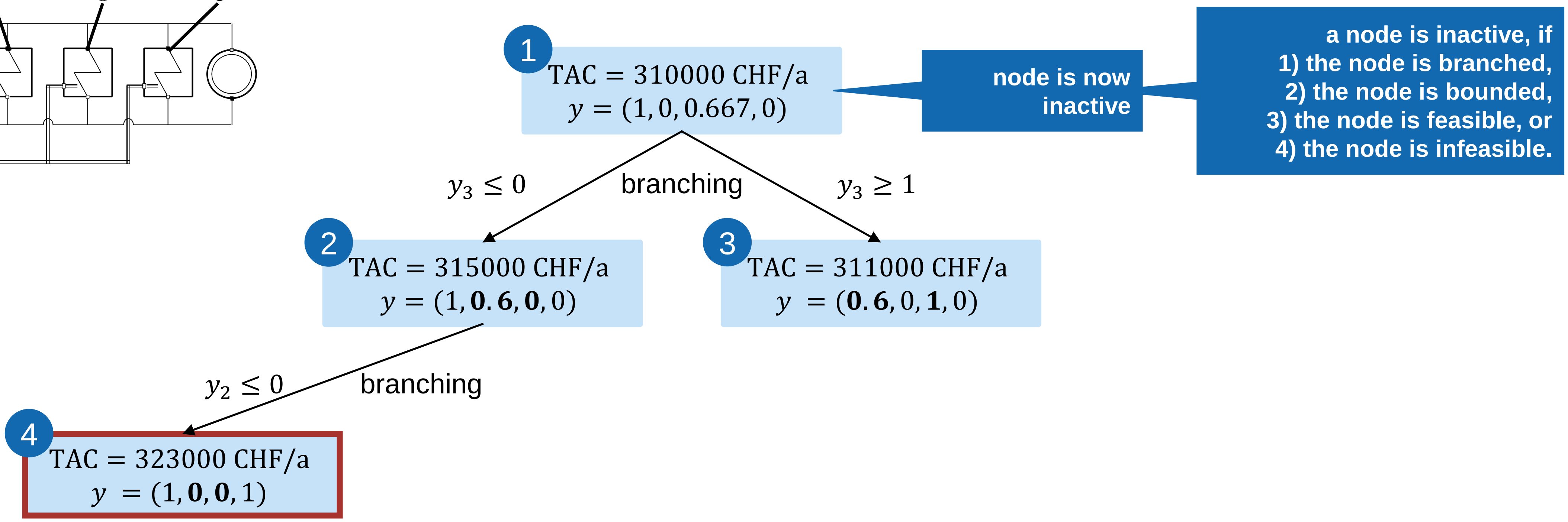
$y_3 \geq 1$

3
$\text{TAC} = 311000\ \text{CHF/a}$
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a				
upper bound	-	-	-				
gap	-	-	-				

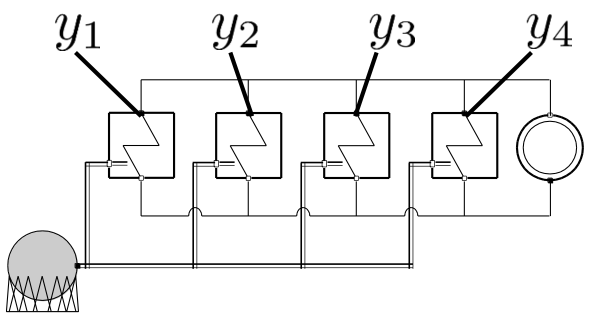
Branch-&-Bound: Lower & upper bound to assess solution quality





node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a	311000 CHF/a			
upper bound	-	-	-	323000 CHF/a			
gap	-	-	-	12000 CHF/a			

Branch-&-Bound: Lower & upper bound to assess solution quality



1
TAC = 310000 CHF/a
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$y_3 \leq 0$ branching $y_3 \geq 1$

2
TAC = 315000 CHF/a
$y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

3
TAC = 311000 CHF/a
$y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

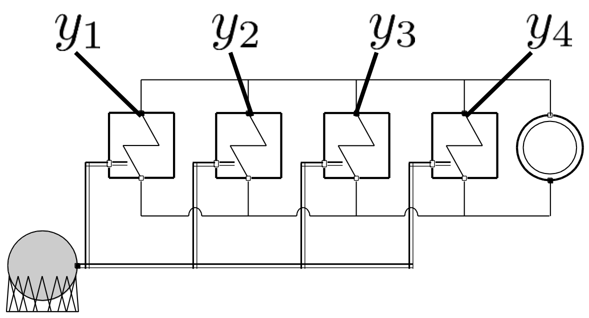
$y_2 \leq 0$ branching $y_2 \geq 1$

4
TAC = 323000 CHF/a
$y = (1, \mathbf{0}, \mathbf{0}, 1)$

5
TAC = 322000 CHF/a
$y = (\mathbf{0.4}, \mathbf{1}, \mathbf{0}, 0)$

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a		
upper bound	-	-	-	323000 CHF/a	323000 CHF/a		
gap	-	-	-	12000 CHF/a	12000 CHF/a		

Branch-&-Bound: Lower & upper bound to assess solution quality



1 TAC = 310000 CHF/a, $y = (1, 0, 0.667, 0)$

node is now inactive

a node is inactive, if
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2) the node is bounded,
3) the node is feasible, or
4) the node is infeasible.

branching: $y_3 \leq 0$ / $y_3 \geq 1$

2 TAC = 315000 CHF/a, $y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

3 TAC = 311000 CHF/a, $y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

branching: $y_2 \leq 0$ / $y_2 \geq 1$

branching: $y_1 \leq 0$

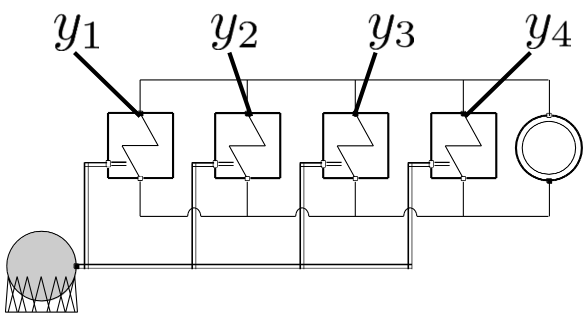
4 TAC = 323000 CHF/a, $y = (1, \mathbf{0}, \mathbf{0}, 1)$

5 TAC = 322000 CHF/a, $y = (\mathbf{0.4}, \mathbf{1}, \mathbf{0}, 0)$

6 TAC = 318000 CHF/a, $y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	
upper bound	-	-	-	323000 CHF/a	323000 CHF/a	323000 CHF/a	
gap	-	-	-	12000 CHF/a	12000 CHF/a	12000 CHF/a	

Branch-&-Bound: Lower & upper bound to assess solution quality



1: TAC = 310000 CHF/a, $y = (1, 0, 0.667, 0)$

node is now inactive

a node is inactive, if
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branching: $y_3 \leq 0$ / $y_3 \geq 1$

2: TAC = 315000 CHF/a, $y = (1, \mathbf{0.6}, \mathbf{0}, 0)$

3: TAC = 311000 CHF/a, $y = (\mathbf{0.6}, 0, \mathbf{1}, 0)$

branching: $y_2 \leq 0$ / $y_2 \geq 1$

branching: $y_1 \leq 0$ / $y_1 \geq 1$

4: TAC = 323000 CHF/a, $y = (1, \mathbf{0}, \mathbf{0}, 1)$

5: TAC = 322000 CHF/a, $y = (\mathbf{0.4}, \mathbf{1}, \mathbf{0}, 0)$

bounding

6: TAC = 318000 CHF/a, $y = (\mathbf{0}, \mathbf{0.4}, \mathbf{1}, 0)$

bounding

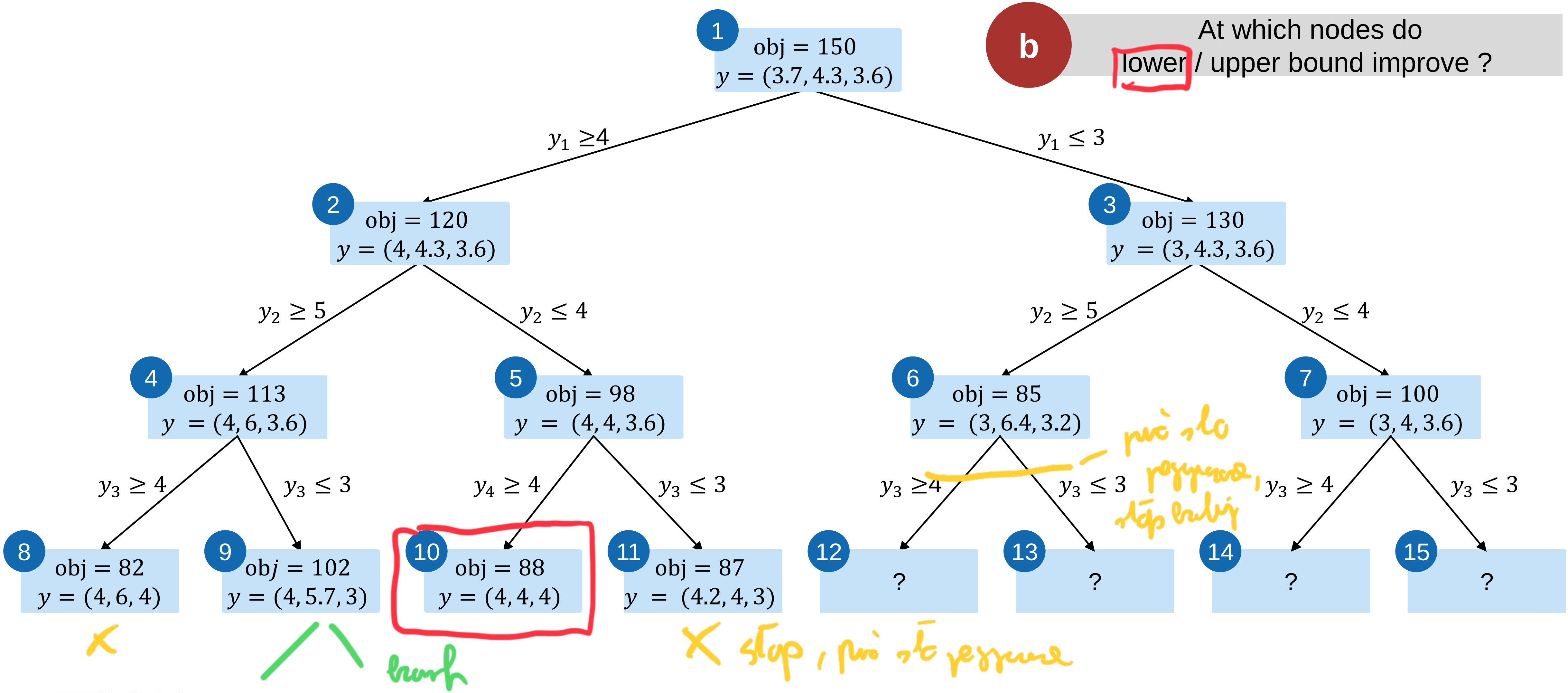
7: TAC = 317000 CHF/a, $y = (\mathbf{1}, 0, \mathbf{1}, 0)$

node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	317000 CHF/a
upper bound	-	-	-	323000 CHF/a	323000 CHF/a	323000 CHF/a	317000 CHF/a
gap	-	-	-	12000 CHF/a	12000 CHF/a	12000 CHF/a	0 CHF/a

Your turn: Branch or Bound?

a Minimization or maximization problem?

b At which nodes do lower / upper bound improve ?



Your turn: Branch or Bound?

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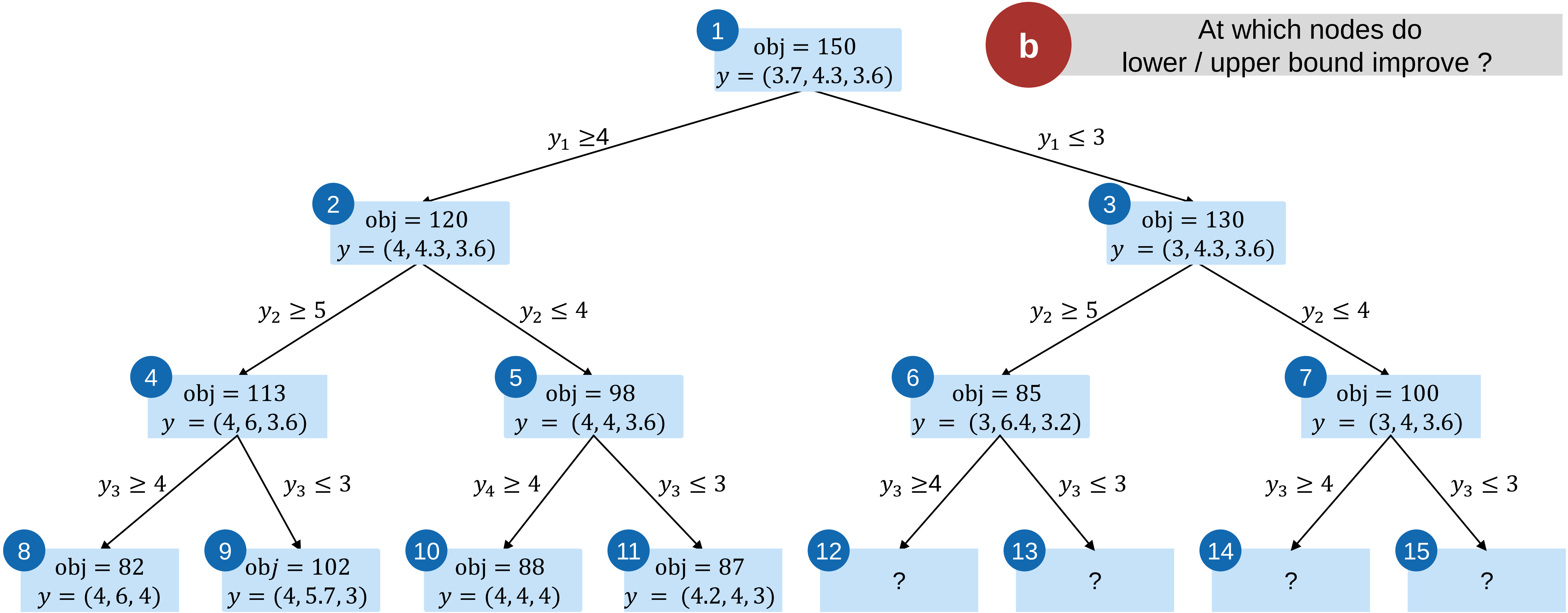
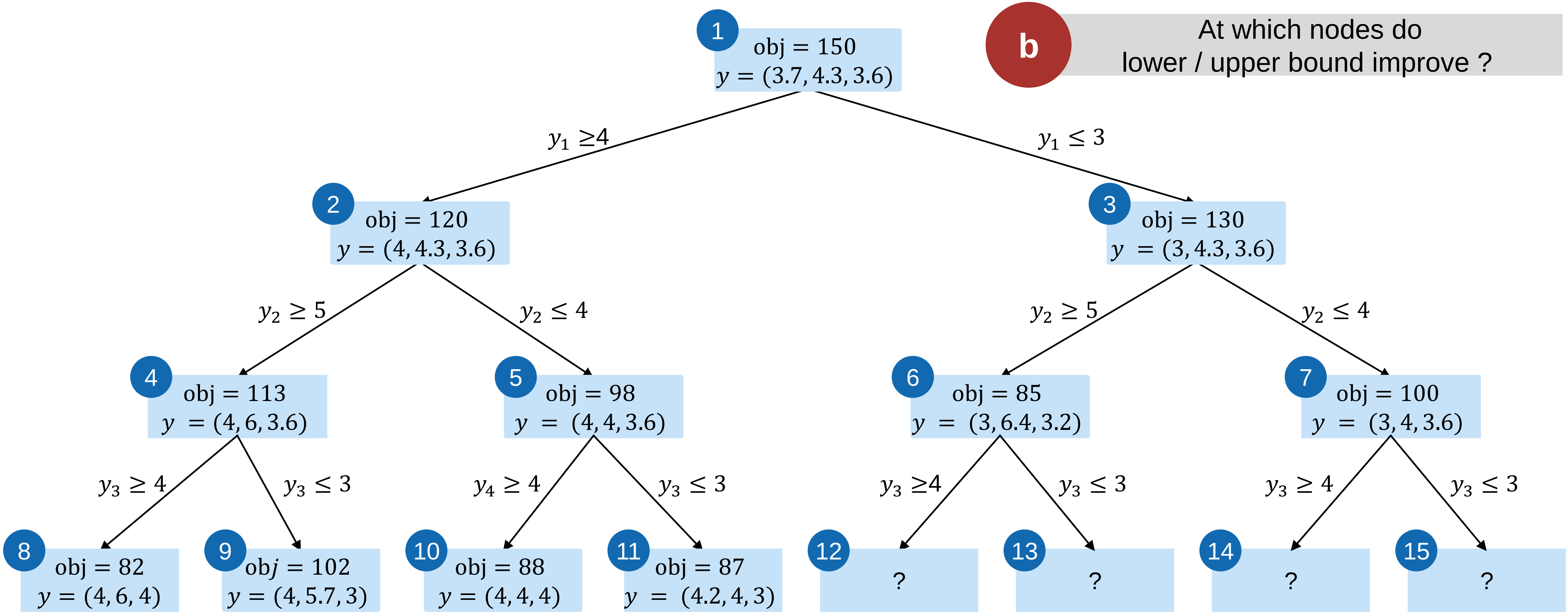


Node	1	2	3	4	5	6	7	8	9	10	11
Upper											
Lower											
gap											

Your turn: Branch or Bound?

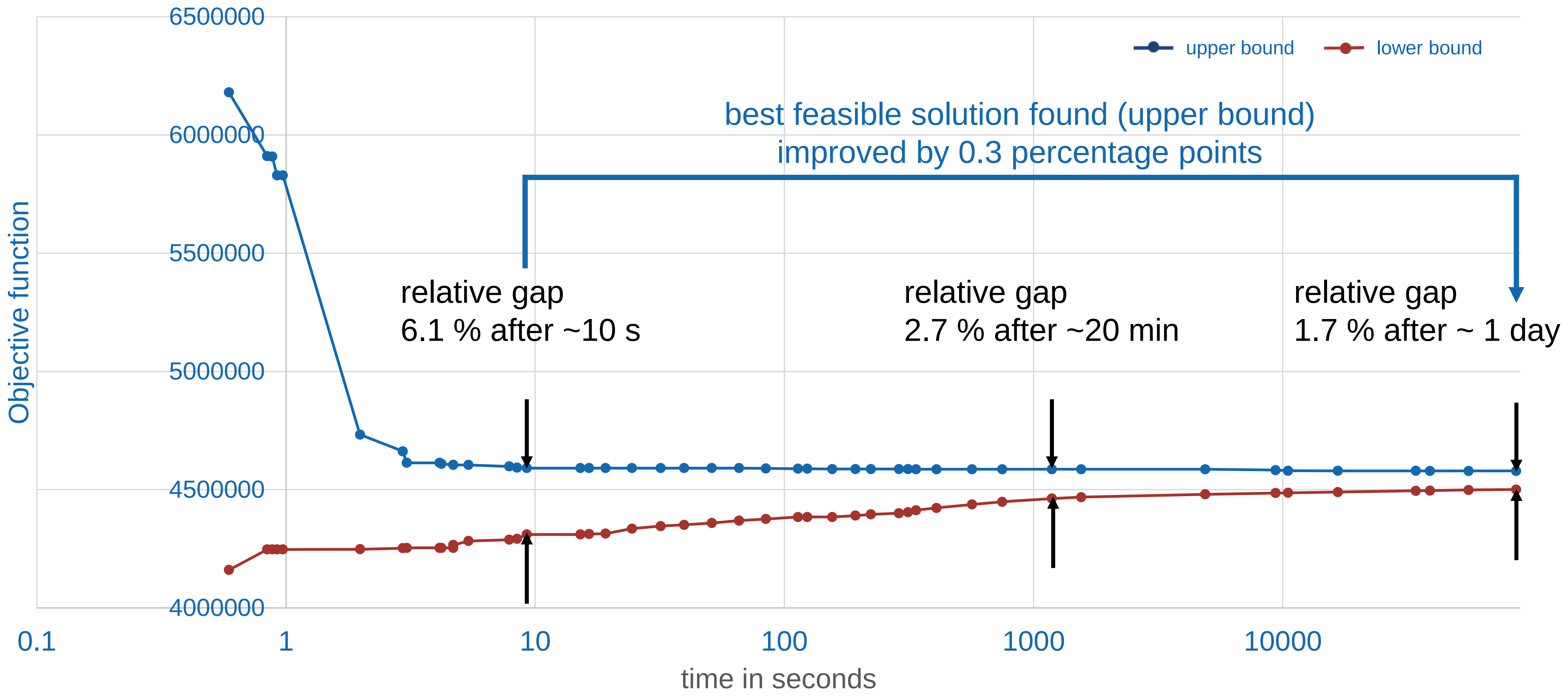
a Minimization or maximization problem?

b At which nodes do lower / upper bound improve ?

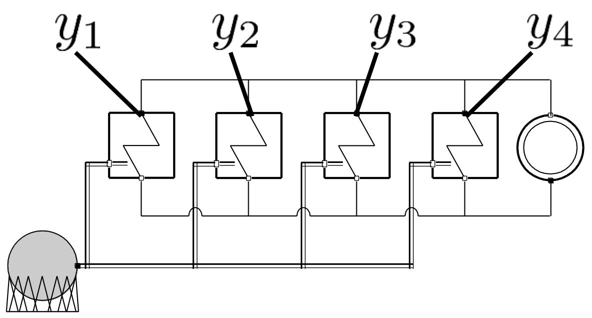


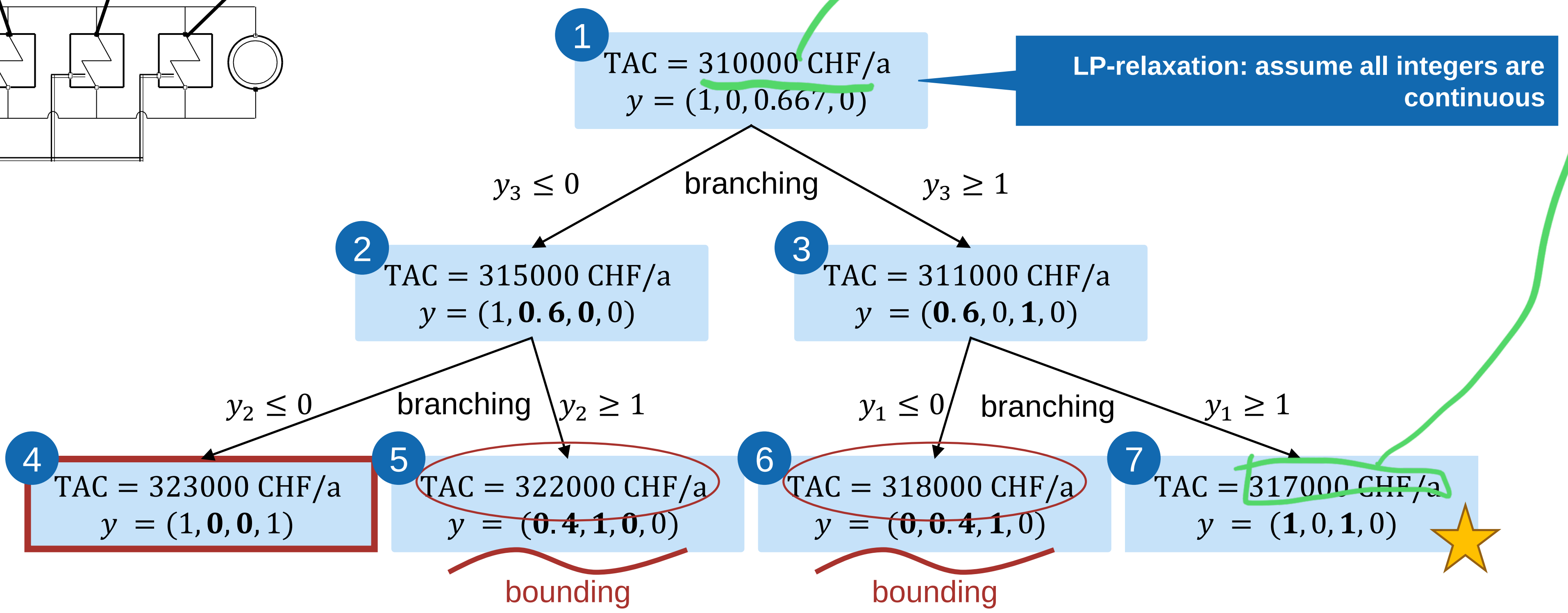
Node	1	2	3	4	5	6	7	8	9	10	11
Upper	150	150	130	130	130	130	113	113	102	102	102
Lower	-	-	-	-	-	-	-	82	82	88	88
gap	-	-	-	-	-	-	-	31	20	14	14

The global optimum – all that matters?
Example: Minimization problem



Branch-&-Bound: “**The integrality gap = LP relaxation – optimum**”





node	1	2	3	4	5	6	7
lower bound	310000 CHF/a	310000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	311000 CHF/a	317000 CHF/a
upper bound	-	-	-	323000 CHF/a	323000 CHF/a	323000 CHF/a	317000 CHF/a

Model to keep integrality gap small

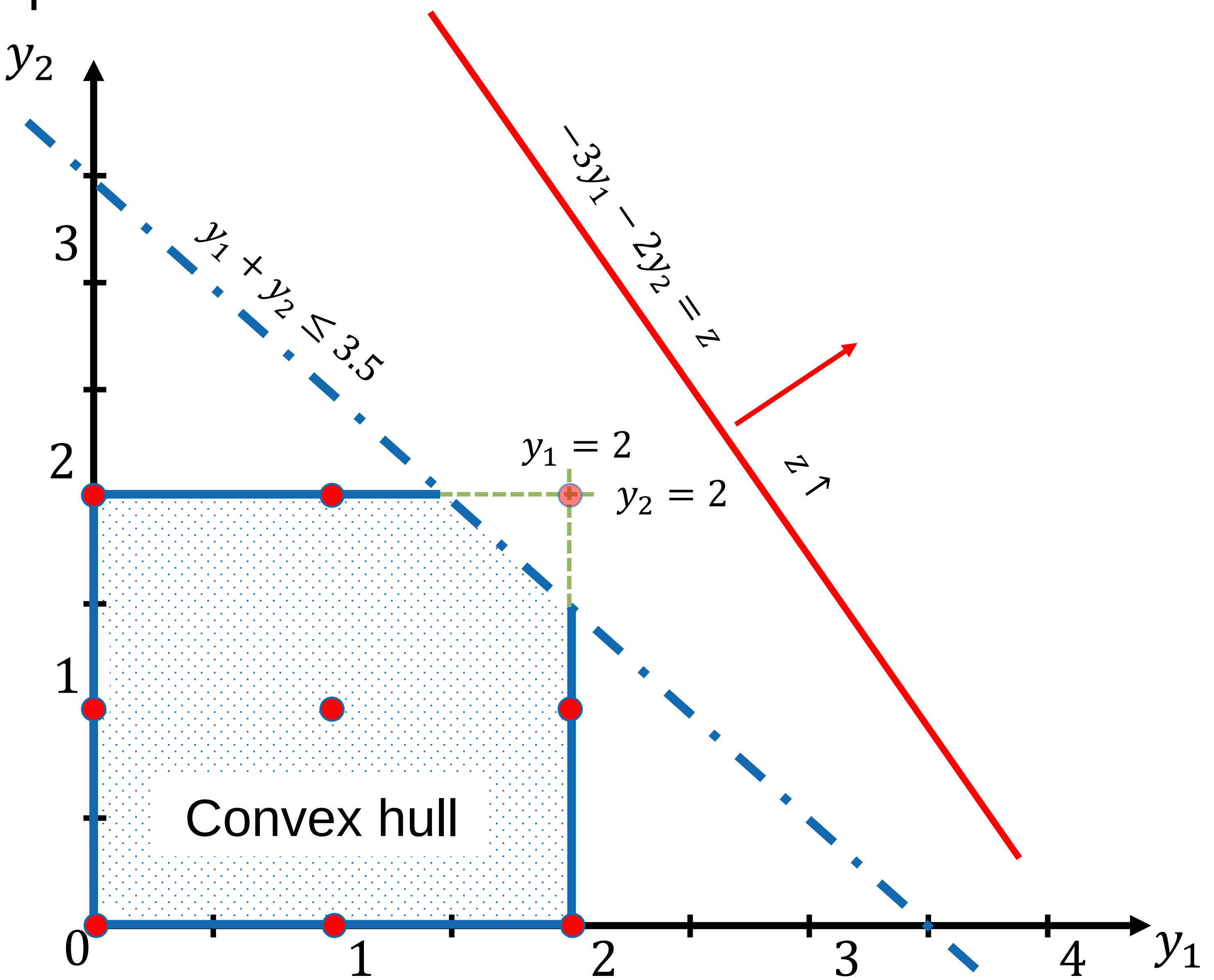
Illustration of the integrality gap

$$\min_{x,y} \quad z = -3y_1 - 2y_2$$

$$\text{s.t.} \quad y_1 + y_2 \le 3.5$$
$$0 \le y_1 \le 2$$
$$0 \le y_2 \le 2$$
$$y_1, y_2 \in \mathbb{Z}^t$$

LP relaxation: $y_1 = 2; y_2 = 1.5; z = -9$

Branch & Bound with 5 LPs
$\Rightarrow$ Optimum : $y_1 = 2; y_2 = 1; z = -8$



Kallrath (2013)

Illustration of the integrality gap

$$\min_{x,y} \quad z = -3y_1 - 2y_2$$

s.t.

$$y_1 + y_2 \leq 3.5$$
$$0 \leq y_1 \leq 2$$
$$0 \leq y_2 \leq 2$$
$$y_1, y_2 \in \mathbb{Z}^t$$

LP relaxation: $y_1 = 2; y_2 = 1.5; z = -9$

Branch & Bound with 5 LPs

$\Rightarrow$ Optimum : $y_1 = 2; y_2 = 1; z = -8$

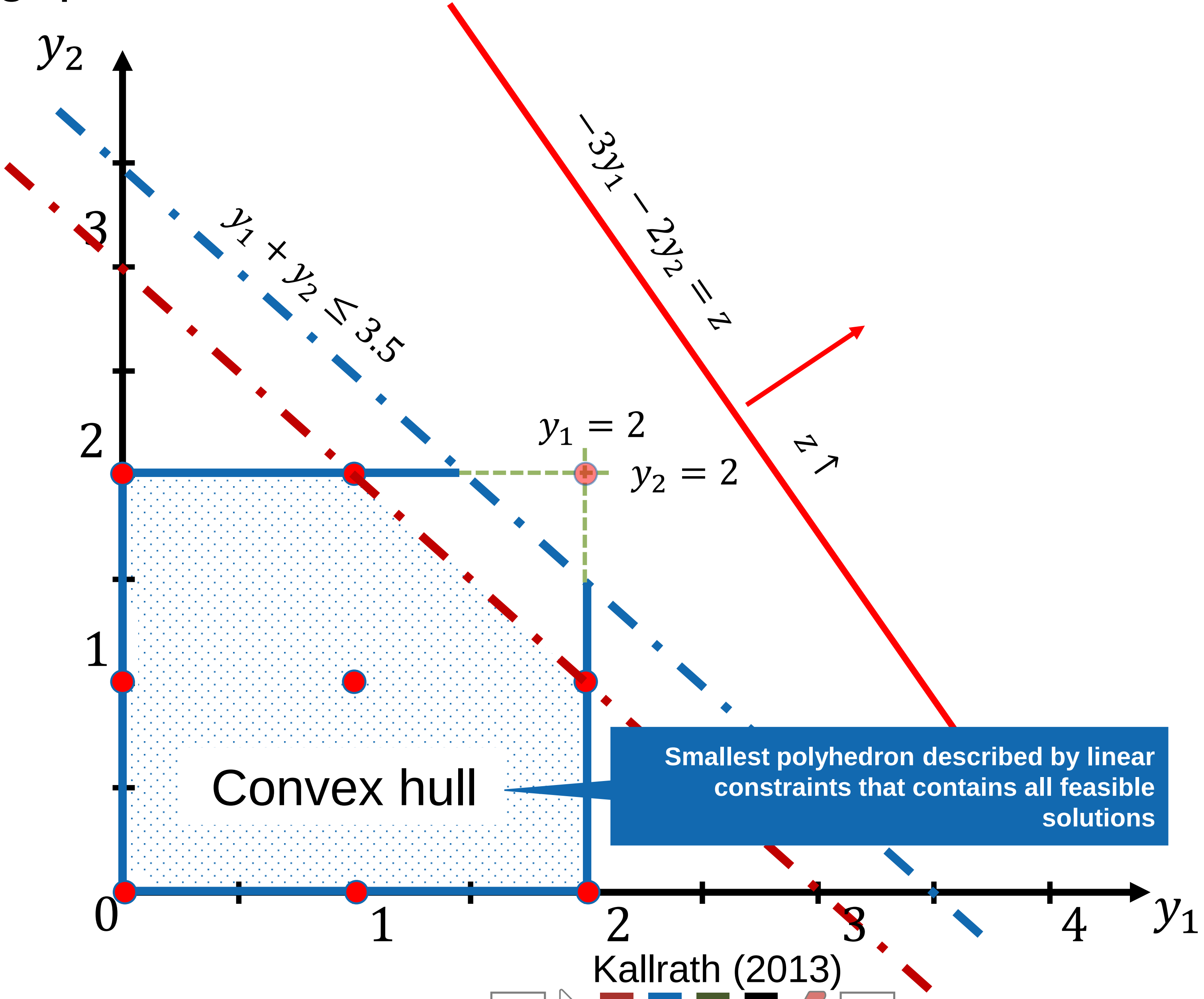
$$\min_{x,y} \quad z = -3y_1 - 2y_2$$

s.t.

$$y_1 + y_2 \leq 3.0$$
$$0 \leq y_1 \leq 2$$
$$0 \leq y_2 \leq 2$$
$$y_1, y_2 \in \mathbb{Z}^t$$

LP relaxation = Optimum ☺

LP relaxation = convex hull



Kallrath (2013)

Illustration of the integrality gap

$$\min_{x,y} \quad z = -3y_1 - 2y_2$$
$$\text{s.t.} \quad y_1 + y_2 \leq 3.5$$
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Branch & Bound with 5 LPs

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$$\text{s.t.} \quad y_1 + y_2 \leq 3.0$$
$$0 \leq y_1 \leq 2$$
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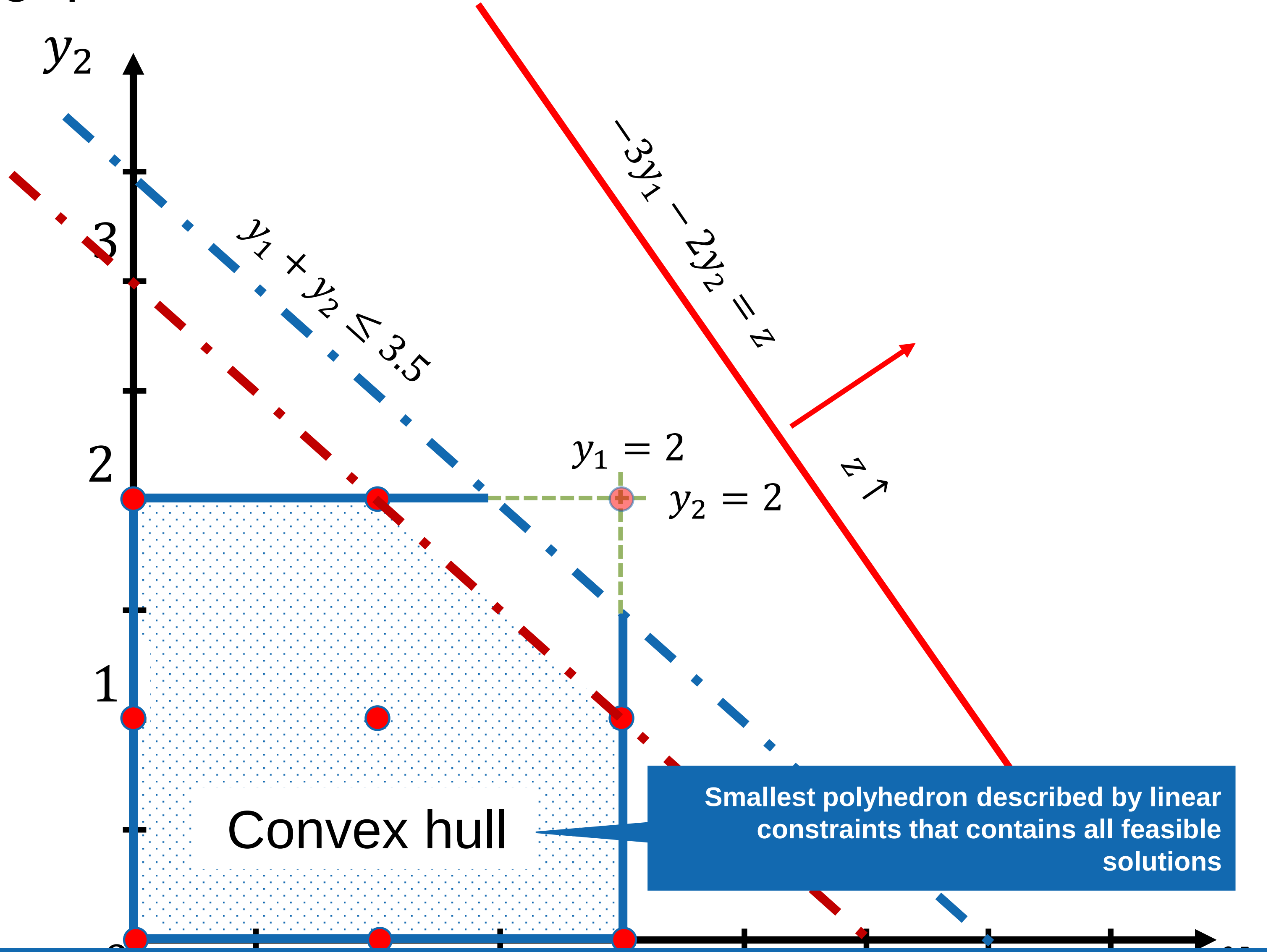


Model to keep integrality gap small

Applying the Branch-and-Bound algorithm

The global optimum of MILPs and MINLPs can be found using the Branch-and-Bound algorithm if the relaxed subproblems can be solved globally.

problem type	MILP	MINLP	
relaxed subproblem type	LP	NLP	
convexity	always convex	convex	non-convex
			convex underestimator required

After this lecture, you will be able to…

- ✓ employ basic **solution methods** for **mixed-integer linear** (MILP) & **nonlinear programming** (MINLP) problems.
- find optimal heat-exchanger networks and near-optimal solutions with **integer cuts**
- discuss **(dis)advantages** of optimization problem classes

Last lecture: Development of optimal HEN

Economic optimization:

min Total costs = Operating costs + Investment costs

Sequential approach :

2nd lecture

1) Targeting: Minimize utility costs (heat integration)

Now

2) Minimize number of heat exchangers (network search)
s.t. Target (minimum utility costs)

Last lecture: Optimization: Number of heat exchangers

$$\min_{\Delta\dot{Q}^*_z,\dot{Q}^{(z)}_{h,c}} \sum_h \sum_c \epsilon_{h,c}$$

Number of stream couplings
≤ Number of heat exchangers

$s.t.$ **Energy balances:**

$$\forall h,z \quad 0 = -\Delta\dot{Q}^*_{h,z} + \Delta\dot{Q}^*_{h,z-1} + \Delta\dot{H}^{(z)}_h - \sum_c \dot{Q}^{(z)}_{h,c},$$

$$0 = \Delta\dot{Q}^*_{h,1},$$

$$0 = \Delta\dot{Q}^*_{h,z_{max}},$$

$$\forall c,z \quad 0 = -\Delta\dot{H}^{(z)}_c + \sum_h \dot{Q}^{(z)}_{h,c}$$

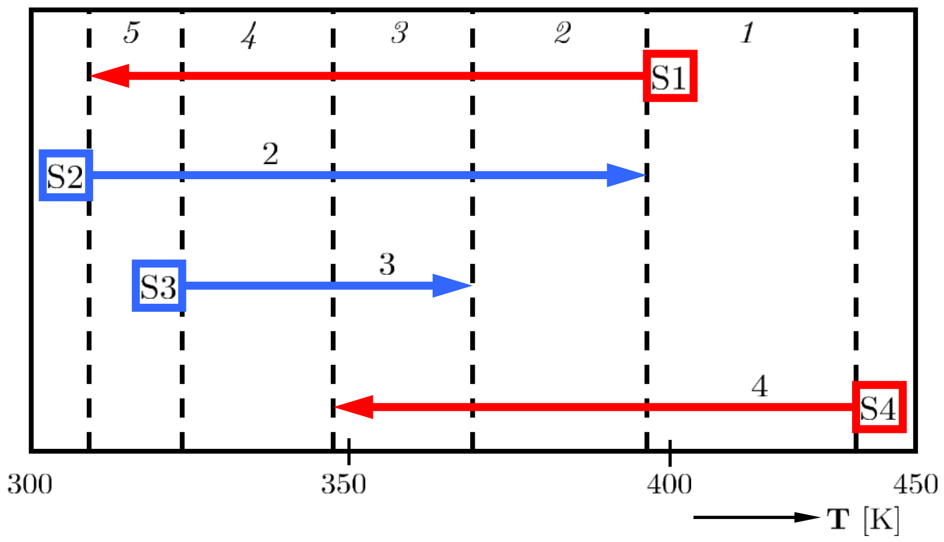
Stream couplings:

$$\forall h,c \quad \sum_z \dot{Q}^{(z)}_{h,c} \leq \epsilon_{h,c} \cdot \Delta\dot{Q}^{max}_{h,c}$$

Papoulias, Grossmann. *A structural optimization approach in process synthesis II: Heat recovery networks.* Comput Chem Eng, *7*:707-721, 1983.

Results example

$$\epsilon_{h,c} = 0, \text{except:}\ \epsilon_{1,2} = 1$$
$$\epsilon_{1,3} = 1$$
$$\epsilon_{1,B} = 1$$
$$\epsilon_{4,3} = 1$$
$$\epsilon_{S,3} = 1$$



[1]

$$\dot{Q}_{h,c} = 0, \text{except:}$$

$$\left(\dot{Q}_{h,c} = \sum_z \dot{Q}_{h,c}^{(z)}\right)$$

$$\dot{Q}_{1,2} = 162\text{kW}(36\text{kW} + 54\text{kW} + 18\text{kW} + 54\text{kW}, z = 2,3,4,5)$$
$$\dot{Q}_{1,3} = 12\text{kW}(10\text{kW} + 2\text{kW}, z = 3,4)$$
$$\dot{Q}_{1,B} = 6\text{kW}(6\text{kW}, z = 5)$$
$$\dot{Q}_{4,3} = 100\text{kW}(62\text{kW} + 38\text{kW}, z = 3,4)$$
$$\dot{Q}_{S,3} = 48\text{kW}(48\text{kW}, z = 3)$$

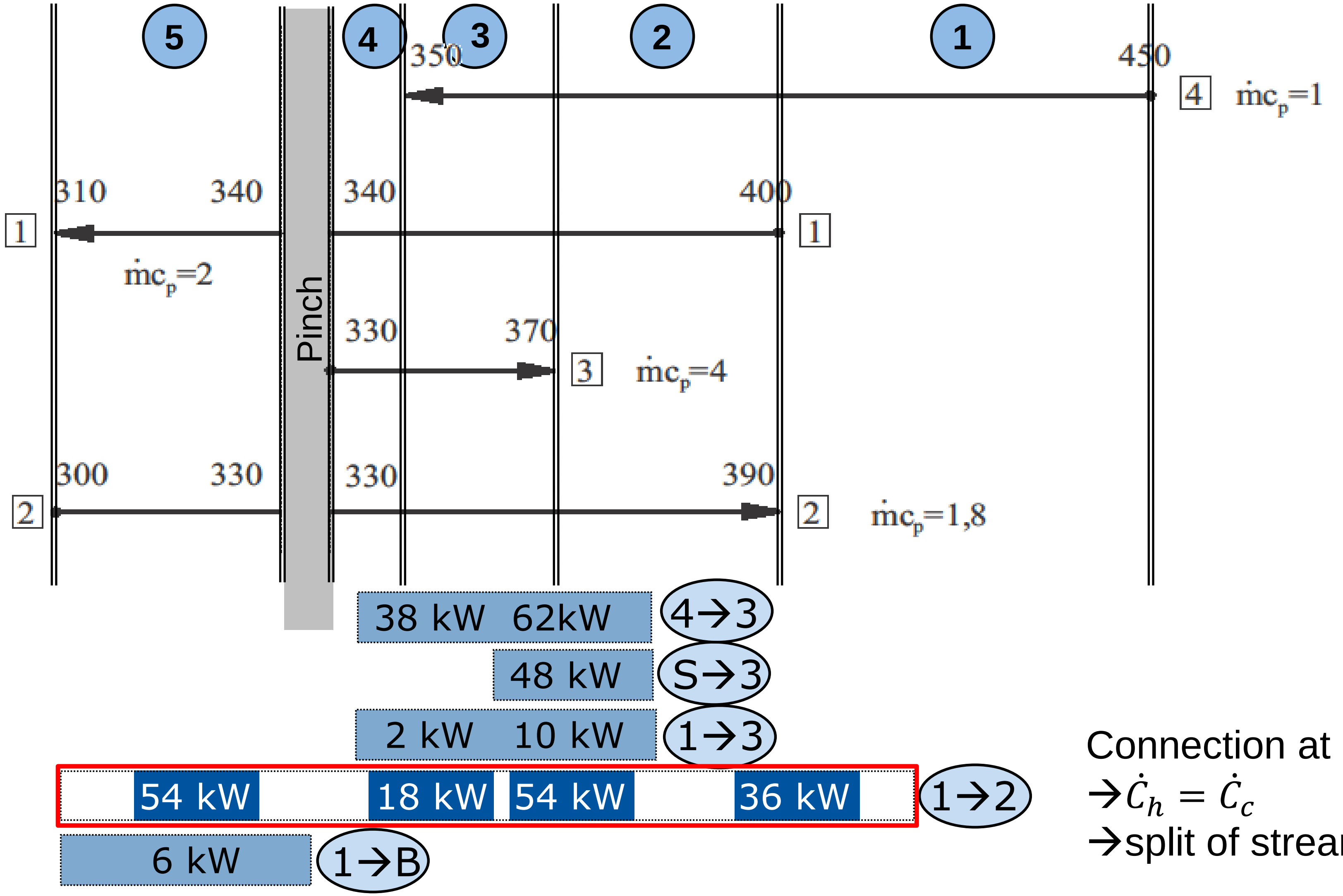
Online optimization tool*

Network Synthesis MILP

Hint: You may get the alternative solution first (see following slides)

*Code and Tutorial provided in Moodle

Connection sequence

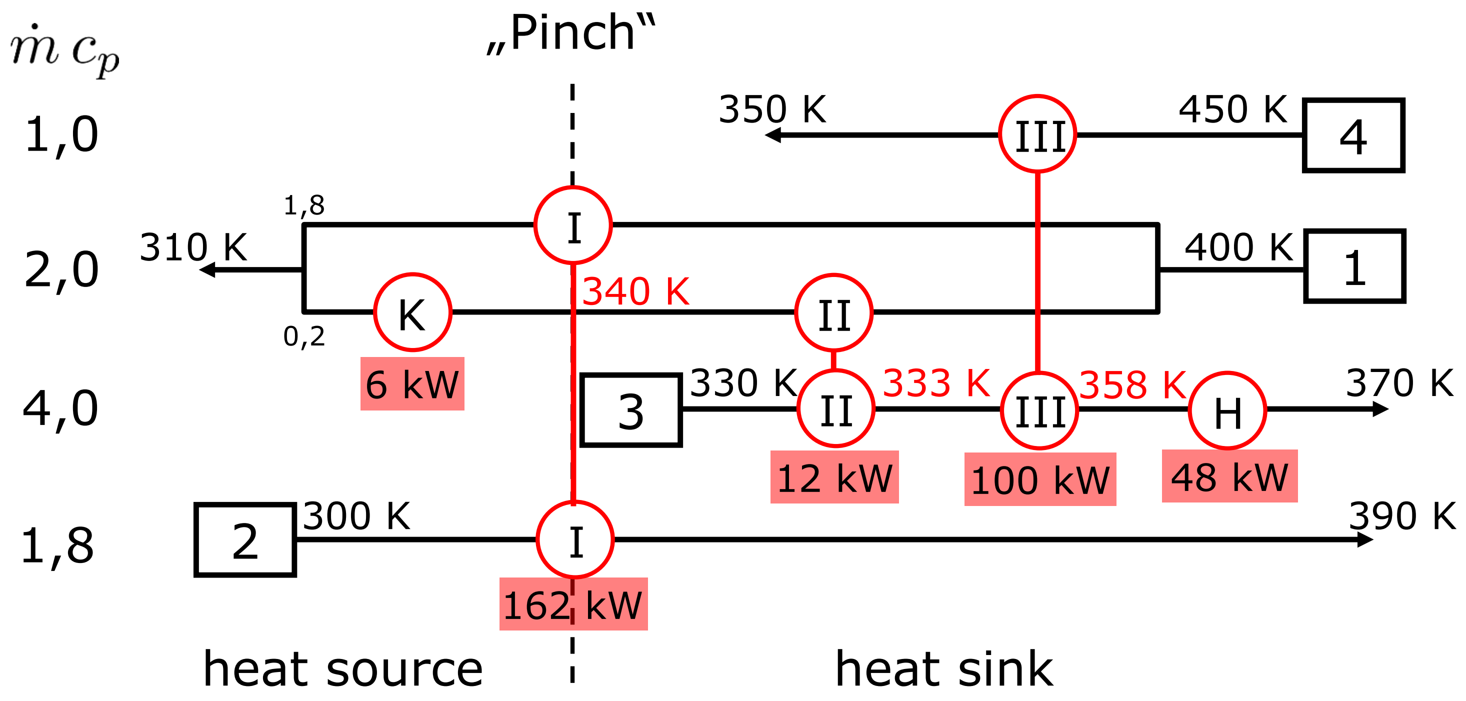


Connection at both sides of the pinch

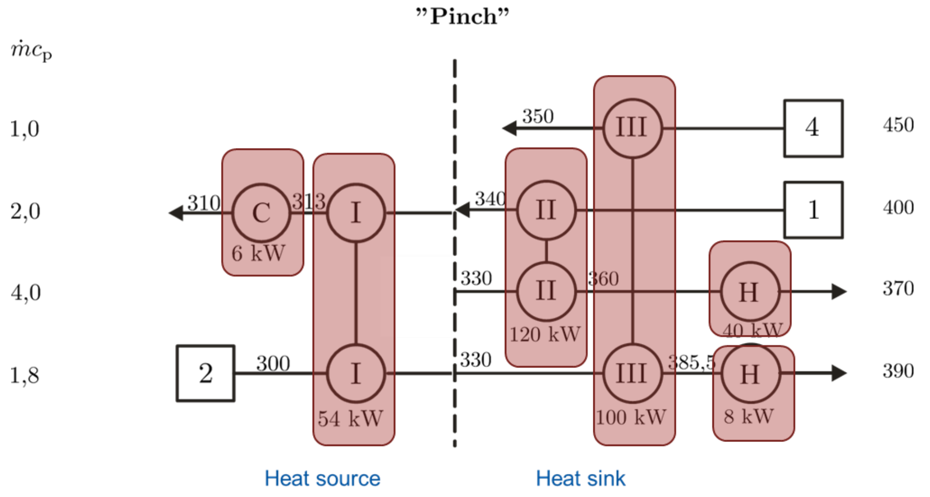
→$\dot{C}_h = \dot{C}_c$

→split of stream necessary

Optimal heat exchanger network



For comparison:
heat exchanger network
from pinch method



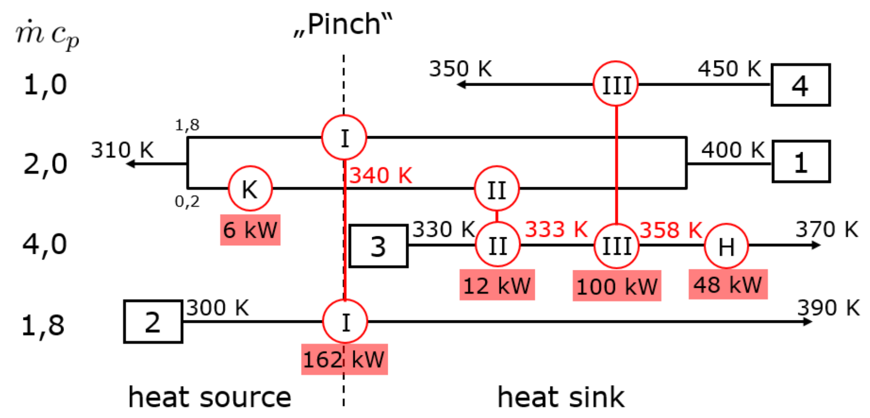
Search for further networks

$$\min_{\Delta\dot{Q}_z^*, \dot{Q}_{h,c}^{(z)}} \sum_h \sum_c \epsilon_{h,c}$$

$$s.t. \qquad \ldots$$

While the known Solution needs to be excluded

$$\epsilon_{1,2} = 1$$
$$\epsilon_{1,3} = 1$$
$$\epsilon_{1,B} = 1$$
$$\epsilon_{4,3} = 1$$
$$\epsilon_{S,3} = 1$$



→ integer-cut constraints:

$$\epsilon_{1,2} + \epsilon_{1,3} + \epsilon_{1,B} + \epsilon_{4,3} + \epsilon_{S,3} \leq 4$$

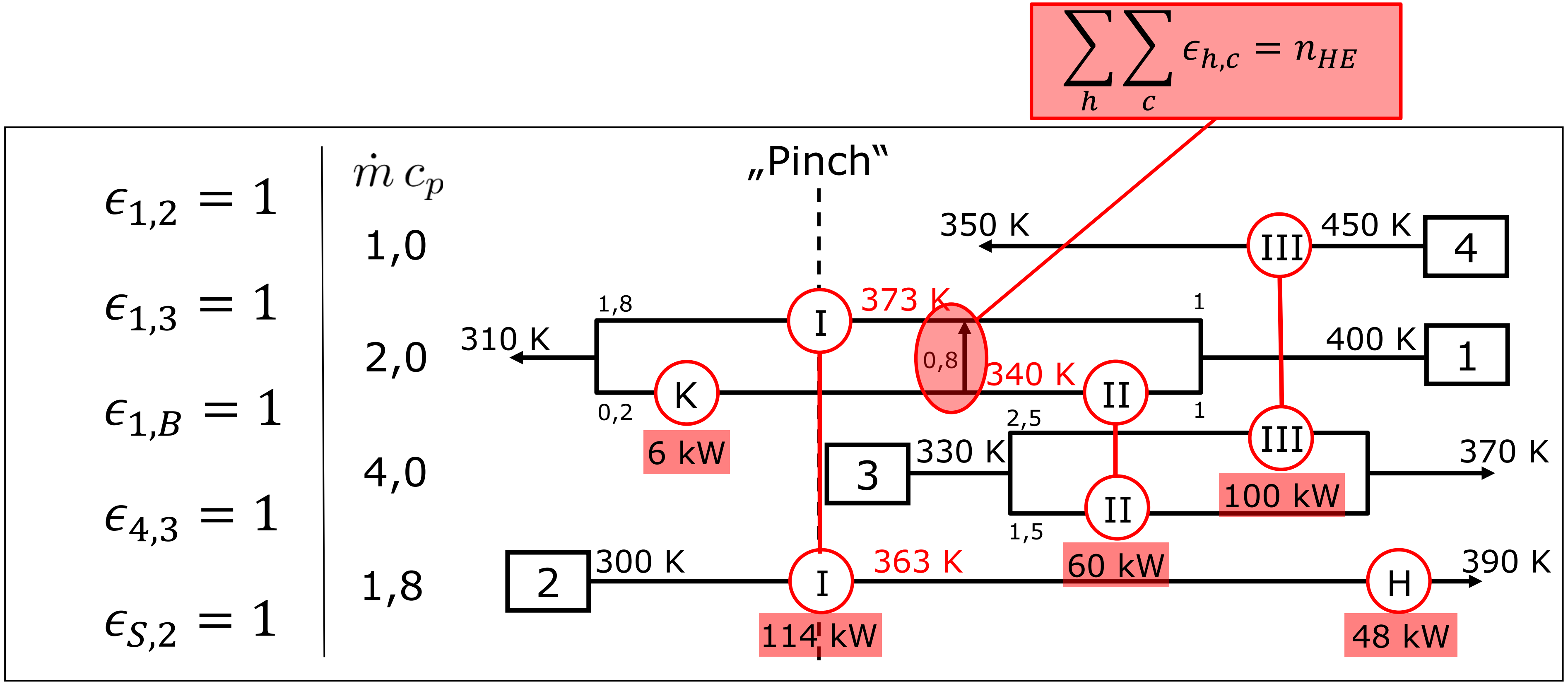
Online optimization tool*

Network Synthesis MILP

Hint: You may get the alternative solution first (see following slides)

*Code and Tutorial provided in Moodle

Search for further networks: result



→ integer-cut constraints:

$$\epsilon_{1,2} + \epsilon_{1,3} + \epsilon_{1,B} + \epsilon_{4,3} + \epsilon_{S,3} \leq 4$$

$$\epsilon_{1,2} + \epsilon_{1,3} + \epsilon_{1,B} + \epsilon_{4,3} + \epsilon_{S,2} \leq 4$$

→ ∅, no further solution

Integer Cuts

- Formula for integer cut on the last slides was special case
- In general:
- Solution k is to be excluded
  - with set of active variables $A = \{y_k | y_k = 1\}$
  - with set of inactive variables $I = \{y_k | y_k = 0\}$

A + I

$$\sum_{i \in A} y_i + \sum_{i \in I} (1 - y_i) \leq |A \cup I| - 1$$

$$\sum_{i \in A} y_i - \sum_{i \in I} y_i \leq |A| - 1$$

Limits of the sequential approach

min total costs = Operating costs + Investment costs

➔ min Number of heat exchangers

s.t. min utility costs

no Trade-Offs!

$\rightarrow$ Consumption of utilities

$\rightarrow$ Number of heat exchangers

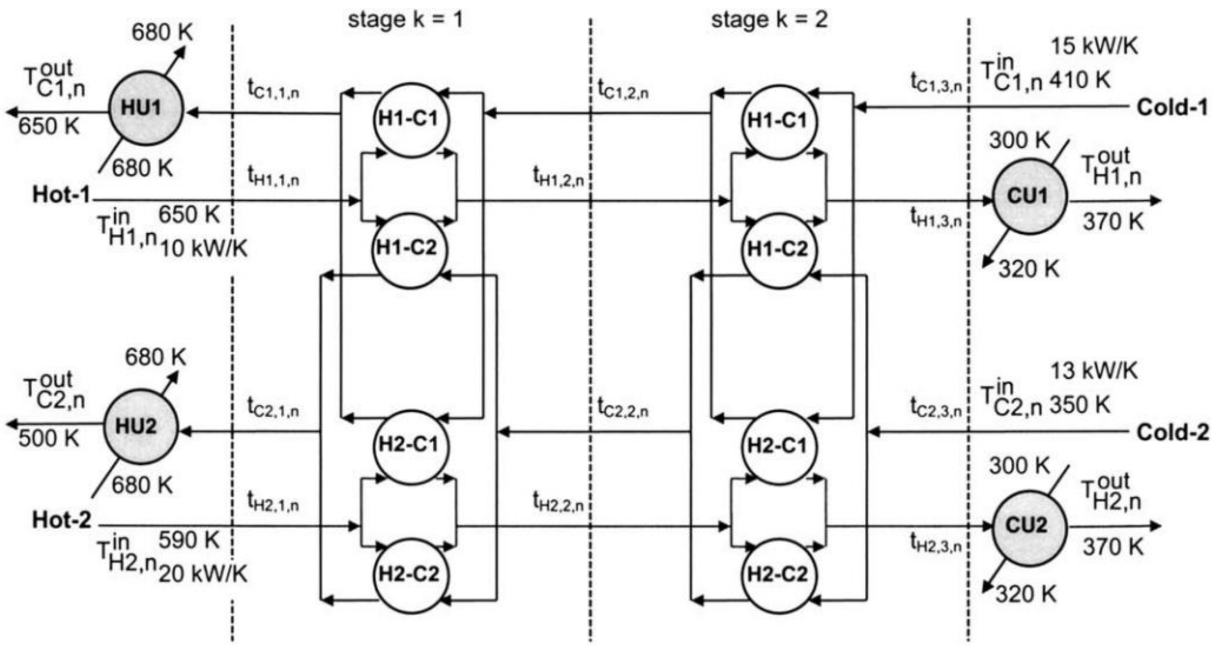
$\rightarrow$ Area heat exchanger

$\rightarrow$ minimal allowed approach temperature

Simultaneous MINLP Model

- Superstructure (example: 2 stages)

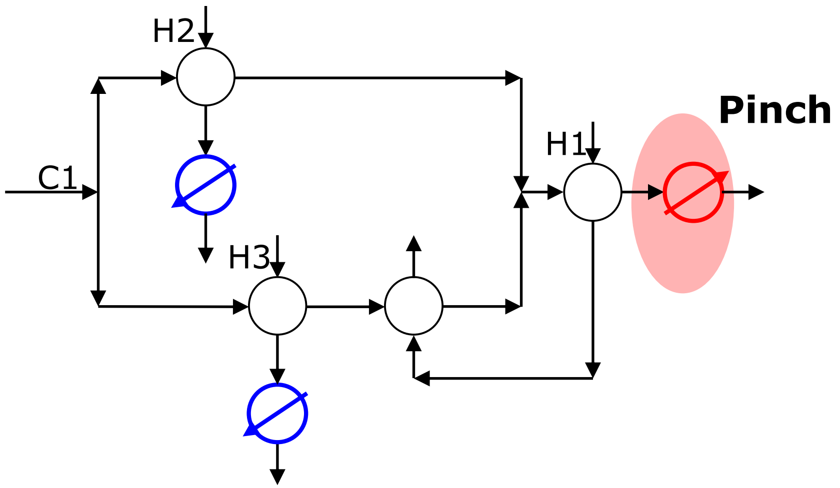
- Number of Stages = Number of temperature intervals
- no default ΔT_{min}
- variable temperatures of the HE outlet streams
  → Assumption: isothermal mixture of outlet flows



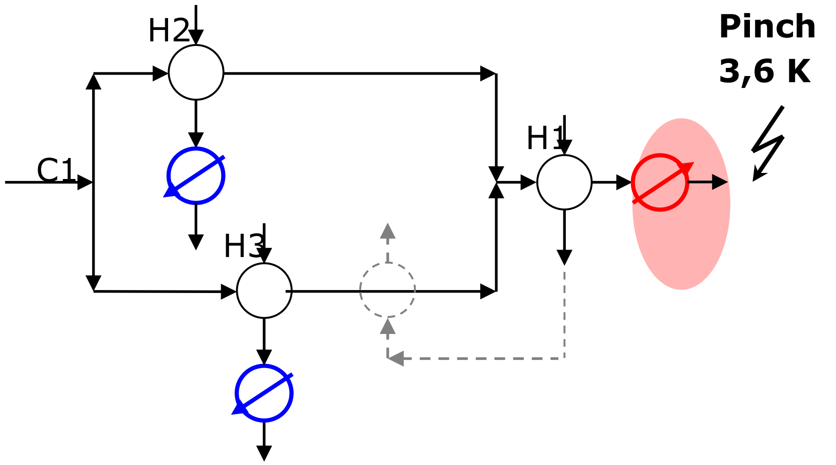
Yee, Terrence F., and Ignacio E. Grossmann. "Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis." *Computers & Chemical Engineering* 14.10 (1990): 1165-1184

Sequential vs. simultaneous approach

Sequential approach(ΔT_{min} = 7.6 K)
- utility costs: \$ 36.000 p.a.
- $\sum A$ = 241 m²
- total costs: \$ 72.000 p.a.



Simultaneous approach
Pinch violated → A_{HE} bigger
→ 1 HE less
- utility costs: \$ 36.000 p.a.
- $\sum A$ = 196.5 m²
- total costs: \$ 68.000 p.a.



Recent developments for heat exchanger networks

ELSEVIER

Computer Aided Chemical Engineering

Volume 48, 2020, Pages 1495-1500

Simultaneous Multiperiod Optimization of Rankine Cycles and Heat Exchanger Networks

Cristina Elsido [a], Emanuele Martelli [*a], Ignacio E. Grossmann [b]

Abstract

This work addresses the multiperiod synthesis and optimization of integrated Heat Exchanger Networks (HEN) and Rankine cycles for plants with demanding operational flexibility requirements. A general and systematic synthesis methodology has been developed to optimize simultaneously the utility systems, Rankine cycles and HENs considering different expected operating modes, seeking for the solution with the minimum Total Annual Costs (TAC). Heat exchangers have been modelled with different approaches depending on the type of control measure (with/without by-pass) in off-design operation. The problem is formulated as a challenging nonconvex MINLP and solved with a bilevel decomposition method, specifically developed to address this class of problems. We present the results of the proposed methodology applied to an extremely challenging problem, with 35 streams and 2 operating modes (periods), consisting in the design of an Integrated Gasification Combined Cycle (IGCC).

https://doi.org/10.1016/B978-0-12-823377-1.50250-0

Heat exchanger networks

→ still hard to solve → MINLP

→ Recent developments consider

- → More streams
- → Multiple periods

The model is based on the SYNHEAT superstructure (Yee and Grossmann, 1990) for the optimal design of heat exchanger networks. The SYNHEAT model is extended to include the streams of the heat recovery cycle, with variable mass flow rate. It should be noted that a steady state condition is assumed in each working period (i.e., no dynamics).

Recent developments in heat integration

Renewable and Sustainable Energy Reviews
Volume 98, December 2018, Pages 439-468

ELSEVIER

New directions in the implementation of Pinch Methodology (PM)

Jiří Jaromír Klemeš, Petar Sabev Varbanov, Timothy G. Walmsley, Xuexiu Jia

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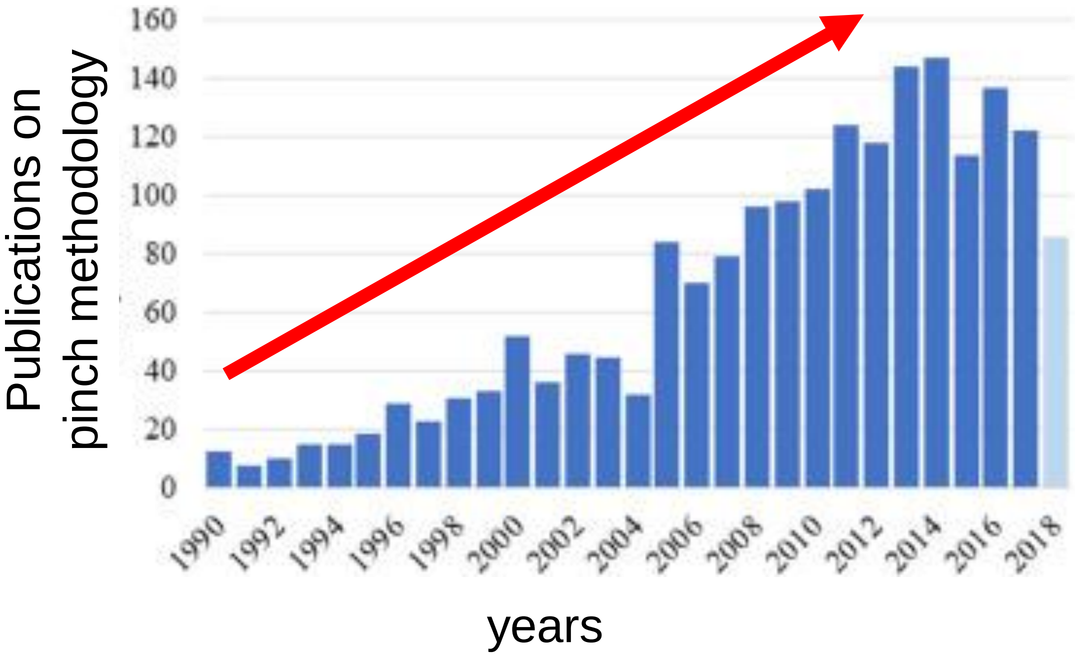
Highlights

- Pinch Analysis – more than 40 yr – systematic thermodynamic-based energy savings.
- Extended – including water, power, hydrogen, supply chains, emissions, Total Sites.
- Reviewed recent developments and suggested directions for future developments.
- Future steps: exploiting the synergy, extend locally integrated regions.
- As well as exergy, emergy, supply chains, targeting emissions and effluents.

https://www.sciencedirect.com/science/article/pii/S1364032118306798



Pinch Analysis

→ Recent developments consider further indicators

→ Lecture 6 (Life-Cycle Assessment)

→ Lecture 7 (Thermoeconomics)

→ Lecture 8 (Risk KPIs)

After this lecture, you will be able to…

- ✓ employ basic **solution methods** for **mixed-integer linear** (MILP) & **nonlinear programming** (MINLP) problems.
- ✓ find optimal heat-exchanger networks and near-optimal solutions with **integer cuts**
- discuss **(dis)advantages** of optimization problem classes

Optimization problem classes

constraints \ variables	continuous	continuous & discrete
linear	linear program (LP)	mixed-integer linear program (MILP)
nonlinear	nonlinear program (NLP)	mixed-integer nonlinear program (MINLP)

Lecture 3

today

Problem types and problem size

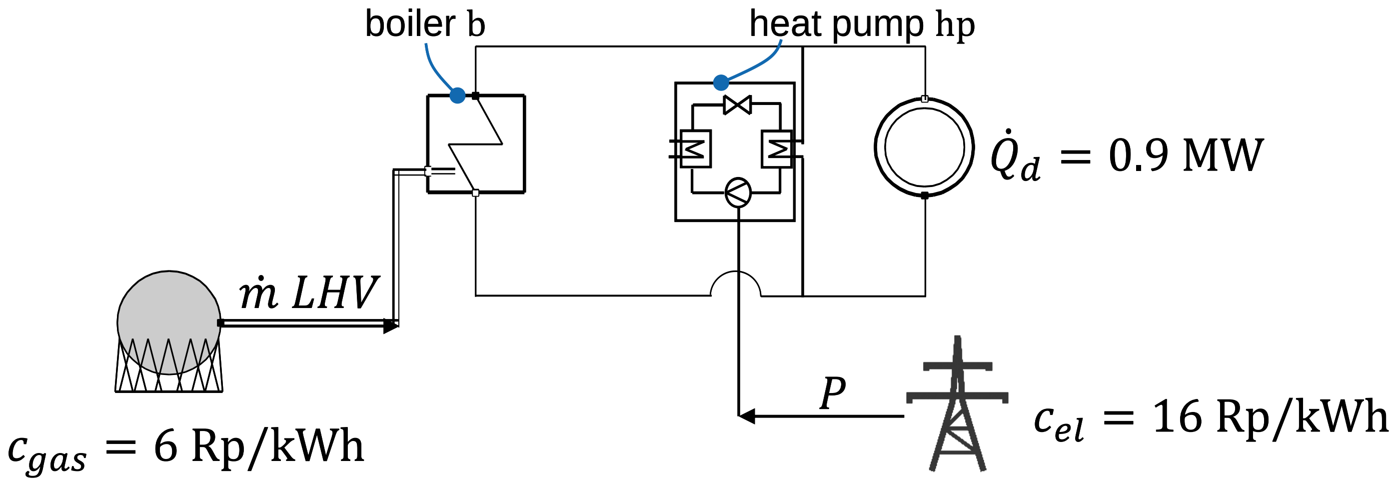
Leyffer-Linderoth-Luedtke (LLL) Complexity

Assuming a problem of type X with a number of Y decision variables:

LLL = The largest number of decision variables Y, for which at least one of the Professors Leyffer, Linderoth or Luedtke is willing to bet $50 that the problem of type X can be solved using a state-of-the-art solver.

	convex	non-convex
MINLP	500	100
NLP	$5 \cdot 10^4$	100
MILP	$2 \cdot 10^4$	-
LP	$5 \cdot 10^7$	-

Structural optimization of a heating system: Boiler or heat pump?



LINEAR

objective function

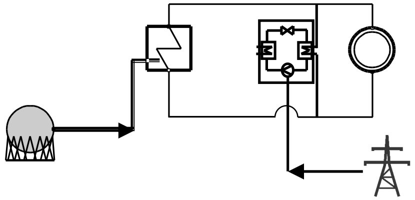
$$\min_{\substack{y_c, \dot{Q}_c,\\ c\in\{b,hp\}}} \ \mathrm{TAC} \ = \underbrace{\sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1}}_{\text{annualized capital cost}} + \underbrace{\int_{t=0}^{T} \left[c_{\mathrm{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\mathrm{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt}_{\text{cost of energy consumption}}$$

variables

$\dot{Q}_c \in \left[0, \dot{Q}_c^N\right], \forall\, c \in \{b, hp\}$ heating output of component i

$y_c \in \{0,1\}, \quad \forall\, c \in \{b, hp\}$ component i is purchased $(= 1)$ or not $(= 0)$

Structural optimization of a heating system: Boiler or heat pump?



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objective function

$$\min_{\substack{y_c, \dot{Q}_c,\\ c\in\{b,hp\}}} \ \mathrm{TAC} \ = \sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1} \quad + \int_{t=0}^{T} \left[c_{\text{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\text{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt$$

MINLP

constraints

$$s.t. \quad 0 \le \dot{Q}_c, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

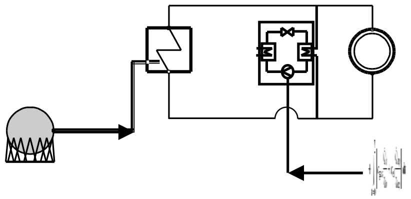
$$\dot{Q}_c \le \dot{Q}_c^N, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

$$\sum_c y_i\, \dot{Q}_c = \dot{Q}_d,$$

A single nonlinearity turns the whole problem into an MINLP!

Product of two variables is nonlinear!

Structural optimization of a heating system:
Boiler or heat pump?



$\dot{Q}_c \in \left[0, \dot{Q}_c^N\right], \forall\, c \in \{b, hp\}$ heating output of component i

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objective function

$$\min_{\substack{y_c, \dot{Q}_c,\\ c\in\{b,hp\}}} \ \text{TAC} = \sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1} + \int_{t=0}^{T} \left[c_{\text{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\text{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt$$

MINLP

constraints

$$s.t. \quad 0 \le \dot{Q}_c, \qquad \forall\, c \in \{\text{b}, \text{hp}\}$$

$$\dot{Q}_c \le \dot{Q}_c^N, \qquad \forall\, c \in \{\text{b}, \text{hp}\}$$

$$\sum_c y_i\, \dot{Q}_c = \dot{Q}_d,$$

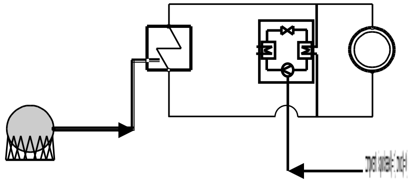
$$0 \le \dot{Q}_c, \qquad \forall\, c \in \{\text{b}, \text{hp}\}$$

$$\dot{Q}_c \le y_i\, \dot{Q}_c^N, \qquad \forall\, c \in \{\text{b}, \text{hp}\}$$

$$\sum_c \cancel{y_i}\, \dot{Q}_c = \dot{Q}_d,$$

Alternative formulation with $\dot{Q}_c^N$ as big-M parameter results in linear constraints.

Structural optimization of a heating system: Boiler or heat pump?



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objective function

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MILP

constraints

$$s.t. \qquad 0 \le \dot{Q}_c, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

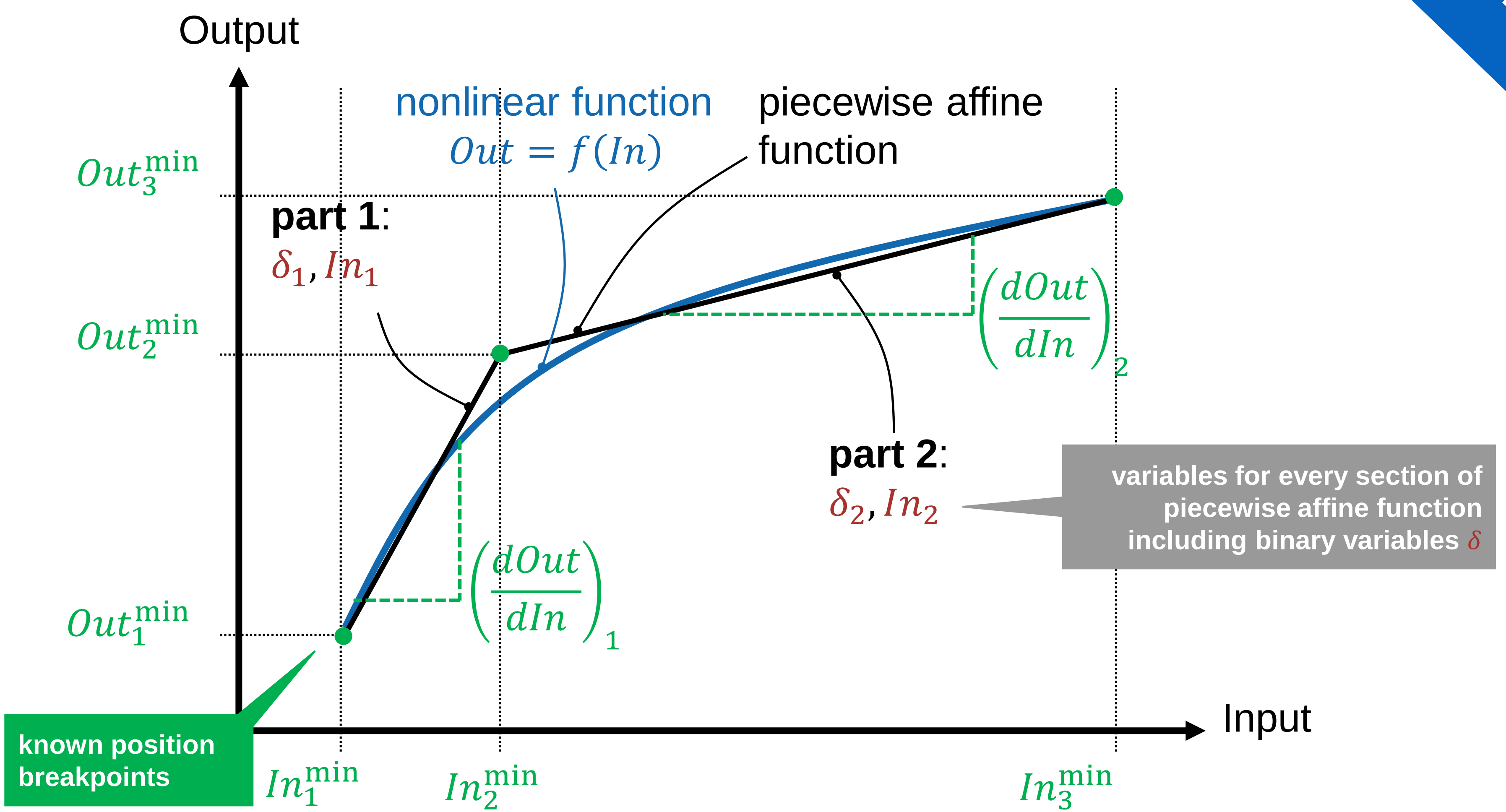
$$\dot{Q}_c \le y_i\, \dot{Q}_c^N, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

$$\sum_c \cancel{y_c}\, \dot{Q}_c = \dot{Q}_d,$$

Exact linearizations allow to transform nonlinear to linear problems ☺

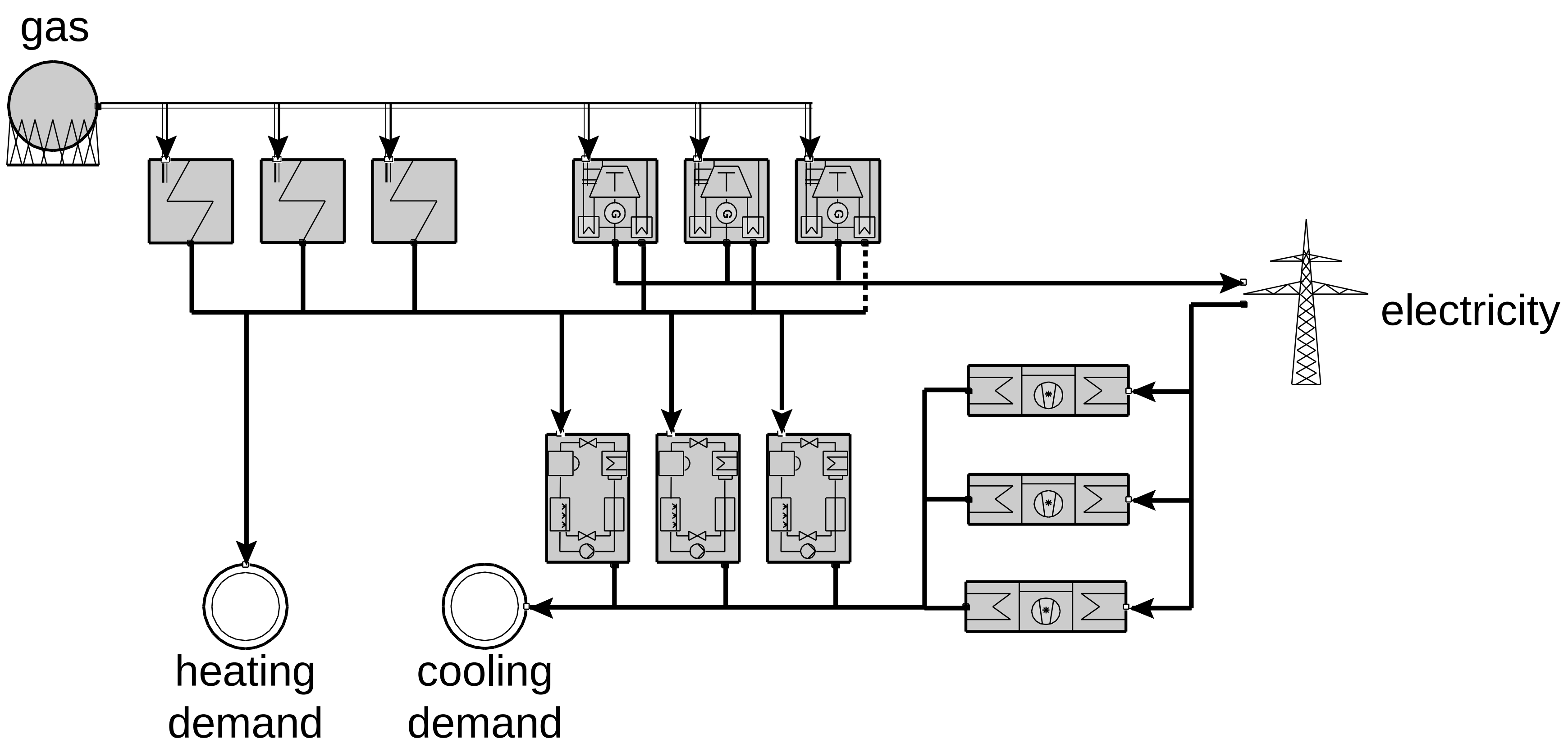
Approximating NLPs with MILPs – Piecewise affine formulation

More details on MILPs in Lectures 9-11!

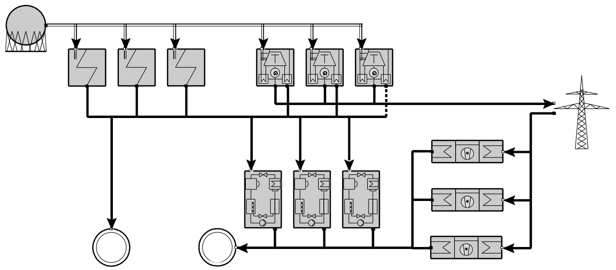


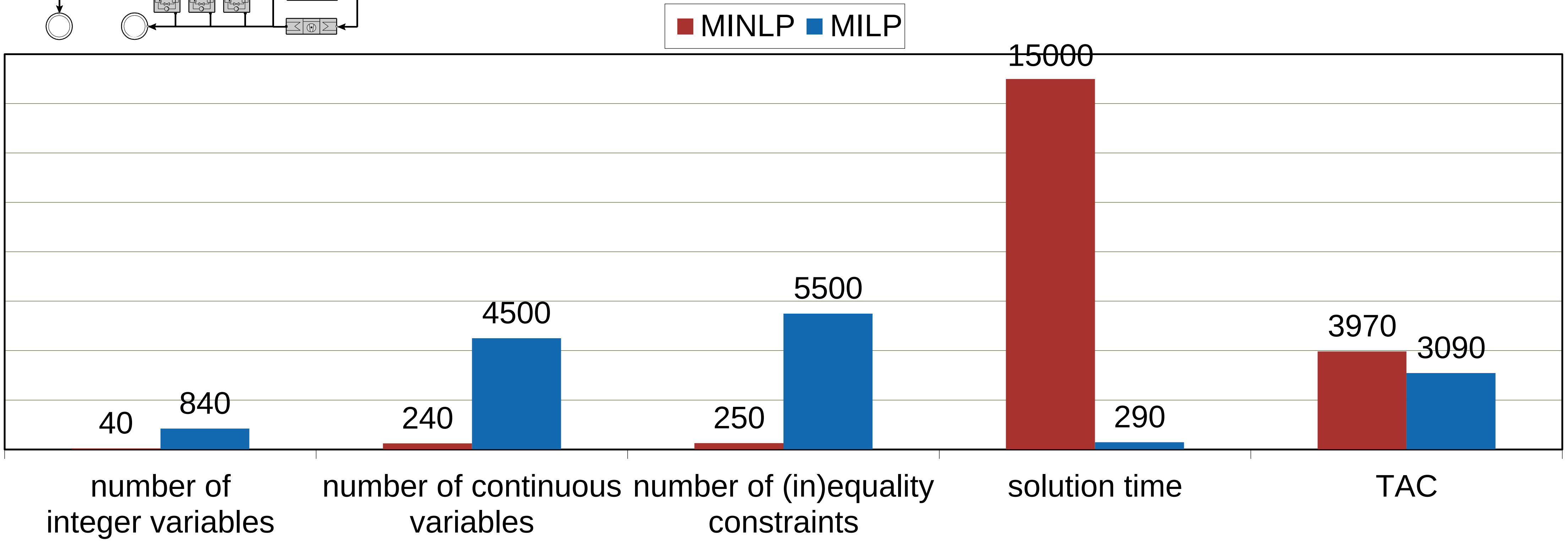
Nonlinear function can be approximated by piecewise-affine functions
⇒ no longer exact
⇒ usually introduces binary variables (but not always)

Solving MINLP vs. MILP – Piecewise linearization in practice



Solving MINLP vs. MILP – Piecewise linearization in practice





Problem class much more important than number of variables & equations

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