ETH zürich

epse ENERGY & PROCESS SYSTEMS ENGINEERING

Introduction to Modeling and Optimization of Sustainable Energy Systems:

Continuous Optimization

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D MAVT

Since the last lecture, you are able to…

- ✓ explain the idea underlying **the heat integration problem**
- ✓ apply the **pinch rules** to heat integration problems.
- ✓ thermodynamically analyze **heat exchangers** with the **pinch method**.
- ✓ integrate **external utilities** by using the grand composite curve
- ✓ interpret **heat integration as optimization problem**

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)	

After this lecture, you are able to…

- identify basic **elements of an optimization problem**.
- distinguish **linear problems** (LP) and **nonlinear problems** (NLP).
- use basic **solution methods** for both NLPs and LPs.
- formulate simple **energy system optimization problems (LP and NLP)**.

Mathematical model types
Summary

increasing complexity →

dimension	0D	1D, 2D, 3D
time	static	dynamic
variables	continuous	discrete
equations	linear	nonlinear
predictability	deterministic	stochastic

There is no single “right” model! The choice of model type depends on the problem at hand!

Optimization problem classes

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

today

in 2 weeks *Discrete Optimization*

Lecture 1: Mathematical modeling: Steam production

How much steam do we produce when boiling?

real system

✓ $\dot{m}_{Steam}$

unknown = **variables**	
known = **parameters**	

Balance equations:

$$0 = \dot{Q}_{stove} - \dot{m}_{Steam} \cdot h''(100\,°C, 1\,bar) - \dot{Q}_{loss}$$

$$\dot{Q}_{Stove} = \dot{m}_{gas} \cdot \Delta h_{gas}$$

$$\dot{Q}_{loss} = A_{\mathrm{w}} \cdot \alpha \cdot (T_{water} - \mathrm{T}_{envir})$$

Variables are only multiplied with parameters. All equations are linear!

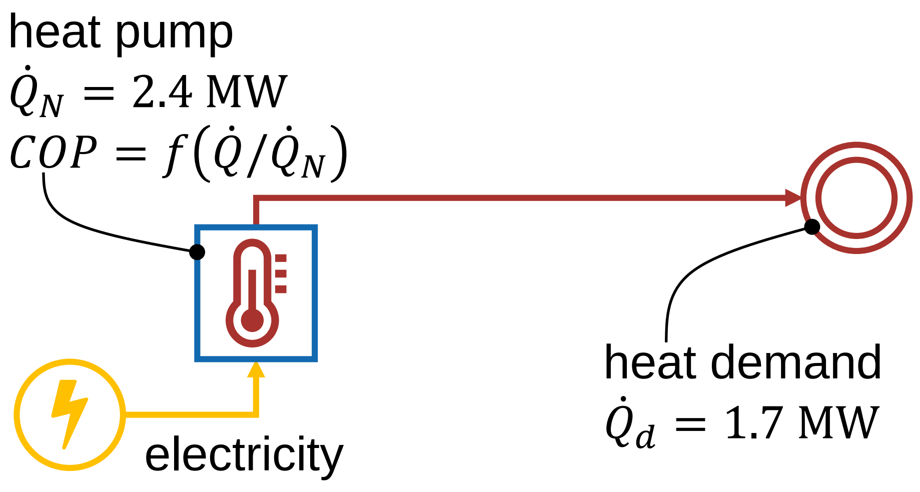
All variables are continuous

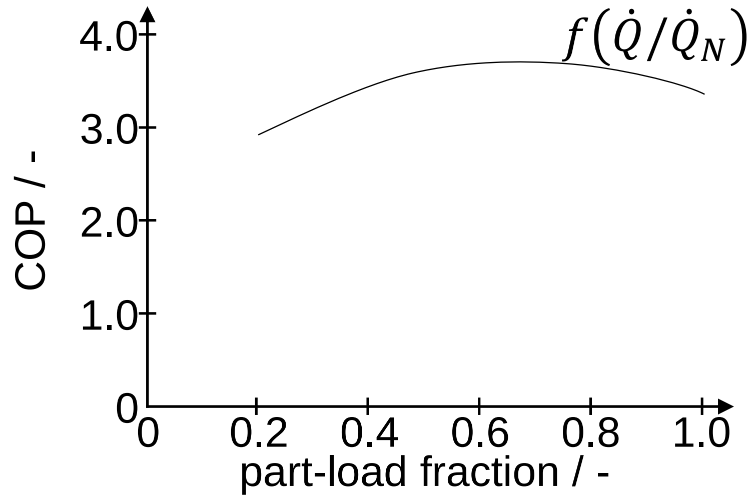
equations	linear
variables	continuous
dimension	0D
time	static
predictability	deterministic

Elements of continuous steady-state models

decision variables		$\boldsymbol{x}$	$\in \mathbb{R}^m$	values decision makers need to determine
constraints	equality	$h_i(\boldsymbol{x}) = 0$	$i = 1, \dots, o$	balance equations (*mass, energy*), component models (*characteristic curves*),…
	inequality	$g_j(\boldsymbol{x}) \leq 0$	$j = 1, \dots, n$	limitations (*physical, technical, mathematical, legal*)

Simulation example: Continuous steady-state model
How much electricity to satisfy heat demand?





System model

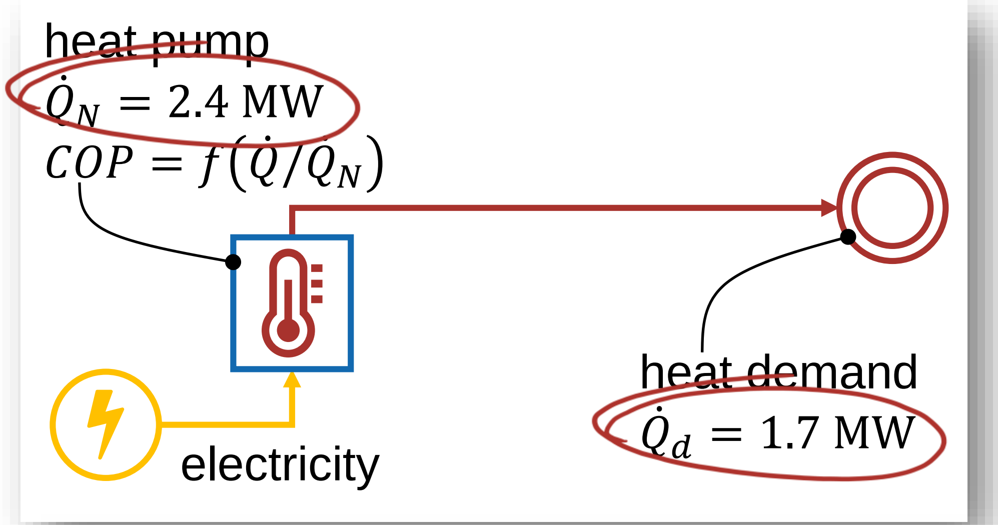
electricity demand

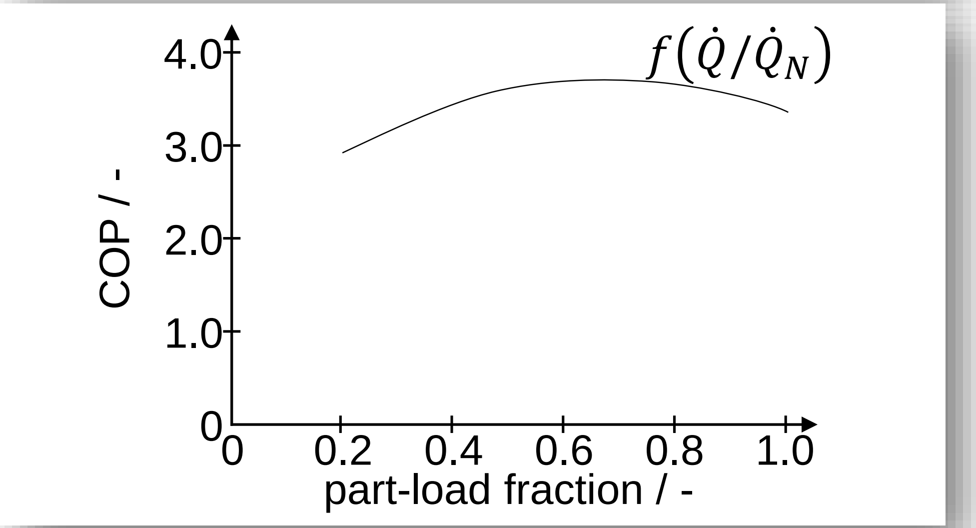
$$P = \frac{\dot{Q}}{COP}$$

additional constraints:

$$\dot{Q} - \dot{Q}_d = 0,$$
$$\dot{Q} \geq 0,$$
$$\dot{Q} \leq \dot{Q}_N,$$
$$COP = f(\underbrace{\dot{Q}/\dot{Q}_N}_{\text{part-load fraction}}),$$

Simulation example: Continuous steady-state model
How much electricity to satisfy heat demand





System model

electricity demand

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$$\dot{Q} \geq 0,$$
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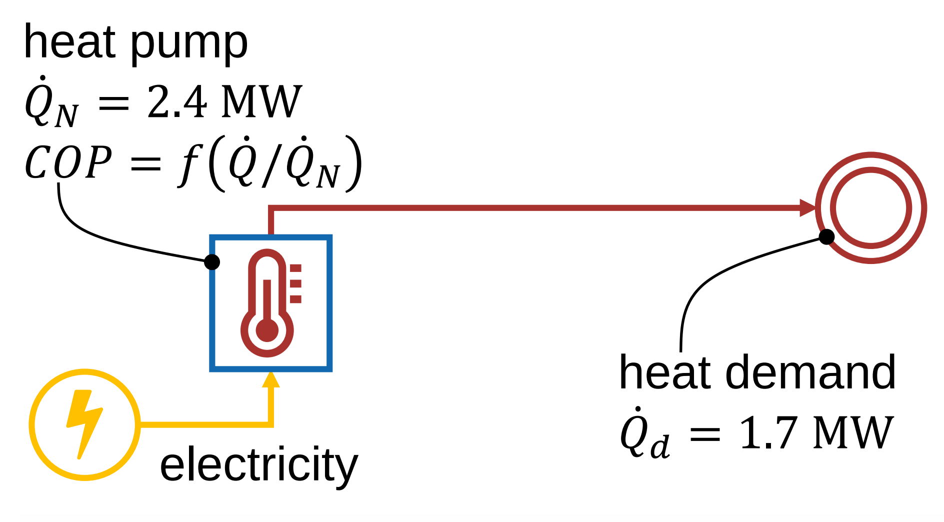
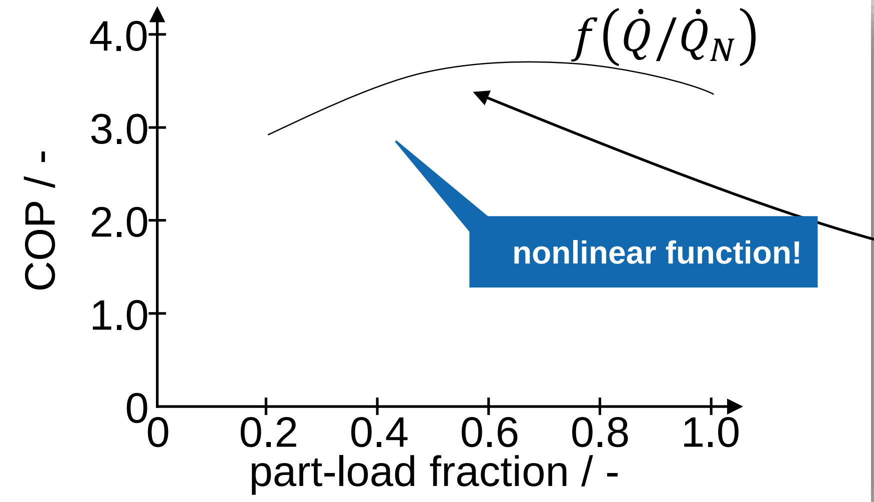
$$COP = f(\underbrace{\dot{Q}/\dot{Q}_N}_{\text{part-load fraction}}),$$

parameter

Simulation example: Continuous steady-state model
How much electricity to satisfy heat demand?





System model

electricity demand

$$P = \frac{\dot{Q}}{COP}$$

nonlinear: division of two variables!

additional constraints:

$$\dot{Q} - \dot{Q}_d = 0,$$
$$\dot{Q} \geq 0,$$
$$\dot{Q} \leq \dot{Q}_N,$$
$$COP = f(\underbrace{\dot{Q}/\dot{Q}_N}_{\text{part-load fraction}}),$$

part-load fraction

variable
parameter

Simulation example: Continuous steady-state model
Degree of freedom analysis

Degree of freedom d of a model
is the difference of number of variables n_x
and number of independent equations n_e.

$$d = n_x - n_e$$

independent equations: 3
variables: 3 $(P, \dot{Q}, COP)$

degree of freedom: $d = 3 - 3 = 0$

$d = 0$:
There is a unique solution!

System model

electricity demand

$$P = \frac{\dot{Q}}{COP}$$

additional constraints:

$$\dot{Q} - \dot{Q}_d = 0,$$
$$\dot{Q} \geq 0,$$
$$\dot{Q} \leq \dot{Q}_N,$$
$$COP = f\left(\dot{Q}/\dot{Q}_N\right),$$

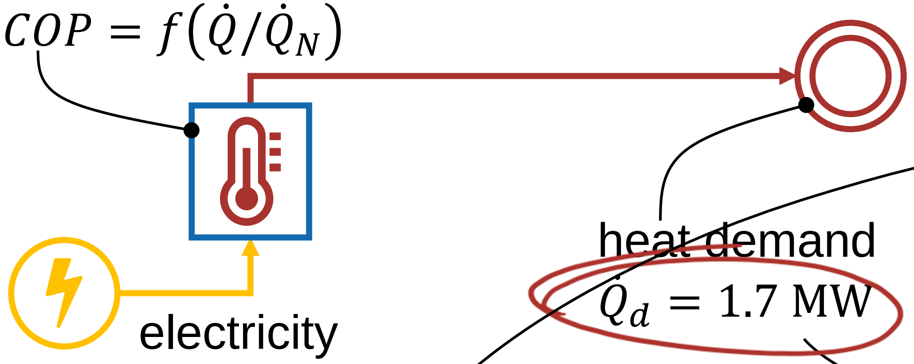
x: variable
x: parameter

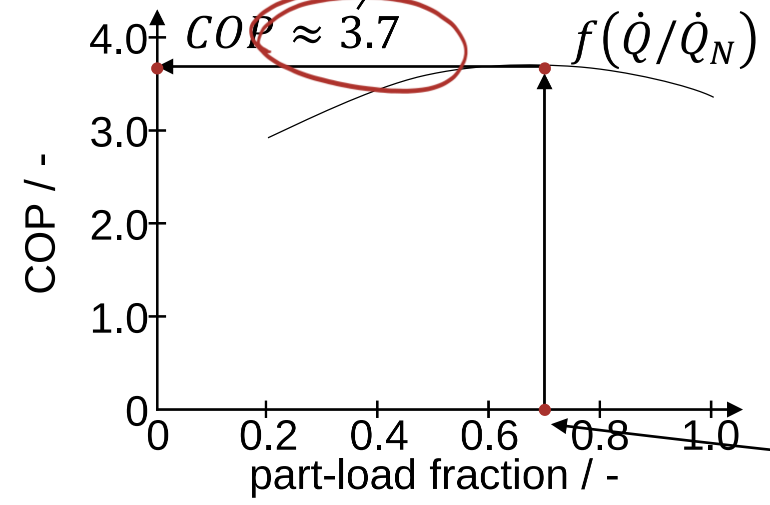
Simulation example: Continuous steady-state model
How much electricity to satisfy heat demand?

heat pump

$\dot{Q}_N = 2.4\ \mathrm{MW}$

$COP = f(\dot{Q}/\dot{Q}_N)$





System model

Our simulation model predicts a primary energy demand of 0.46 MW.

electricity demand

$$P = \frac{\dot{Q}}{COP}$$

$$P = 1.7\ \mathrm{MW}/3.7 = 0.46\ \mathrm{MW}$$

additional constraints:

$$\dot{Q} - \dot{Q}_d = 0, \quad \Rightarrow \dot{Q} = 1.7\ \mathrm{MW}$$

$$\dot{Q} \geq 0,$$

$$\dot{Q} \leq \dot{Q}_N,$$

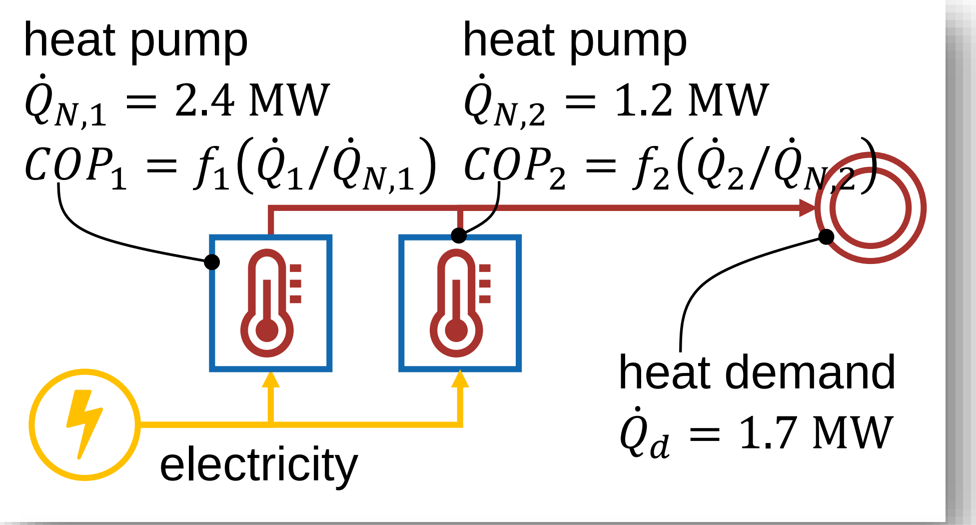
$$COP = f(\dot{Q}/\dot{Q}_N),$$

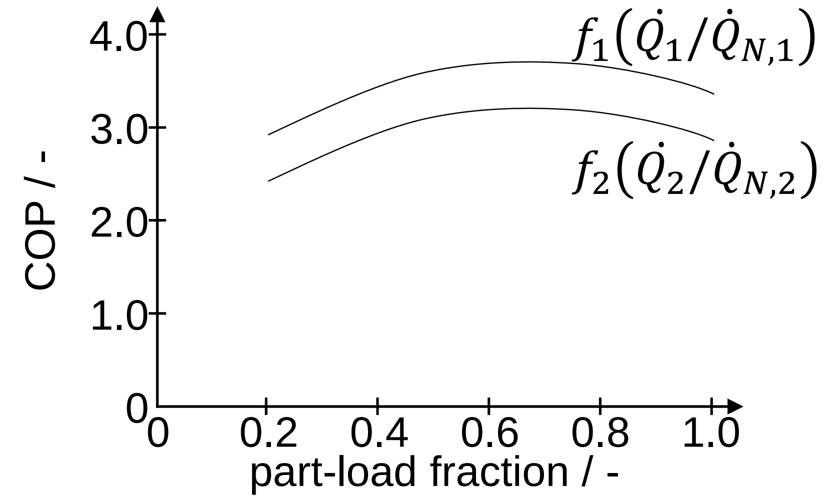
$$\dot{Q}/\dot{Q}_N = 1.7\ \mathrm{MW}/2.4\ \mathrm{MW} \approx 0.71$$

variable

parameter

Optimization example: Continuous steady-state model
How much electricity to satisfy heat demand?





System model

$$P = \underbrace{\frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

$$\begin{aligned}
&\dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0,\\
&\dot{Q}_1 \geq 0,\\
&\dot{Q}_2 \geq 0,\\
&\dot{Q}_1 \leq \dot{Q}_{N,1},\\
&\dot{Q}_2 \leq \dot{Q}_{N,2},\\
&COP_1 = f_1(\dot{Q}_1/\dot{Q}_{N,1}),\\
&COP_2 = f_2(\dot{Q}_2/\dot{Q}_{N,2})
\end{aligned}$$

variable
parameter

Degree of freedom analysis

Degree of freedom d of a model
is the difference of number of variables n_x
and number of independent equations n_e.

$$d = n_x - n_e$$

independent equations: 4

variables: 5 $(P, \dot{Q}_1, \dot{Q}_2, COP_1, COP_2)$

degree of freedom: $d = 5 - 4 = 1$

$d > 0$:
There is no unique solution!
Which one of many solutions is the best?

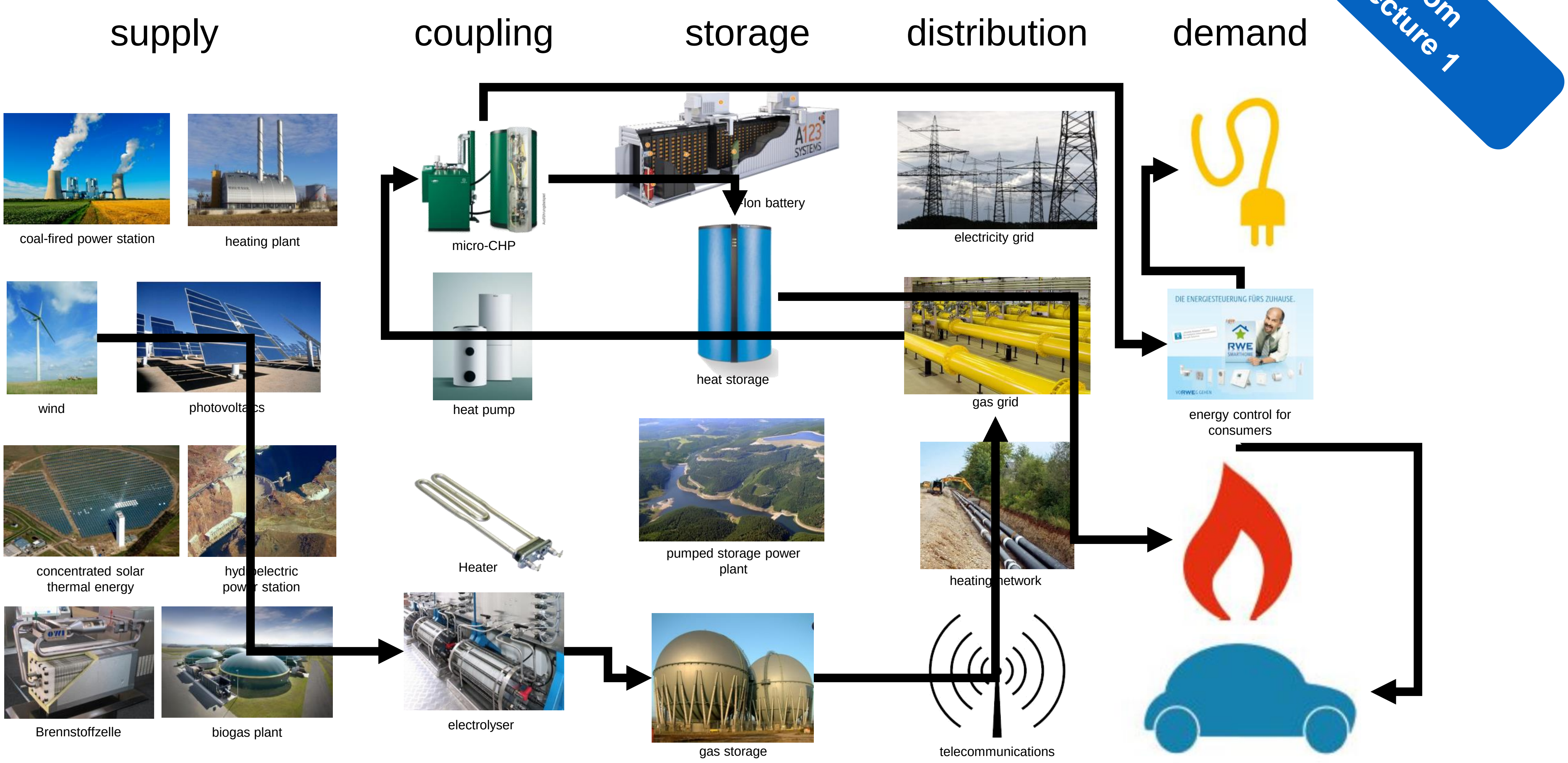
System model

$$\underbrace{P = \frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

$$\dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0,$$
$$\dot{Q}_1 \geq 0,$$
$$\dot{Q}_2 \geq 0,$$
$$\dot{Q}_1 \leq \dot{Q}_{N,1},$$
$$\dot{Q}_2 \leq \dot{Q}_{N,2},$$
$$COP_1 = f_1(\dot{Q}_1/\dot{Q}_{N,1}),$$
$$COP_2 = f_2(\dot{Q}_2/\dot{Q}_{N,2})$$

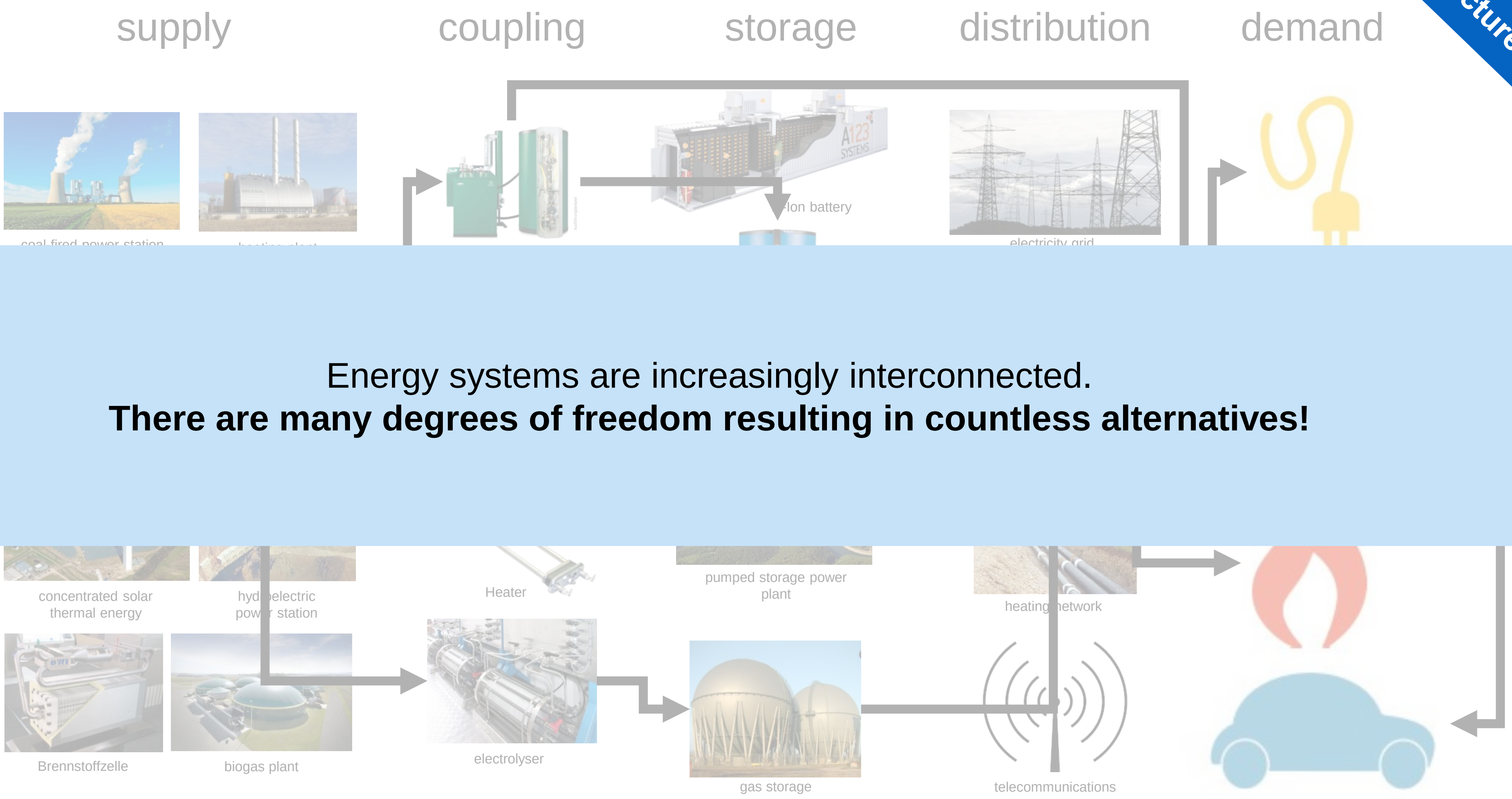
variable
parameter

Energy systems today: Which one of many solutions is the best?



Energy systems today: Which one of many solutions is the best?

From Lecture 1



Energy systems are increasingly interconnected.
There are many degrees of freedom resulting in countless alternatives!

Elements of continuous **optimization problems**

If there is no unique solution, optimize to find the best one!

objective function		z	$\mathbb{R}^m \rightarrow \mathbb{R}$	quantity to be minimized/maximized
decision variables		$\boldsymbol{x}$	$\in \mathbb{R}^m$	values decision makers need to determine
constraints	equality	$h_i(\boldsymbol{x}) = 0$	$i = 1, \dots, o$	balance equations (*mass, energy*), component models (*characteristic curves*),…
	inequality	$g_j(\boldsymbol{x}) \leq 0$	$j = 1, \dots, n$	limitations (*physical, technical, mathematical, legal*)

objective function		z	$\mathbb{R}^m \rightarrow \mathbb{R}$	quantity to be minimized/maximized
decision variables		$\boldsymbol{x}$	$\in \mathbb{R}^m$	values decision makers need to determine
constraints	equality	$h_i(\boldsymbol{x}) = 0$	$i = 1, \dots, o$	balance equations (*mass, energy*), component models (*characteristic curves*),…
	inequality	$g_j(\boldsymbol{x}) \leq 0$	$j = 1, \dots, n$	limitations (*physical, technical, mathematical, legal*)

we write

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

$$\min_x z = \max_x(-z)$$

"subject to"

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

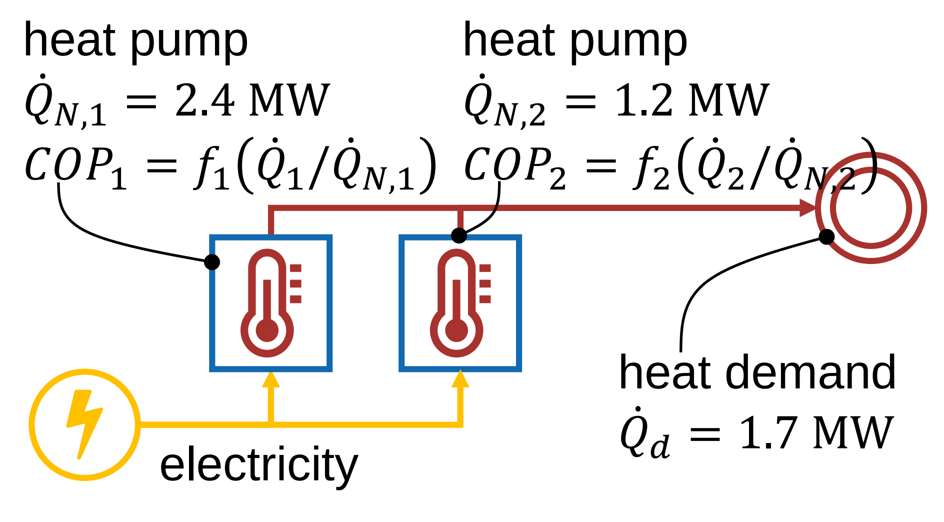
Discussion

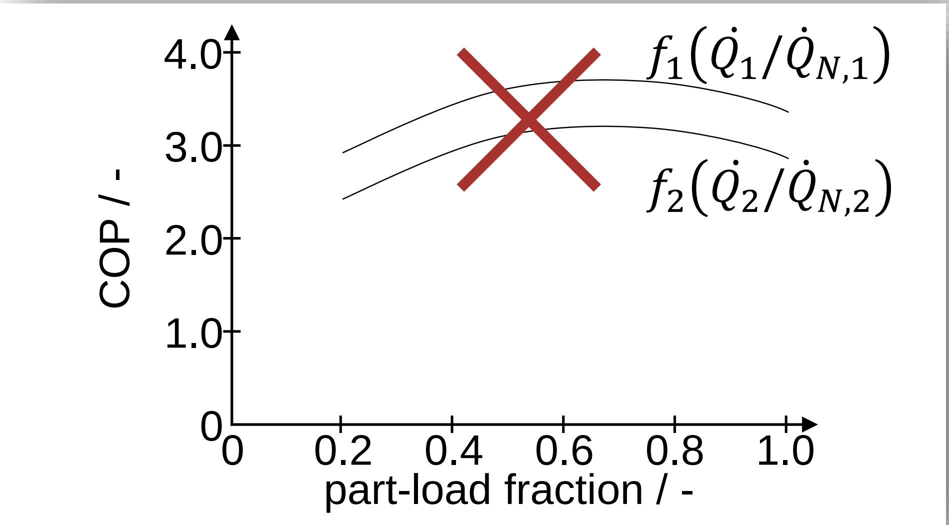
The lead engineer of an energy company has designed an efficient heat pump for residential use. The engineer wants to estimate the gas savings of the heat pump compared to an existing boiler. Therefore, the engineer models the boiler to calculate electricity demand based on the measured heating demand of a typical household throughout a year.

Which of the following statements is false?

- **a** Mass balances in the model of the heat pump can be modeled as equality constraints.
- **b** The maximum electricity input of the heat pump can be modeled using an inequality constraint.
- **c** The objective function is to minimize the consumption of electricity throughout the year.
- **d** The measured heating demand of the household is a parameter in the model.

Optimization example: Continuous steady-state model
How much electricity to satisfy heat demand?





Optimization problem

objective function:

$$P = \underbrace{\frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

constraints:

$$
\begin{aligned}
\text{s.t.} \quad & \dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0, \\
& \dot{Q}_1 \geq 0, \\
& \dot{Q}_2 \geq 0, \\
& \dot{Q}_1 \leq \dot{Q}_{N,1}, \\
& \dot{Q}_2 \leq \dot{Q}_{N,2}, \\
& COP_1 = f_1(\cancel{\dot{Q}_1/\dot{Q}_{N,1}}), \\
& COP_2 = f_2(\cancel{\dot{Q}_2/\dot{Q}_{N,2}})
\end{aligned}
$$

For simplicity, assume constant COP $COP_1 = 3.5,\ COP_2 = 2.7$

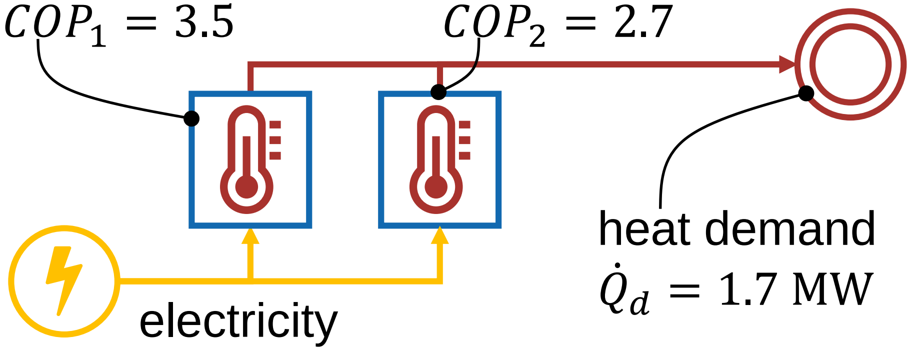
variable

parameter

Optimization example: Continuous linear steady-state model
How much electricity to satisfy heat demand?

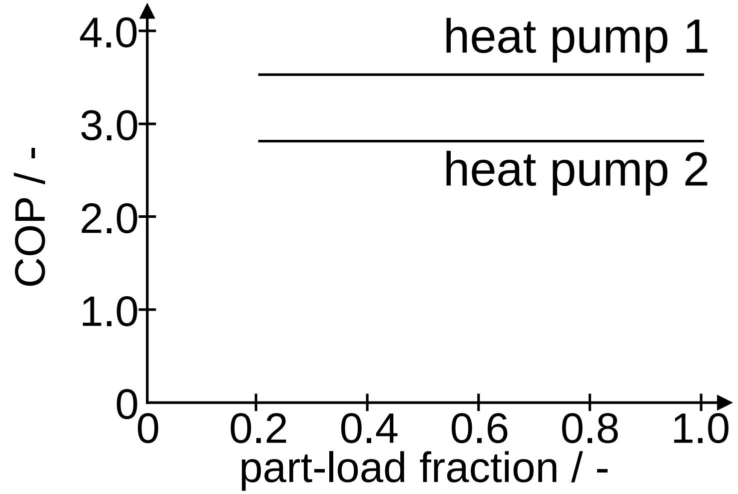
heat pump
$\dot{Q}_{N,1} = 2.4$ MW
$COP_1 = 3.5$

heat pump
$\dot{Q}_{N,2} = 1.2$ MW
$COP_2 = 2.7$



heat demand
$\dot{Q}_d = 1.7$ MW

electricity



Optimization problem

objective function:

$$P = \underbrace{\frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

linear!

constraints:

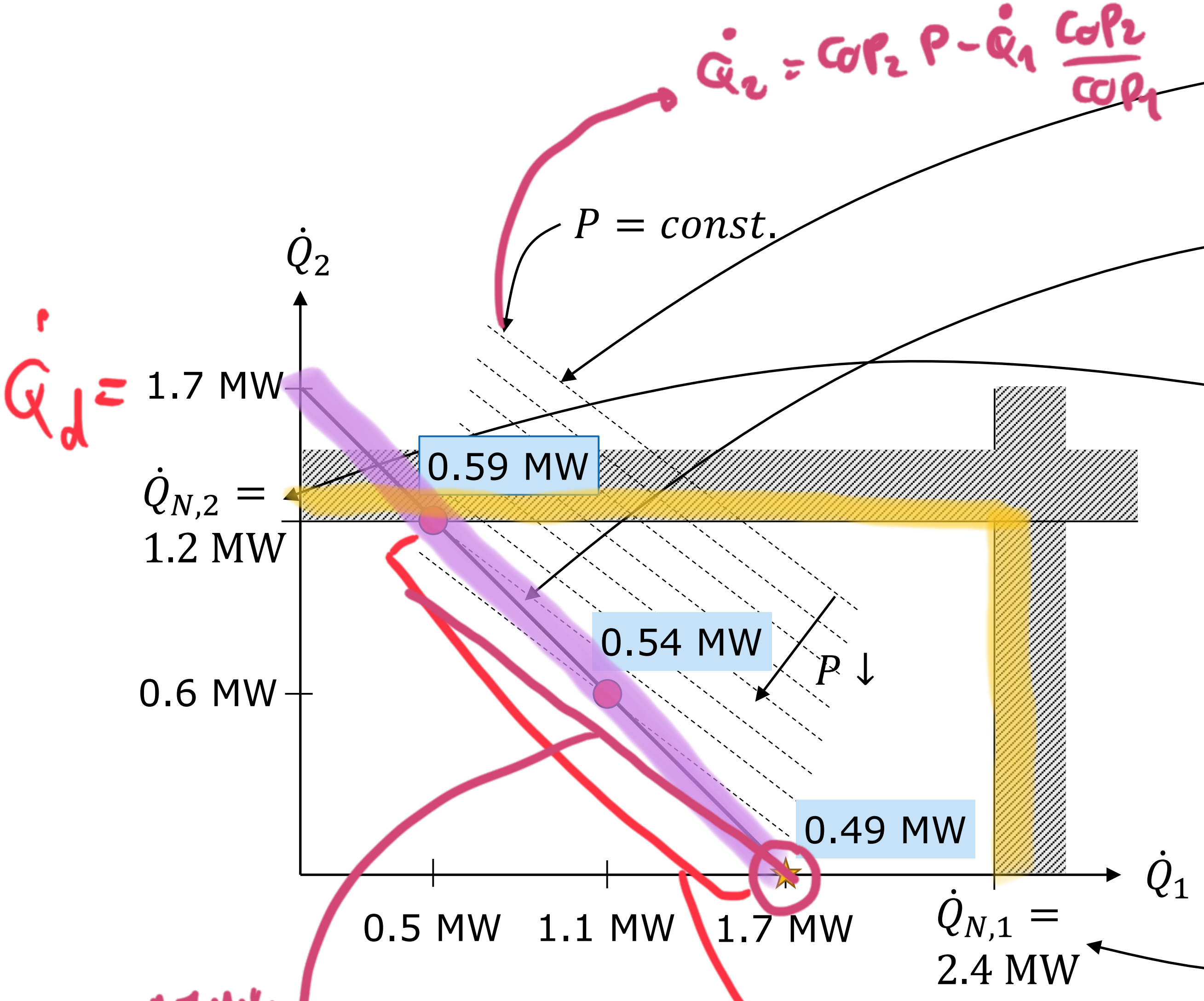
$$\text{s.t.} \quad \dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0,$$
$$\dot{Q}_1 \geq 0,$$
$$\dot{Q}_2 \geq 0,$$
$$\dot{Q}_1 \leq \dot{Q}_{N,1},$$
$$\dot{Q}_2 \leq \dot{Q}_{N,2},$$
$$COP_1 = 3.5,$$
$$COP_2 = 2.7$$

Degree of freedom is still 1.
Check for yourself!

variable
parameter

linear!

Mini-example: Graphical solution method



$$\min_{\dot{Q}_1,\dot{Q}_2} P = \frac{\dot{Q}_1}{COP_1} + \frac{\dot{Q}_2}{COP_2}$$

$$\text{s.t.} \quad \dot{Q}_1 + \dot{Q}_2 - \underbrace{\dot{Q}_d}_{1.7\,\text{MW}} = 0,$$
$$\dot{Q}_1 \geq 0,$$
$$\dot{Q}_2 \geq 0,$$
$$\dot{Q}_1 \leq \dot{Q}_{N,1},$$
$$\dot{Q}_2 \leq \dot{Q}_{N,2},$$
$$COP_1 = 3.5,$$
$$COP_2 = 2.7$$

1,7 MW
↳ [illegible]

All solutions in this interval or line

Linear programming (LP)

Properties

- ✓ all variables continuous
- ✓ all functions f linear:

↳ $y = mx + q$

Linear program (LP)

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

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

$$E\boldsymbol{x} = \boldsymbol{f}$$

$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{c} \in \mathbb{R}^m,$$
$$A \in \mathbb{R}^{n \times m}, \boldsymbol{b} \in \mathbb{R}^n,$$
$$E \in \mathbb{R}^{o \times m}, \boldsymbol{f} \in \mathbb{R}^o$$

cost coefficients

$$z = c_1 x_1 + c_2 x_2 + \dots + c_m x_m$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & \ddots & & \vdots \\ \vdots & & & \\ a_{n1} & \cdots & & a_{nm} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} \leq \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\begin{pmatrix} e_{11} & e_{12} & \cdots & e_{1m} \\ e_{21} & \ddots & & \vdots \\ \vdots & & & \\ e_{o1} & \cdots & & e_{om} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_o \end{pmatrix}$$

$$\min_{\dot{Q}_1, \dot{Q}_2} P = \underbrace{\frac{\dot{Q}_1}{COP_1} + \frac{\dot{Q}_2}{COP_2}}_{\text{const.}}$$

s.t.

$$\dot{Q}_1 \geq 0,$$
$$\dot{Q}_2 \geq 0,$$
$$\dot{Q}_1 \leq \dot{Q}_{N,1},$$
$$\dot{Q}_2 \leq \dot{Q}_{N,2},$$
$$\dot{Q}_1 + \dot{Q}_2 - \underbrace{\dot{Q}_d}_{1.7\text{ MW}} = 0,$$

LINEAR PROGRAM

$$\min_{\dot{Q}_1, \dot{Q}_2} P = \frac{1}{COP_1}\dot{Q}_1 + \frac{1}{COP_2}\dot{Q}_2$$

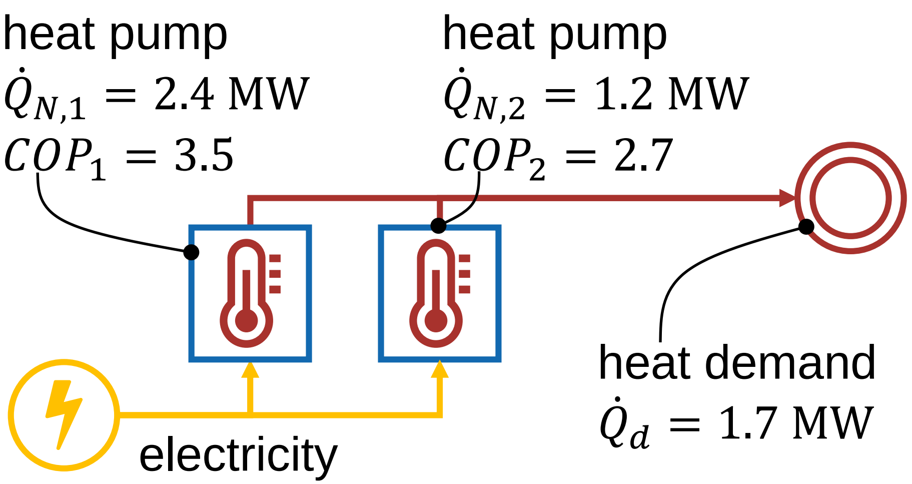
s.t.

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \dot{Q}_1 \\ \dot{Q}_2 \end{pmatrix} \leq \begin{pmatrix} 0 \\ 0 \\ \dot{Q}_{N,1} \\ \dot{Q}_{N,2} \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} \dot{Q}_1 \\ \dot{Q}_2 \end{pmatrix} = \begin{pmatrix} \dot{Q}_d \end{pmatrix}$$

$Ax \leq b$
$Ex \geq f$
$Ex \leq f$

LP in practice?

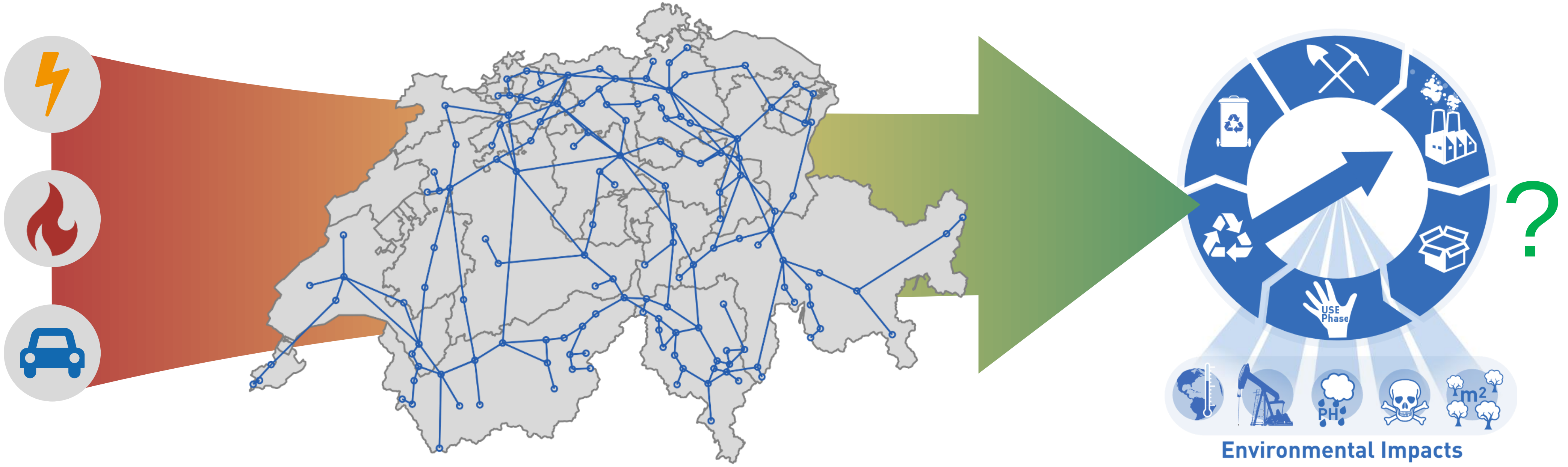


$$\min_{\dot{Q}_1,\dot{Q}_2} P = \frac{\dot{Q}_1}{COP_1} + \frac{\dot{Q}_2}{COP_2}$$

$$\begin{aligned}
\text{s.t.} \quad & \dot{Q}_1 + \dot{Q}_2 - \underbrace{\dot{Q}_d}_{1.7\ \mathrm{MW}} = 0, \\
& \dot{Q}_1 \geq 0, \\
& \dot{Q}_2 \geq 0, \\
& \dot{Q}_1 \leq \dot{Q}_{N,1}, \\
& \dot{Q}_2 \leq \dot{Q}_{N,2}, \\
& COP_1 = 3.5, \\
& COP_2 = 2.7
\end{aligned}$$

? Are linear problems (LPs) actually useful?

Transition of the Swiss energy system to net-zero emissions



minimize **total annualized costs**
reduce operational **GHG emissions** to zero by 2050

Transition of the Swiss energy system to net-zero emissions

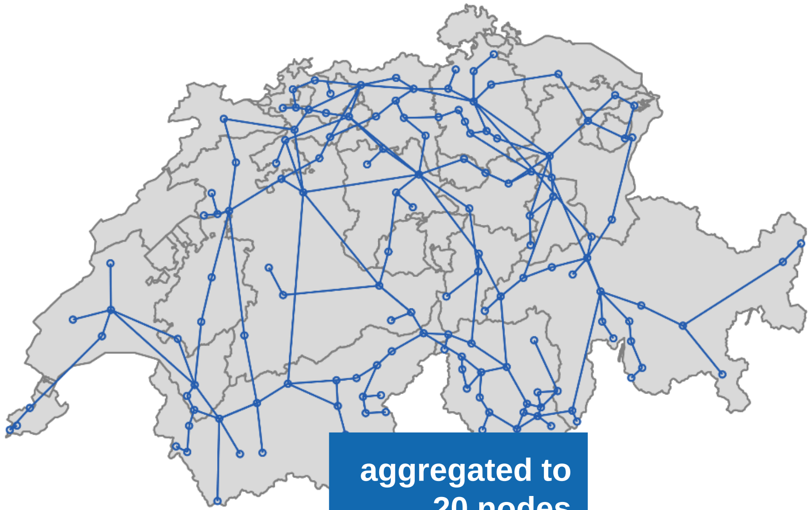
sectors

electricity
- 10 generation technologies
- power-to-fuel
- direct air capture

building & industrial heat
- 5 heating technologies
- industrial heat on three temperature levels

private mobility
- 5 transport technologies
- fossil- or electricity based

resolution



aggregated to 20 nodes

- 148 nodes connected by transmission grid
- 8760 time steps
- island system

aggregated to 120 typical time steps

life cycle assessment

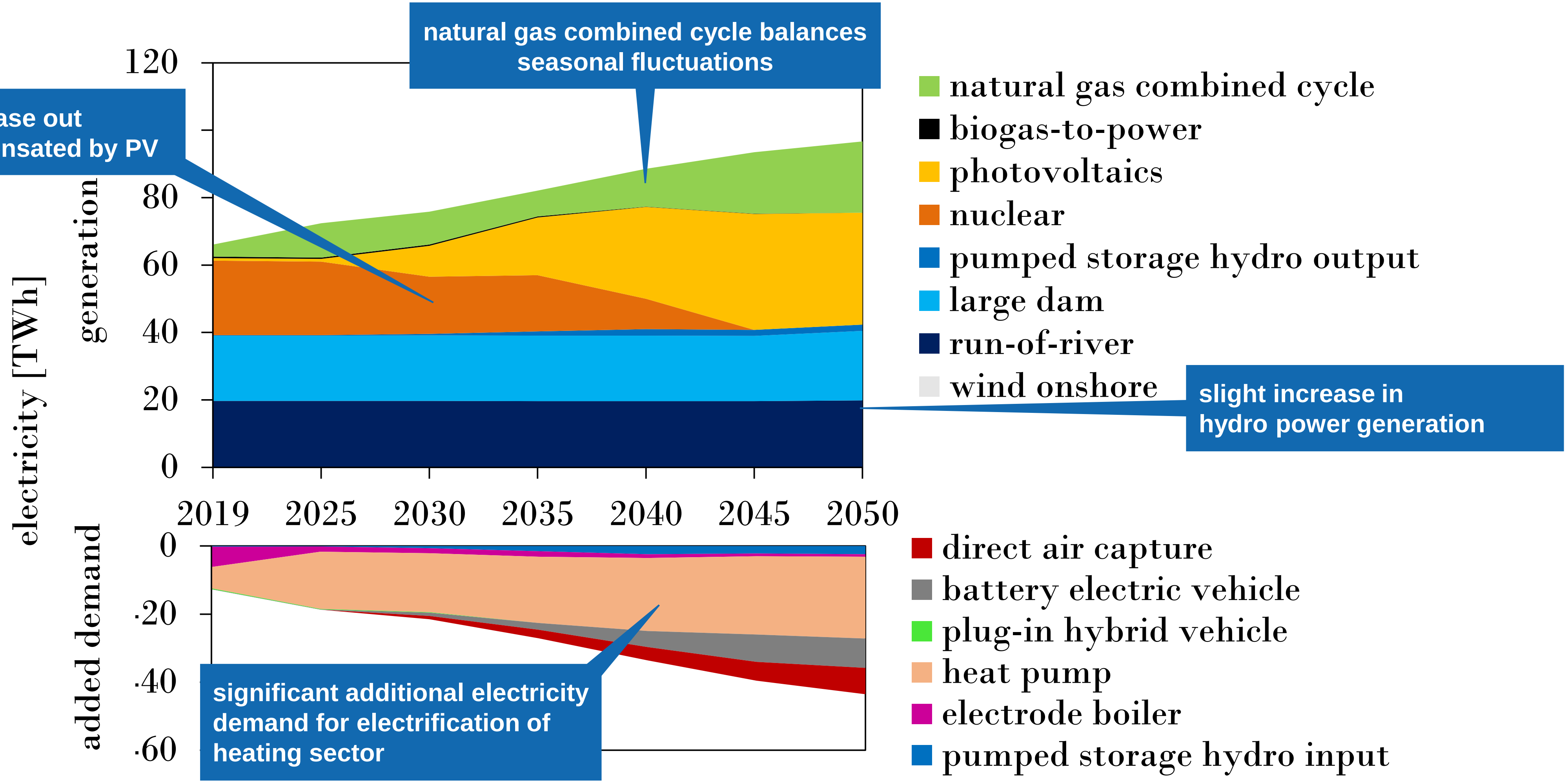
based on ecoinvent 3.7.1

Impact categories based on Environmental Footprint

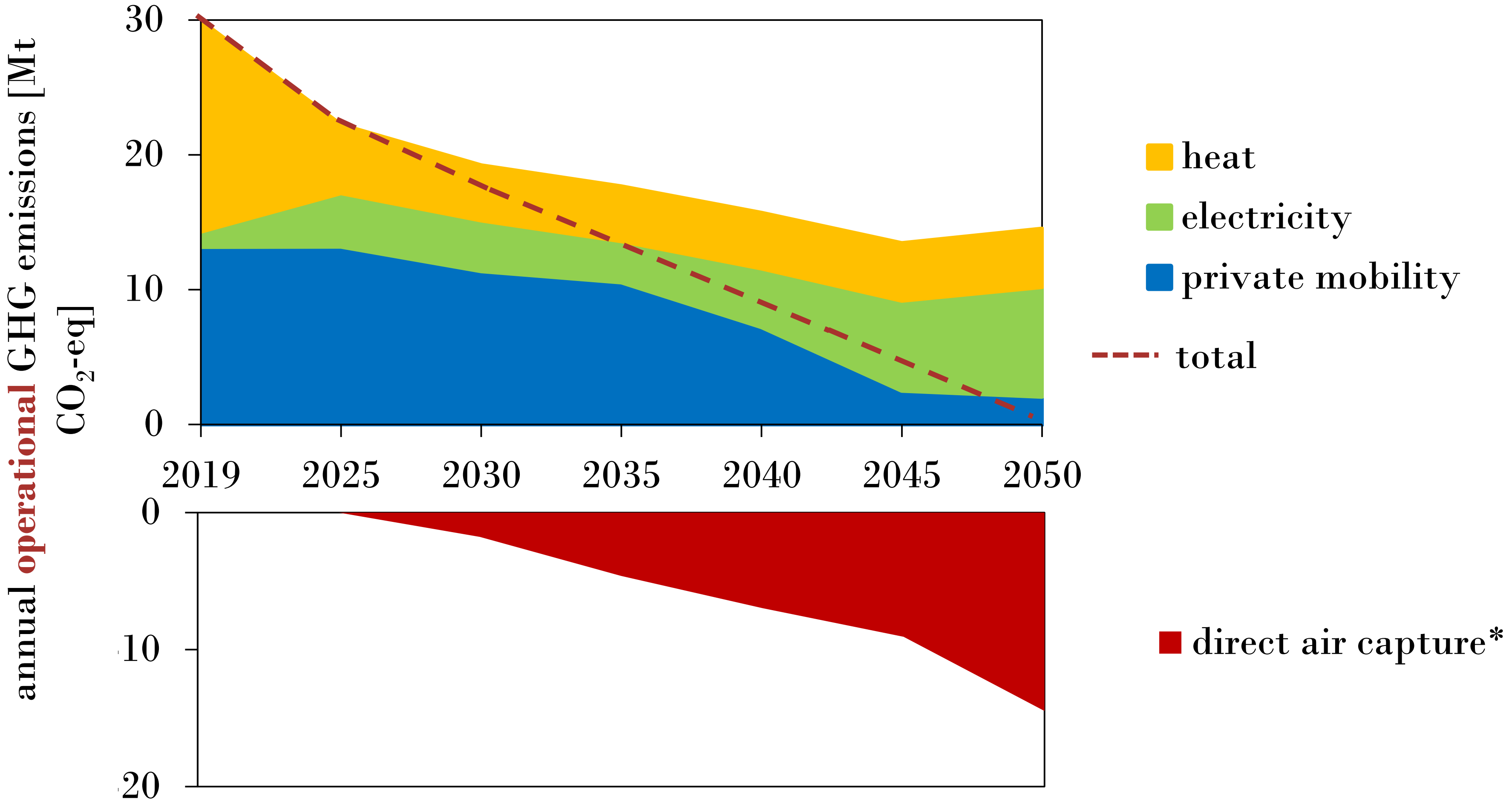
operational GHG emission reduced to net-zero by 2050

Reinert et al. *Optimization of Regionally Resolved Energy Systems by Spatial Aggregation and Disaggregation. In* 16. Symposiu -12 - 2020-02-14.
Bahl et al. *Rigorous synthesis of energy systems by decomposition via time-series aggregation.* In *Comput Chem Eng 2018;*112:70–81.

Electricity sector transformation driven by PV & natural gas

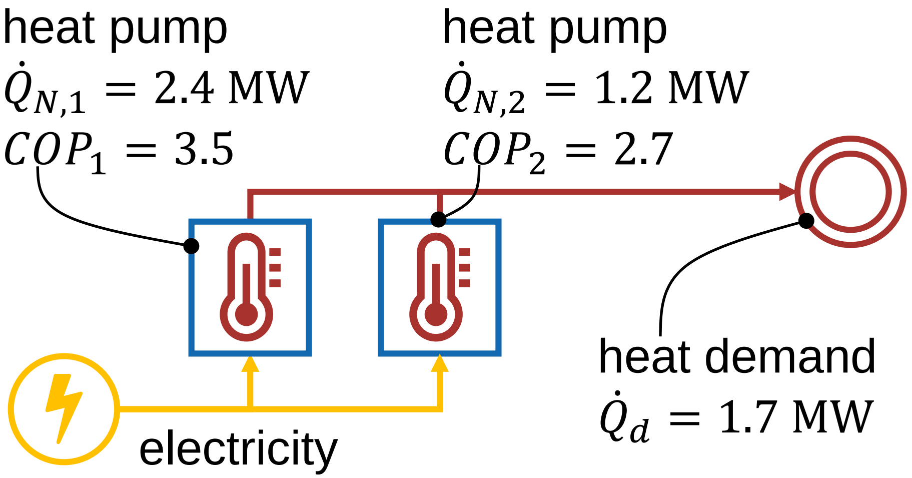


Net-zero scenario relies on natural gas combined cycle & DAC



* Deutz and Bardow *Life-cycle assessment of an industrial direct air capture process based on temperature–vacuum swing adsorption*. Nature Energy 2021;6(2):203–13.
Fasihi et al. *Techno-economic assessment of CO2 direct air capture plants*. Journal of Cleaner Production 2019;224:957–80.

LP in practice?



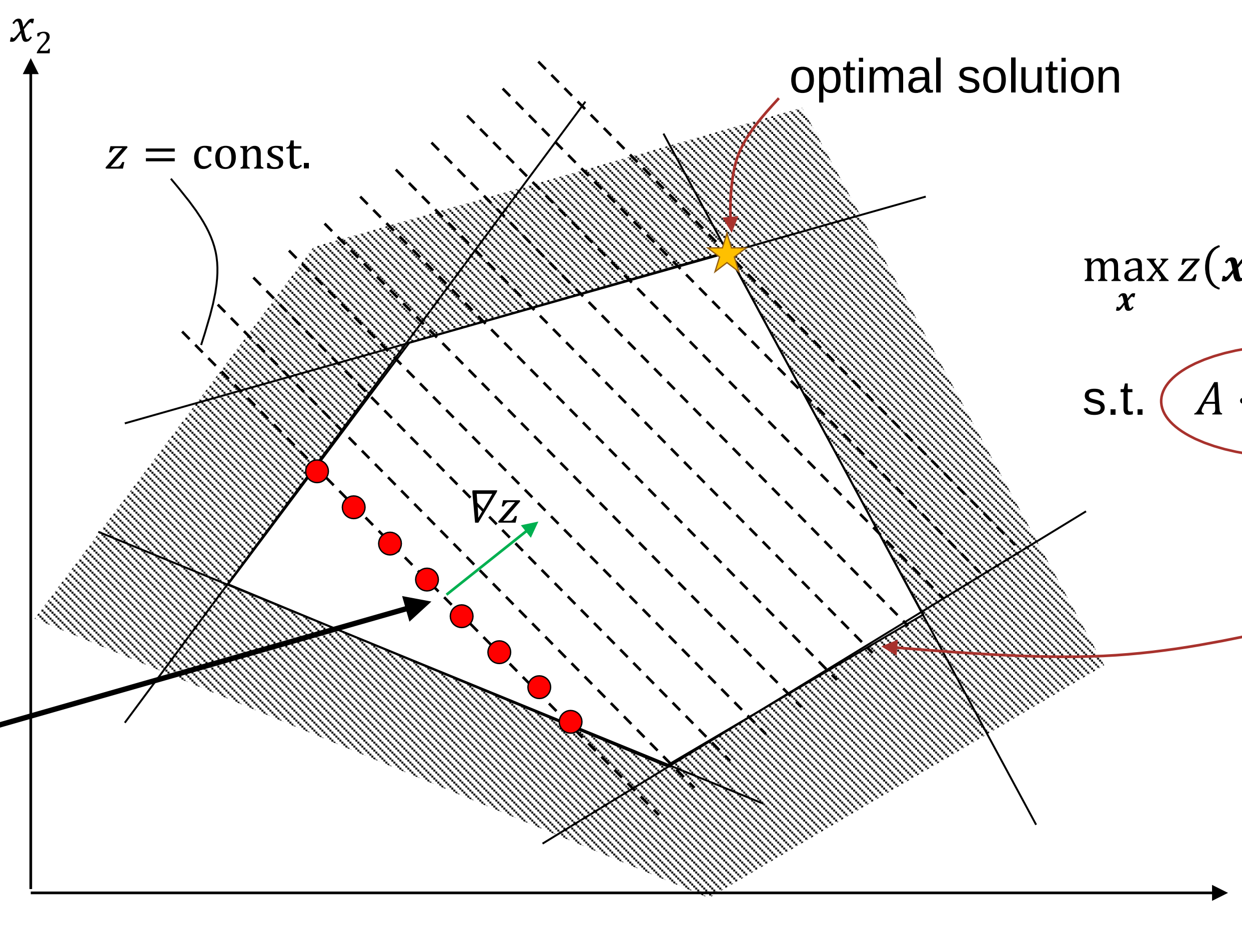
$$\min_{\dot{Q}_1,\dot{Q}_2} P = \frac{\dot{Q}_1}{COP_1} + \frac{\dot{Q}_2}{COP_2}$$

$$\begin{aligned}
\text{s.t.} \quad & \dot{Q}_1 + \dot{Q}_2 - \underbrace{\dot{Q}_d}_{1.7\text{ MW}} = 0, \\
& \dot{Q}_1 \geq 0, \\
& \dot{Q}_2 \geq 0, \\
& \dot{Q}_1 \leq \dot{Q}_{N,1}, \\
& \dot{Q}_2 \leq \dot{Q}_{N,2}, \\
& COP_1 = 3.5, \\
& COP_2 = 2.7
\end{aligned}$$

? **Are linear problems (LPs) actually useful?** ✓

? **Do LPs always have a (unique) solution?**

Solving linear programming problems (unique solution)



$$\max_{\boldsymbol{x}} z(\boldsymbol{x}) = c_1 x_1 + c_2 x_2$$

s.t. $A \cdot \boldsymbol{x} \leq \boldsymbol{b}$

"solution-polyhedron"
(feasible region)

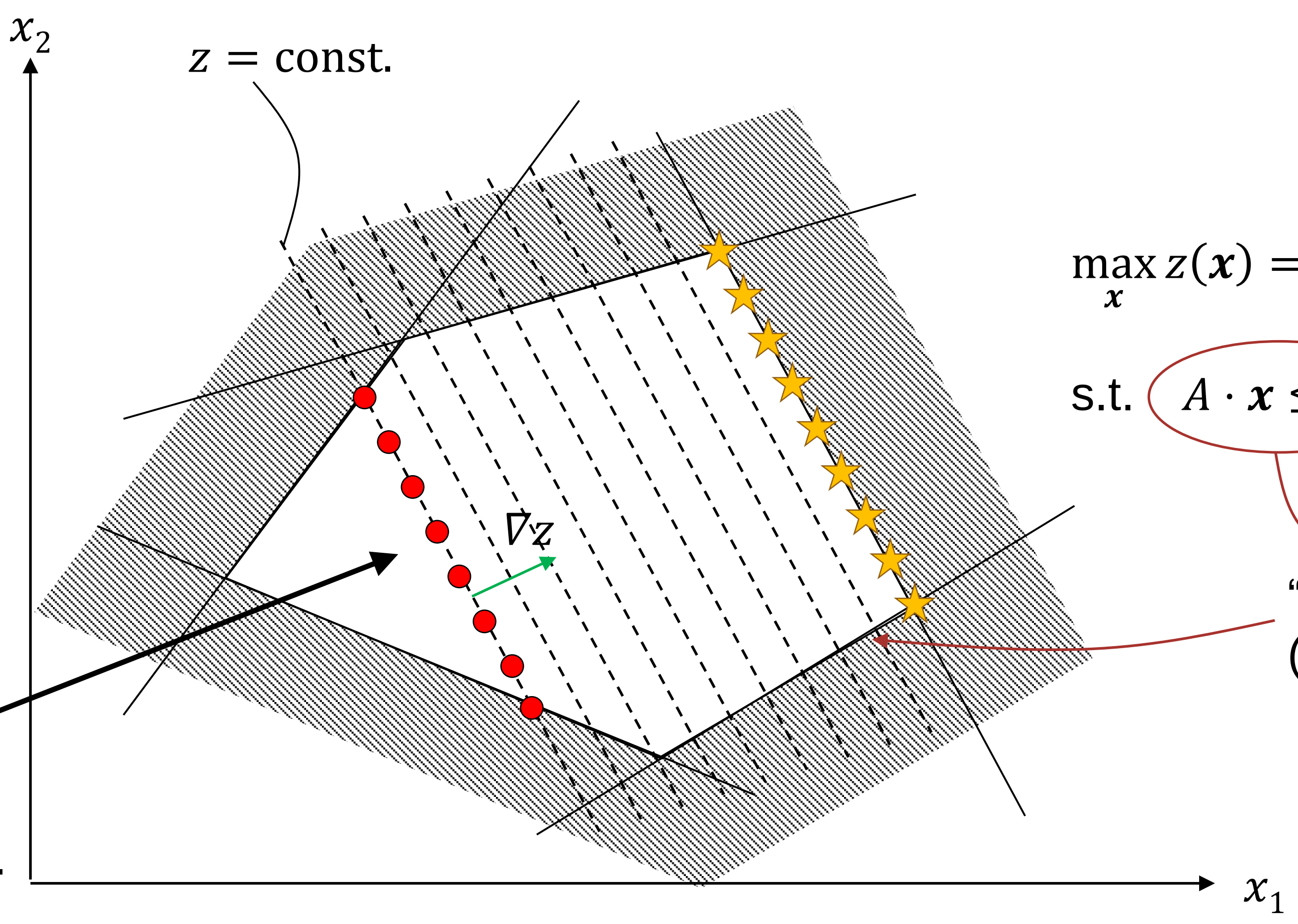
depends on

slope of objective function

$$\vec{\nabla} z = \left(\frac{\partial z}{\partial x_1}, \dots, \frac{\partial z}{\partial x_n}\right)^{\mathrm{T}} = \text{const.}$$
$$= (c_1, c_2)^T$$

cost coefficients!

Solving linear programming problems (infinite solutions)



$$\max_{\boldsymbol{x}} z(\boldsymbol{x}) = c_1 x_1 + c_2 x_2$$

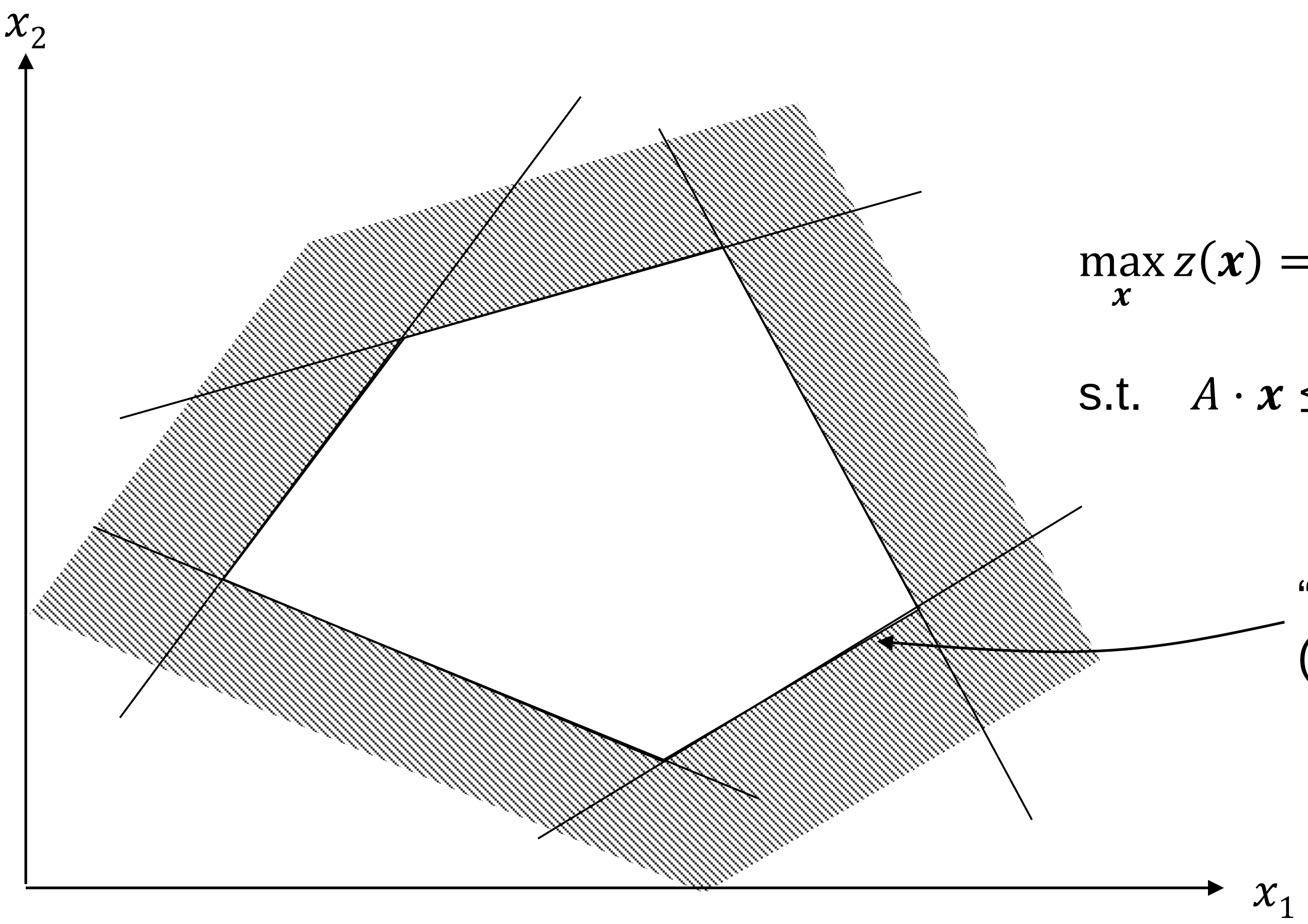
s.t. $A \cdot \boldsymbol{x} \leq \boldsymbol{b}$

"solution-polyhedron" (feasible region)

slope of objective function

$$\vec{\nabla} z = \left(\frac{\partial z}{\partial x_1}, \ldots, \frac{\partial z}{\partial x_n}\right)^{\mathrm{T}} = \text{const.}$$
$$= (c_1, c_2)^T$$

Solving linear programming problems (no solution)



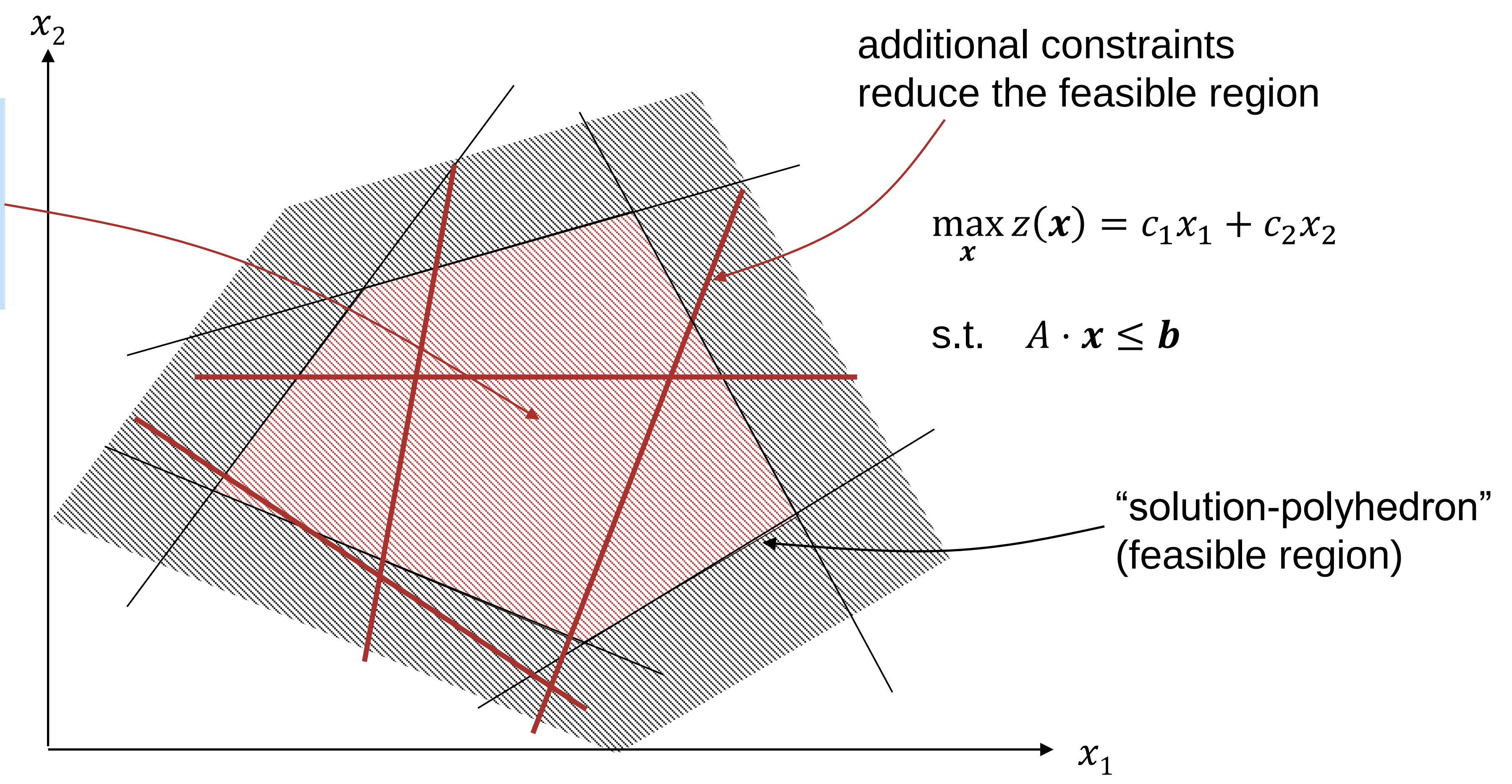
$$\max_{\boldsymbol{x}} z(\boldsymbol{x}) = c_1 x_1 + c_2 x_2$$

s.t. $A \cdot \boldsymbol{x} \leq \boldsymbol{b}$

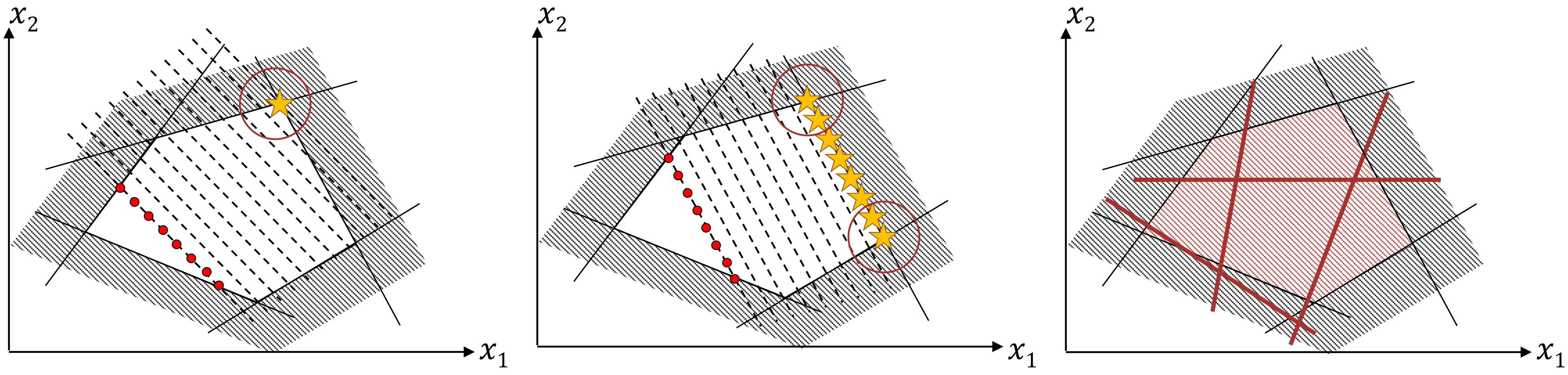
"solution-polyhedron"
(feasible region)

Solving linear programming problems (no solution)

no solution
if no feasible region
("infeasible problem")

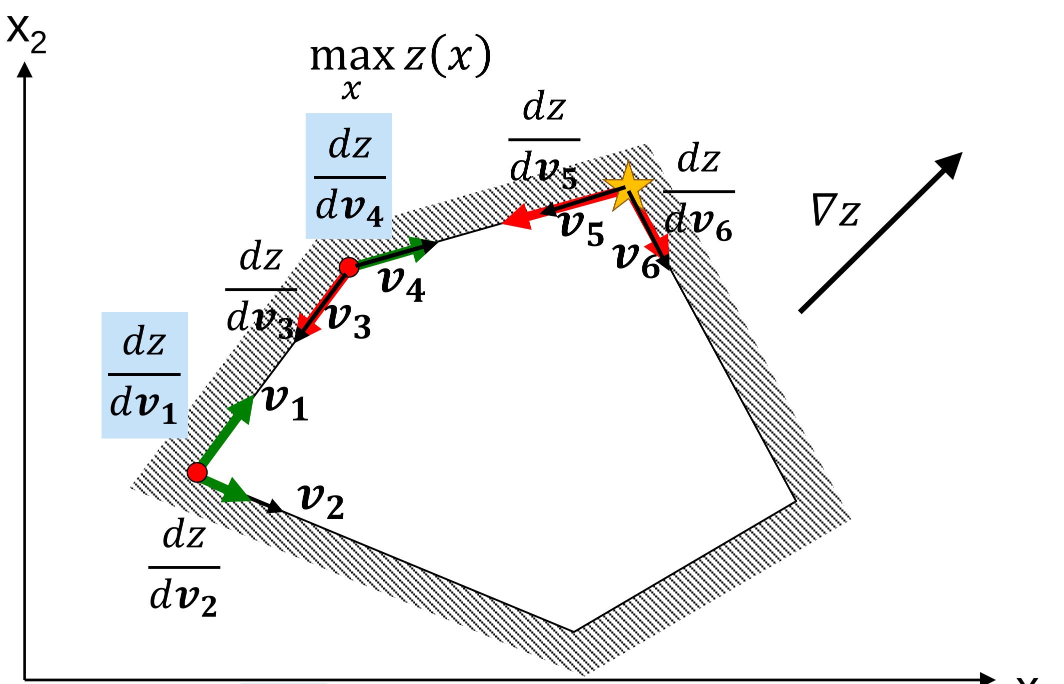


Solving linear programming problems



If an optimal solution exists,
an optimal solution lies on a **corner of the solution-polyhedron**!

Idea behind Simplex algorithm



$$\frac{dz}{d\boldsymbol{v}_1} > \frac{dz}{d\boldsymbol{v}_2} > 0$$

$$\frac{dz}{d\boldsymbol{v}_4} > 0 > \frac{dz}{d\boldsymbol{v}_3}$$

$$0 > \frac{dz}{d\boldsymbol{v}_6} > \frac{dz}{d\boldsymbol{v}_5}$$

1. find a corner of the solution-polyhedron
2. from the corner, follow the edge that improves the objective the most until the next corner
3. repeat step 2 until no further improvement is possible

Linear programming (LP)

Properties

- ✓ all variables continuous
- ✓ all (in)equalities linear

Linear program (LP)

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

$$\text{s.t.} \quad A\boldsymbol{x} \le \boldsymbol{b}$$

$$E\boldsymbol{x} = \boldsymbol{f}$$

$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{c} \in \mathbb{R}^m,$$
$$A \in \mathbb{R}^{n\times m}, \boldsymbol{b} \in \mathbb{R}^n,$$
$$E \in \mathbb{R}^{o\times m}, \boldsymbol{f} \in \mathbb{R}^o$$

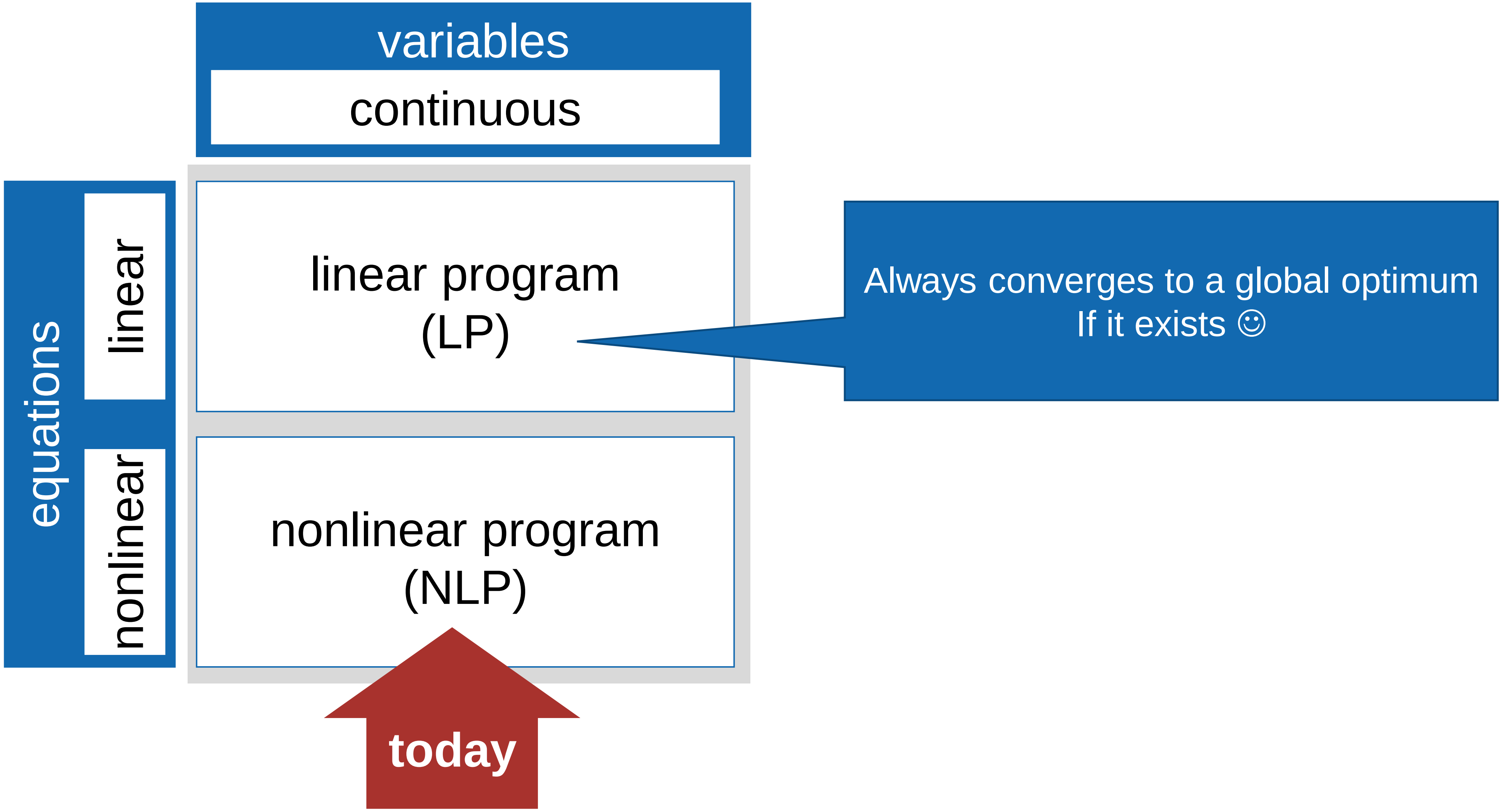
solve with simplex method!

$$z = c_1 \ldots + c_m x_m$$

$$\begin{pmatrix} a_{11} & a_{12} & & a_{1m} \\ a_{21} & \ddots & & \vdots \\ \vdots & & & \\ a_{n1} & \cdots & & a_{nm} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} \le \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\begin{pmatrix} e_{11} & e_{12} & \cdots & e_{1m} \\ e_{21} & \ddots & & \vdots \\ \vdots & & & \\ e_{o1} & \cdots & & e_{om} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_o \end{pmatrix}$$

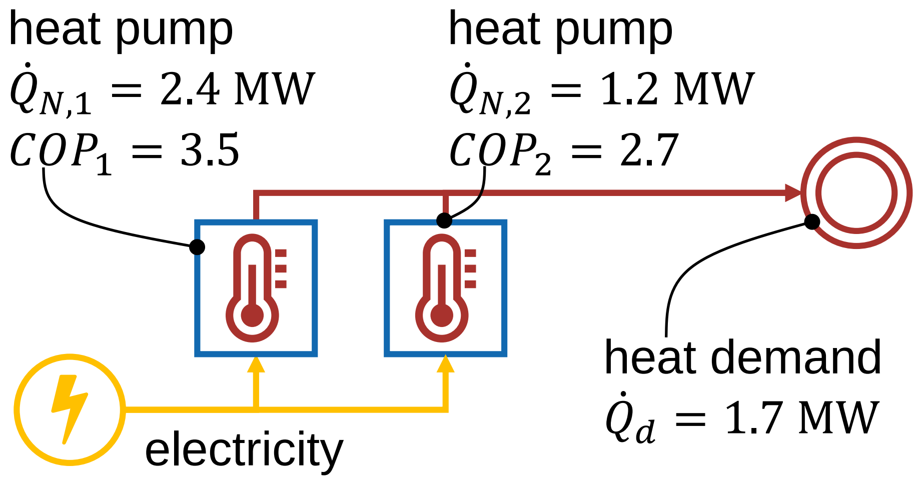
Optimization problem classes

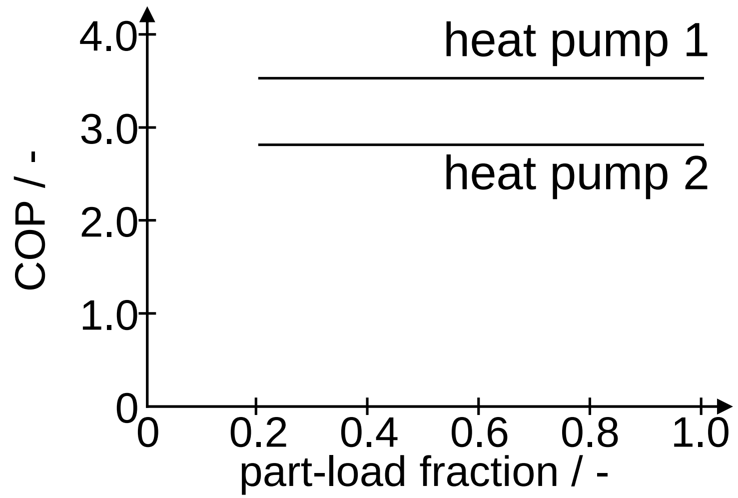


After this lecture, you are able to…

- ✓ identify basic **elements of an optimization problem**.
- distinguish **linear problems** (LP) and **nonlinear problems** (NLP).
- use basic **solution methods** for both LPs and NLPs.
- formulate simple **energy system optimization problems (LP and NLP)**

Optimization example: Continuous steady-state model
How much electricity to satisfy heat demand?





Optimization problem

objective function:

$$P = \underbrace{\frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

linear!

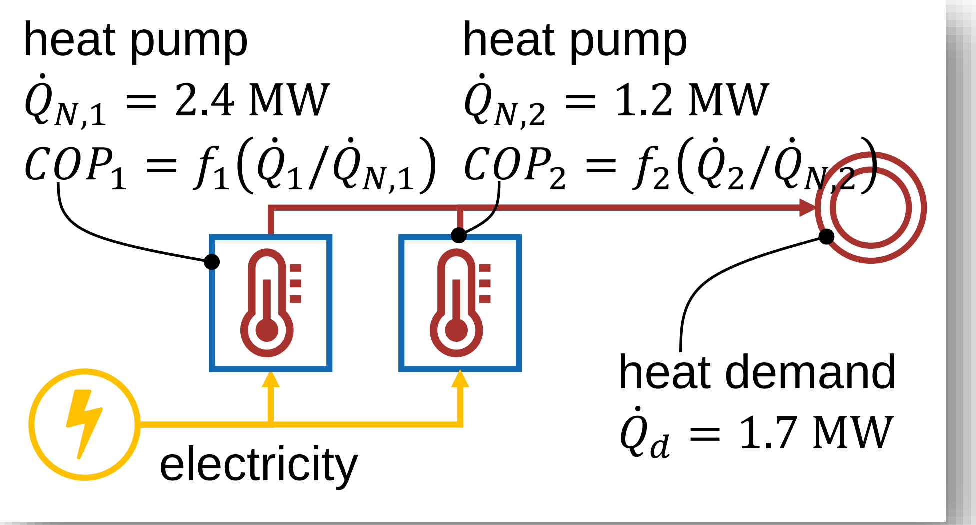
constraints:

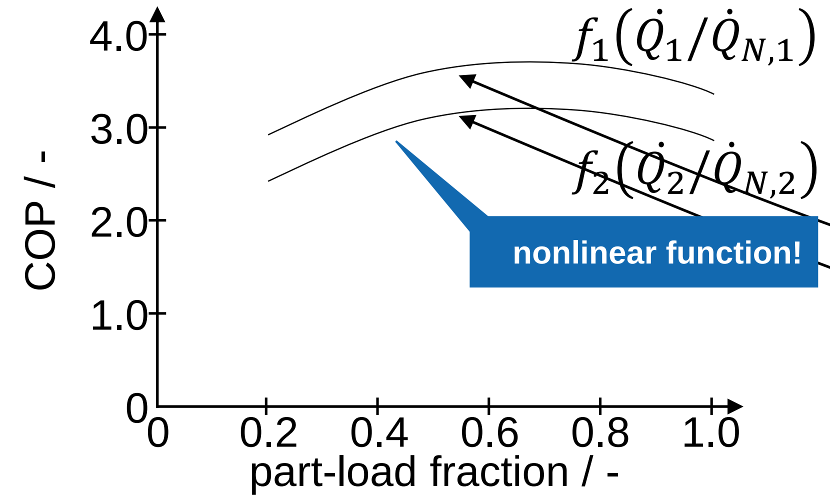
$$\begin{aligned} \text{s.t.} \quad & \dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0, \\ & \dot{Q}_1 \geq 0, \\ & \dot{Q}_2 \geq 0, \\ & \dot{Q}_1 \leq \dot{Q}_{N,1}, \\ & \dot{Q}_2 \leq \dot{Q}_{N,2}, \\ & COP_1 = 3.5, \\ & COP_2 = 2.7 \end{aligned}$$

variable
parameter

linear!

Optimization example: Continuous steady-state model
How much electricity to satisfy heat demand?





System model

$$P = \underbrace{\frac{\dot{Q}_1}{COP_1}}_{\text{electricity demand heat pump 1}} + \underbrace{\frac{\dot{Q}_2}{COP_2}}_{\text{electricity demand heat pump 2}}$$

nonlinear: division of two variables!

$$\dot{Q}_1 + \dot{Q}_2 - \dot{Q}_d = 0,$$
$$\dot{Q}_1 \geq 0,$$
$$\dot{Q}_2 \geq 0,$$
$$\dot{Q}_1 \leq \dot{Q}_{N,1},$$
$$\dot{Q}_2 \leq \dot{Q}_{N,2},$$
$$COP_1 = f_1(\dot{Q}_1/\dot{Q}_{N,1}),$$
$$COP_2 = f_2(\dot{Q}_2/\dot{Q}_{N,2})$$

variable
parameter

Nonlinear programming (NLP)

Properties

- ✓ all variables continuous
- ✓ all functions f linear:

Linear program (LP)

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

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

$$E\boldsymbol{x} = \boldsymbol{f}$$

$$z = c_1 \ldots + c_m x_m$$

$$\begin{pmatrix} a_{11} & a_{12} & & a_{1m} \\ a_{21} & \ddots & & \vdots \\ \vdots & & & \\ a_{n1} & \cdots & & a_{nm} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} \leq \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\begin{pmatrix} e_{11} & e_{12} & \cdots & e_{1m} \\ e_{21} & \ddots & & \vdots \\ \vdots & & & \\ e_{o1} & \cdots & & e_{om} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_o \end{pmatrix}$$

$$\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{c} \in \mathbb{R}^m, \quad A \in \mathbb{R}^{n \times m}, \boldsymbol{b} \in \mathbb{R}^n, \quad E \in \mathbb{R}^{o \times m}, \boldsymbol{f} \in \mathbb{R}^o$$

solve with simplex method!

Properties

- ✓ all variables continuous
- ✓ some functions $g_j(\boldsymbol{x})$, $h_i(\boldsymbol{x})$ nonlinear

  e.g.:
  $x_i^n, \prod_i x_i, \ln x, \sin(x), e^x, \ldots$

Nonlinear programming

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

$$\text{s.t.} \quad g_j(\boldsymbol{x}) \leq 0, \quad j = 1, \ldots, n$$

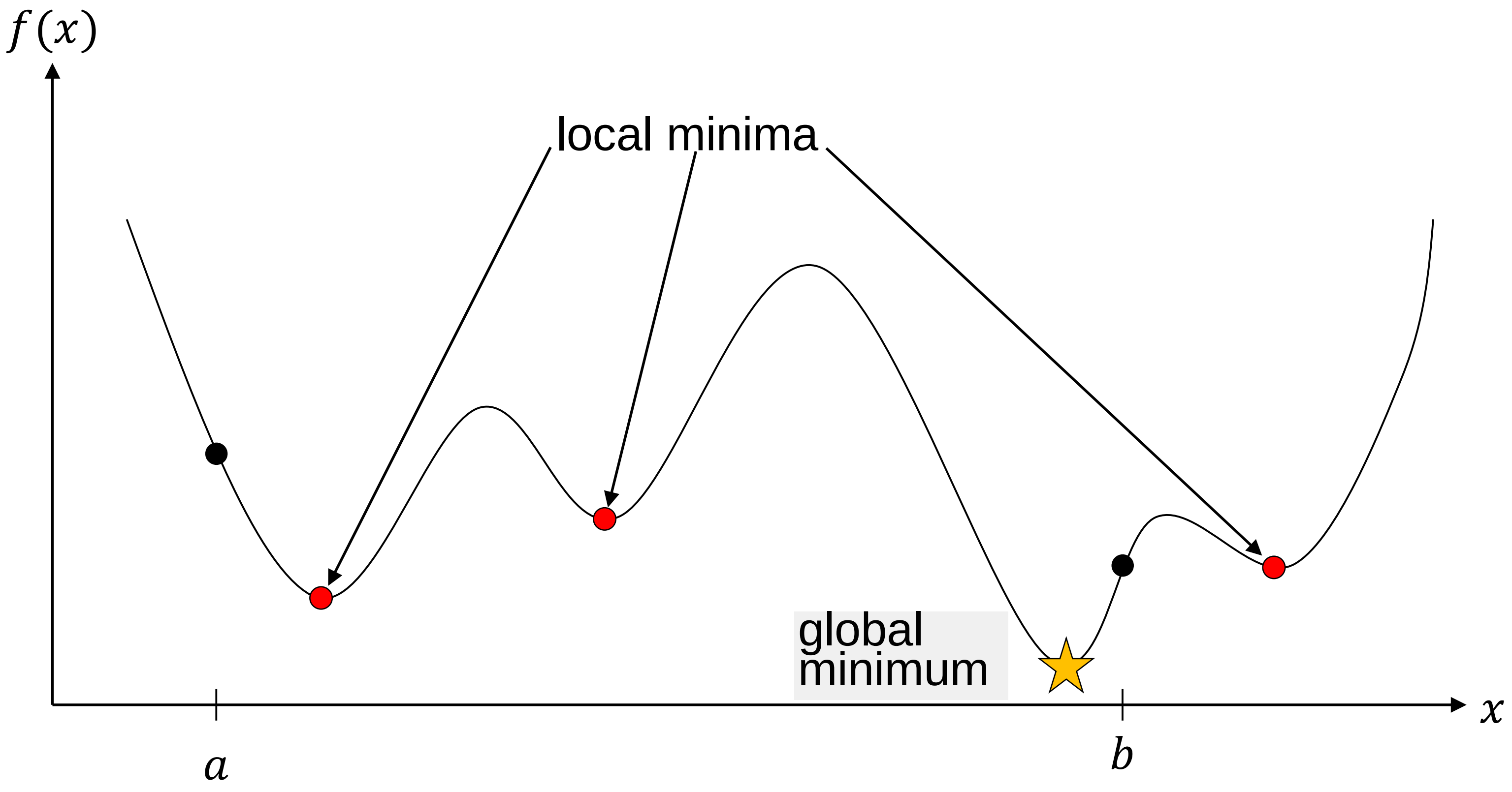
$$h_i(\boldsymbol{x}) = 0, \quad i = 1, \ldots, o$$

$$\boldsymbol{x} \in \mathbb{R}^m$$

How to solve?

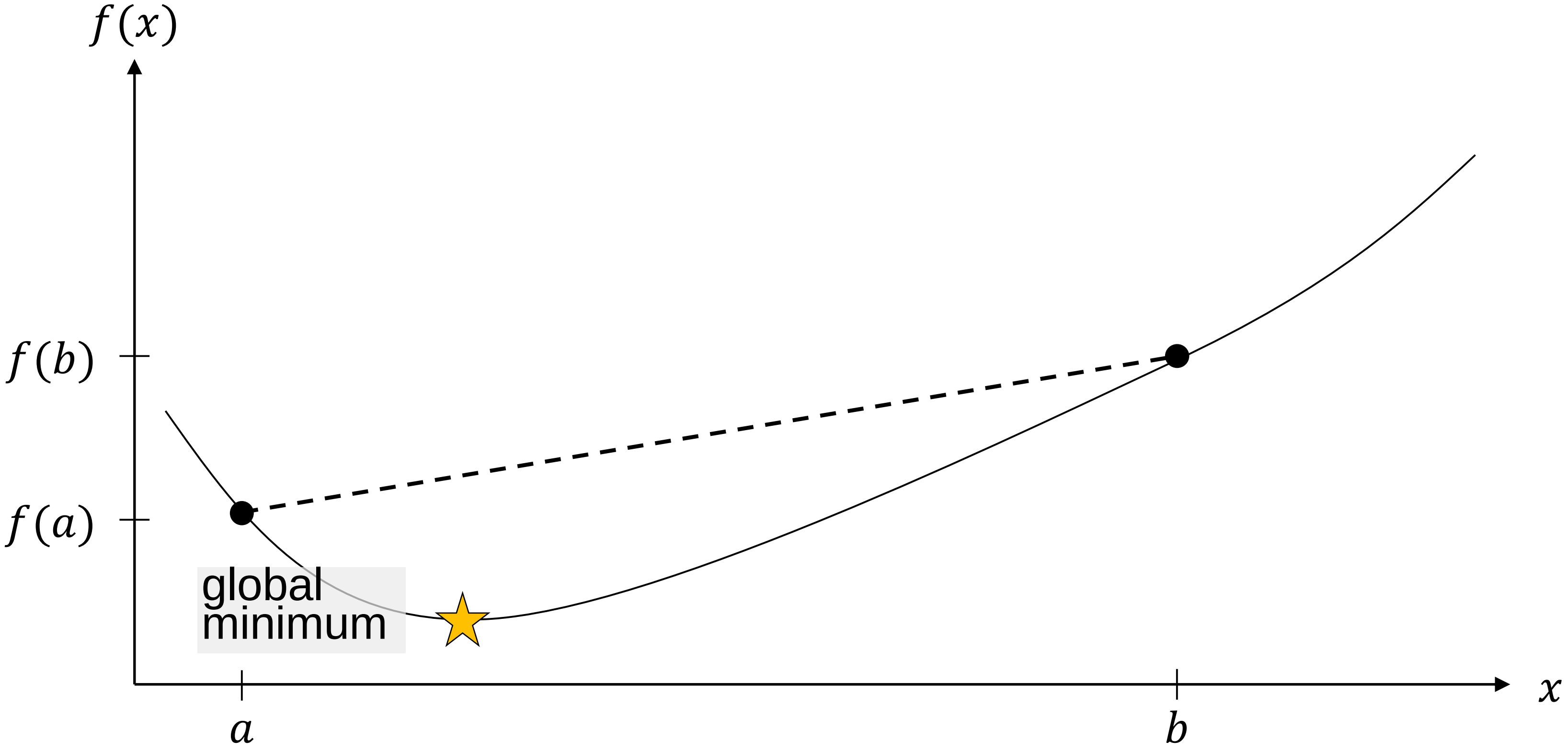
No longer in matrix form!

Multimodal nonlinear functions



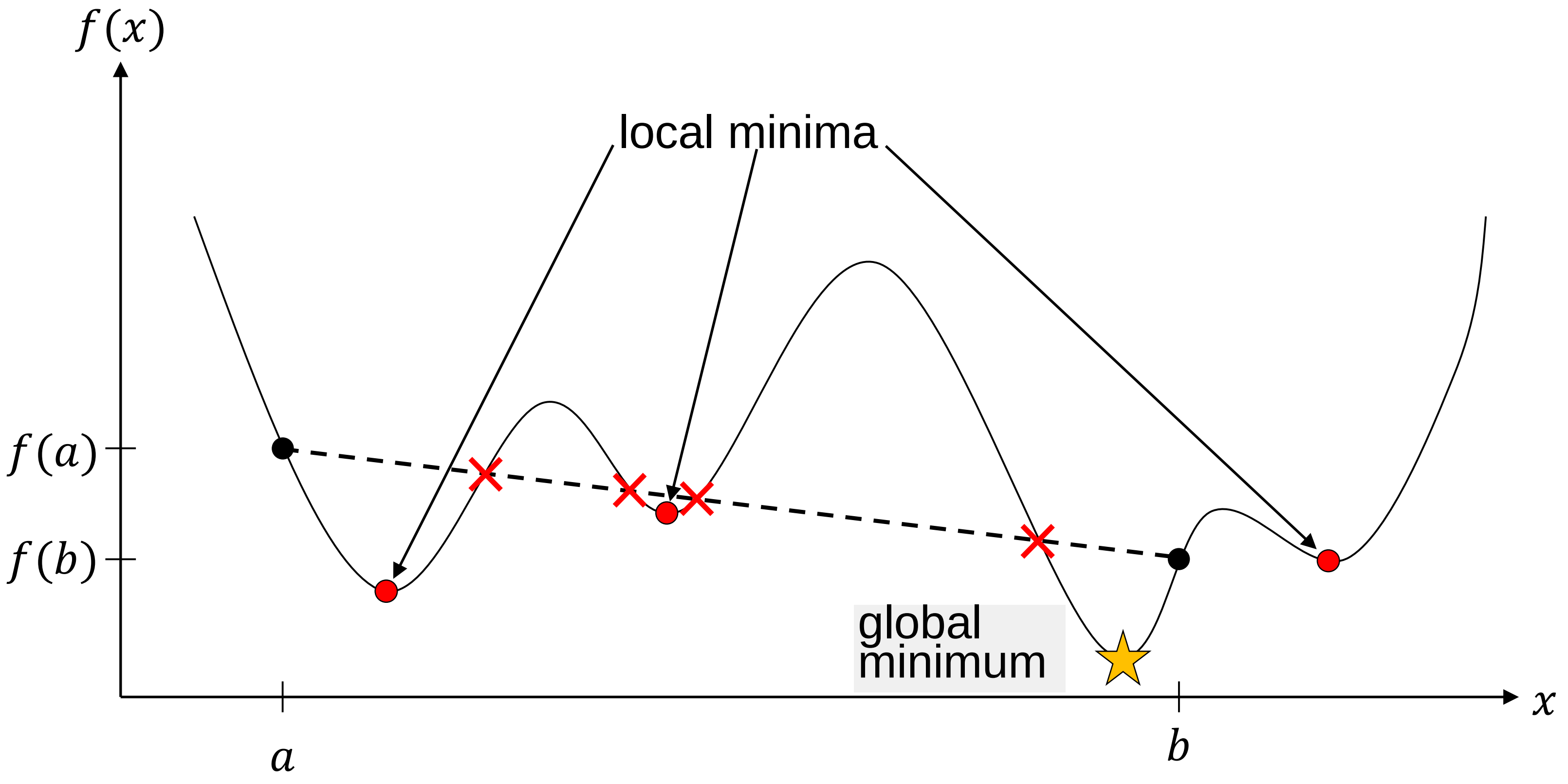
Convex functions

$$f(x) \leq f(a) + \frac{f(b) - f(a)}{b - a}(x - a), \qquad \forall x \in [a, b]$$



Multimodal nonlinear functions

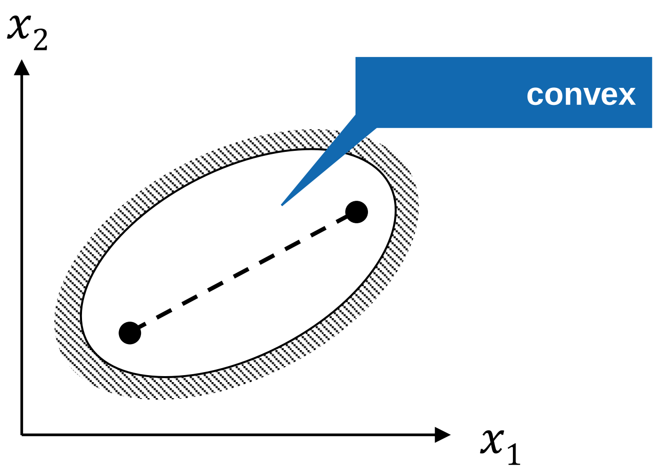
$$f(x) \leq f(a) + \frac{f(b) - f(a)}{b - a}(x - a), \qquad \cancel{\forall} x \in [a, b]$$

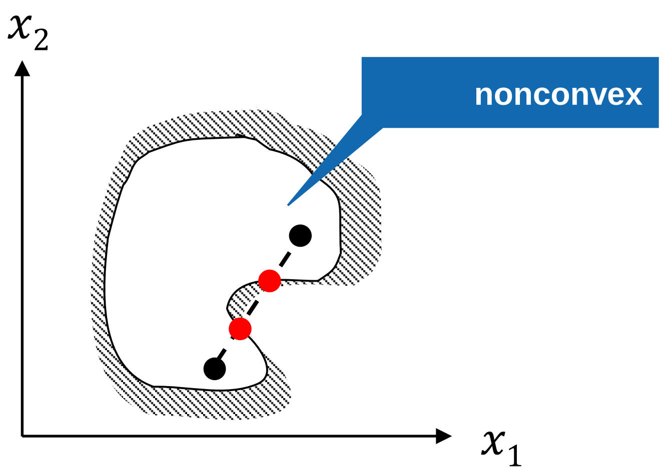


Convex optimization problems

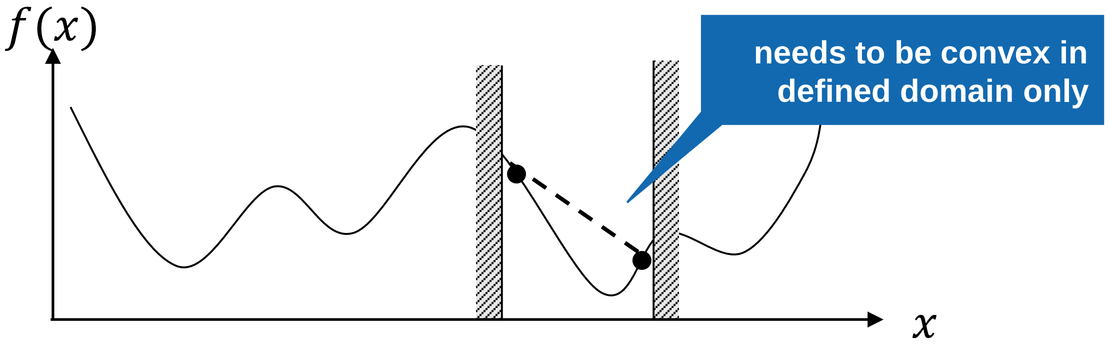
1 convex feasible region

F is convex if and only if
$\forall x_1, x_2 \in F$;
$x = \alpha x_1 + (1-\alpha) x_2 \in F$

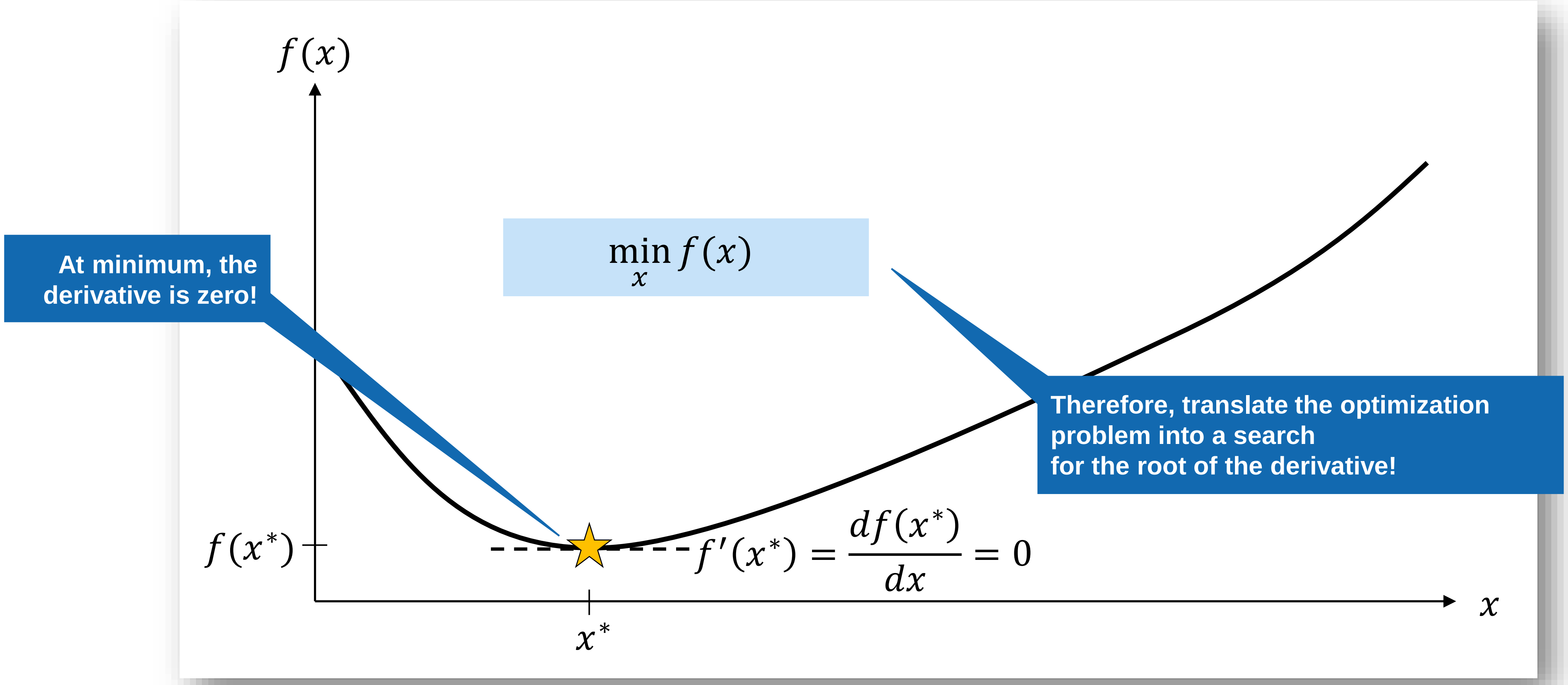




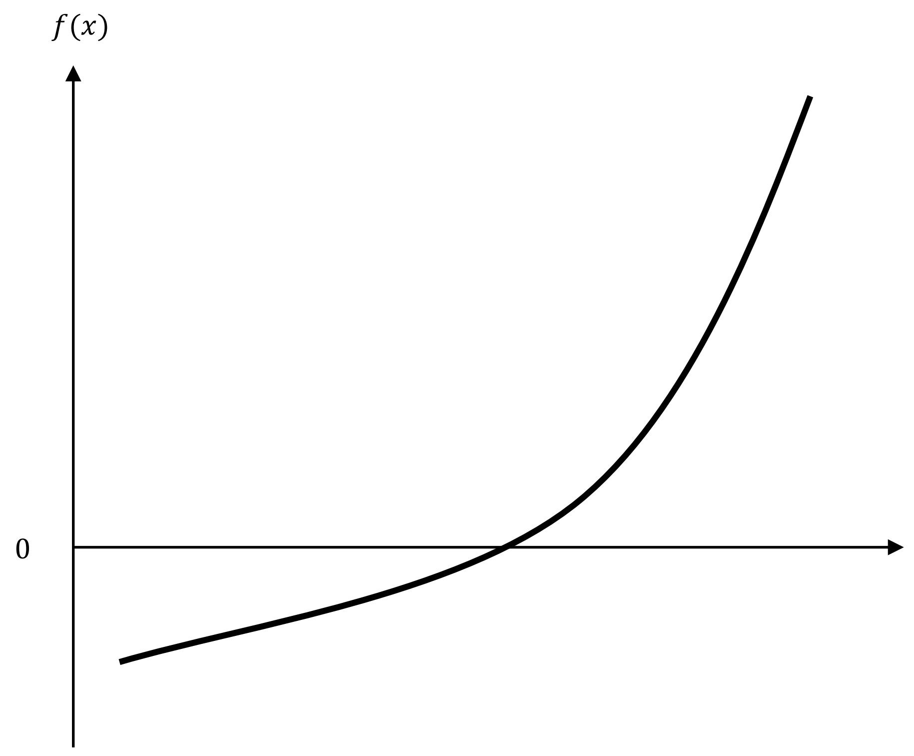
2 convex objective function



Solving convex unconstrained optimization problems



Solving convex unconstrained optimization problems: Newton's method



Newton's method: Finding roots iteratively

First-order Taylor series expansion:

$$f(x) \approx f(x_0) + \frac{df(x_0)}{dx}(x - x_0)$$

Root of first-order Taylor polynomial:

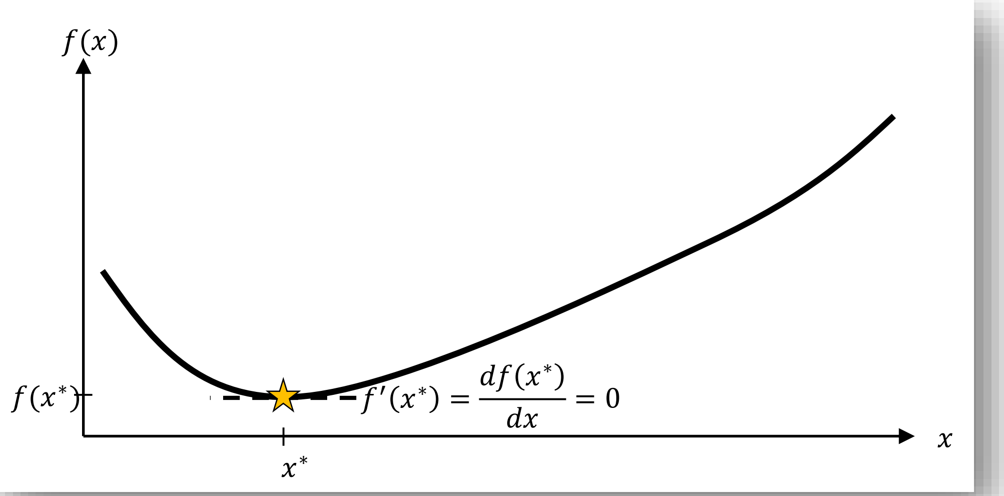
$$f(x_0) + \frac{df(x_0)}{dx}(x - x_0) = 0$$

$$\Leftrightarrow x = x_0 - \frac{f(x_0)}{\left(\frac{df(x_0)}{dx}\right)}$$

Iterate to approximate root of $g(x)$

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{\left(\frac{df(x_n)}{dx}\right)}}$$

Solving convex unconstrained optimization problems: Newton's method



$$\min_x f(x)$$

$$f'(x) = 0$$

Newton's method: Finding roots iteratively

First-order Taylor series expansion:

$$f(x) \approx f(x_0) + \frac{df(x_0)}{dx}(x - x_0)$$

Root of first-order Taylor polynomial:

$$f(x_0) + \frac{df(x_0)}{dx}(x - x_0) = 0$$

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Iterate to approximate root of $f(x)$

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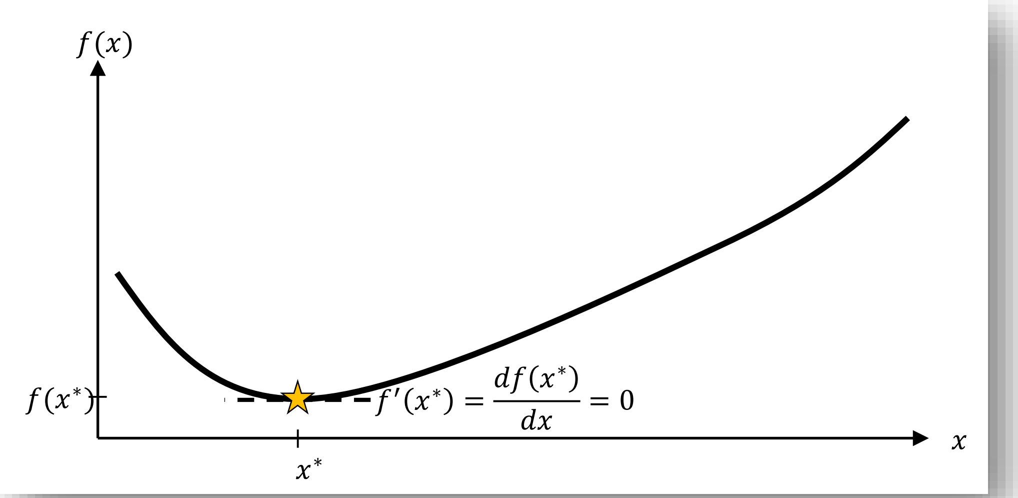
Solving convex unconstrained optimization problems: Newton's method



$\min_x f(x)$ ▶ $f'(x) = 0$

Reminder:
need to find the root of $f'(x)$

Newton's method:
Finding roots iteratively

Iterate to approximate root of $g(x)$

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{\left(\frac{df(x_n)}{dx}\right)}}$$

for $f'(x)$

Iterate to approximate root of $f'(x)$

$$x_{n+1} = x_n - \frac{f'(x_n)}{\left(\frac{df'(x_n)}{dx}\right)}$$

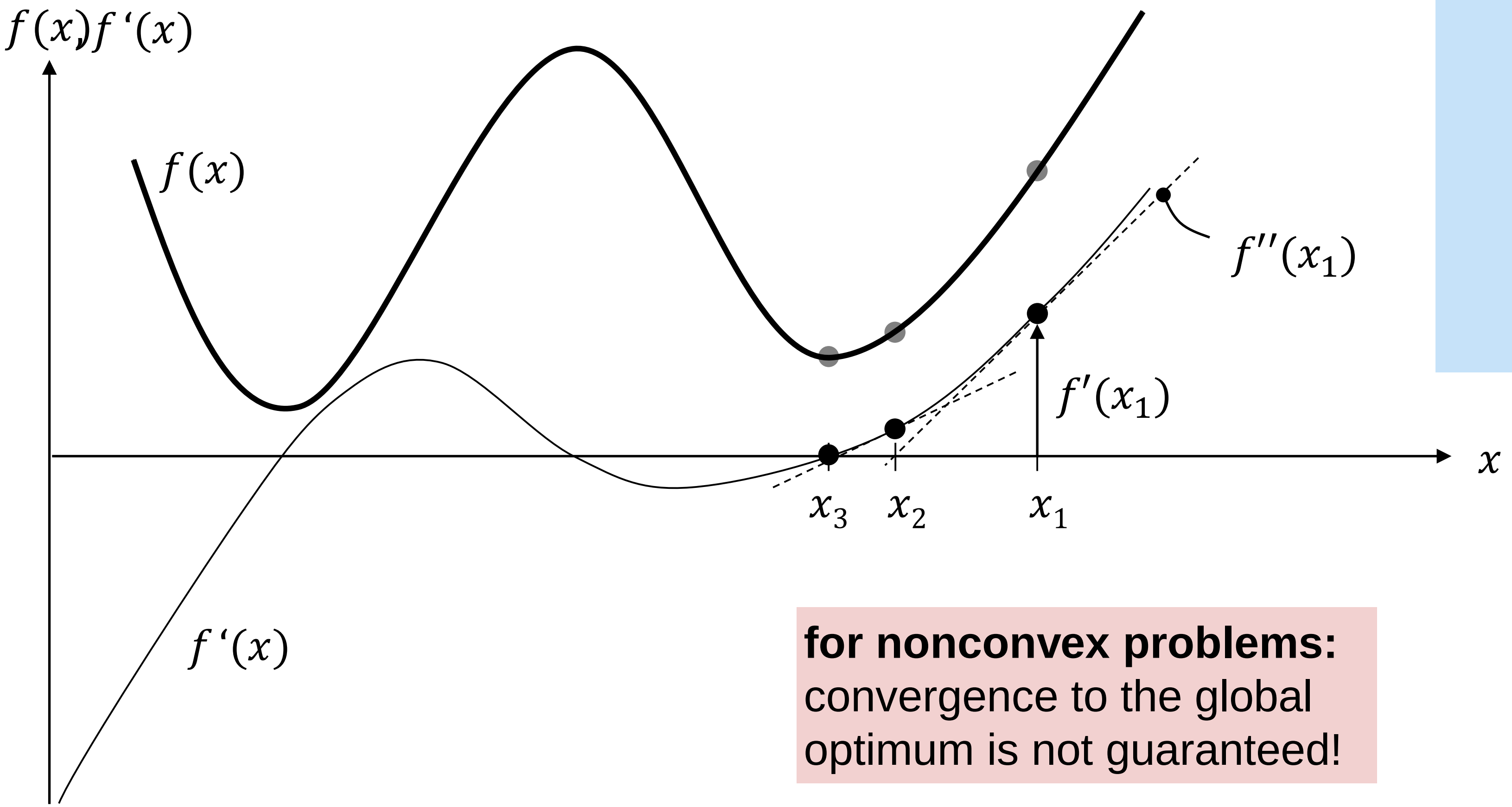
$$= x_n - \frac{f'(x_n)}{f''(x_n)}$$

Discussion

In the previous example, we applied Newton's Method to a convex optimization problem. What happens if it is applied to a nonconvex problem?

- **a** — **Newton's Method is based on the first order Taylor series expansion and will thus always converge to the global optimum.**
- **b** — **Newton's Method may converge to a solution. But the solution may be the global minimum, a local minimum, or a saddle point.**
- **c** — **If applied to nonconvex problems, the method will fail to find a meaningful solution.**

Solving nonconvex unconstrained optimization problems: Newton's method



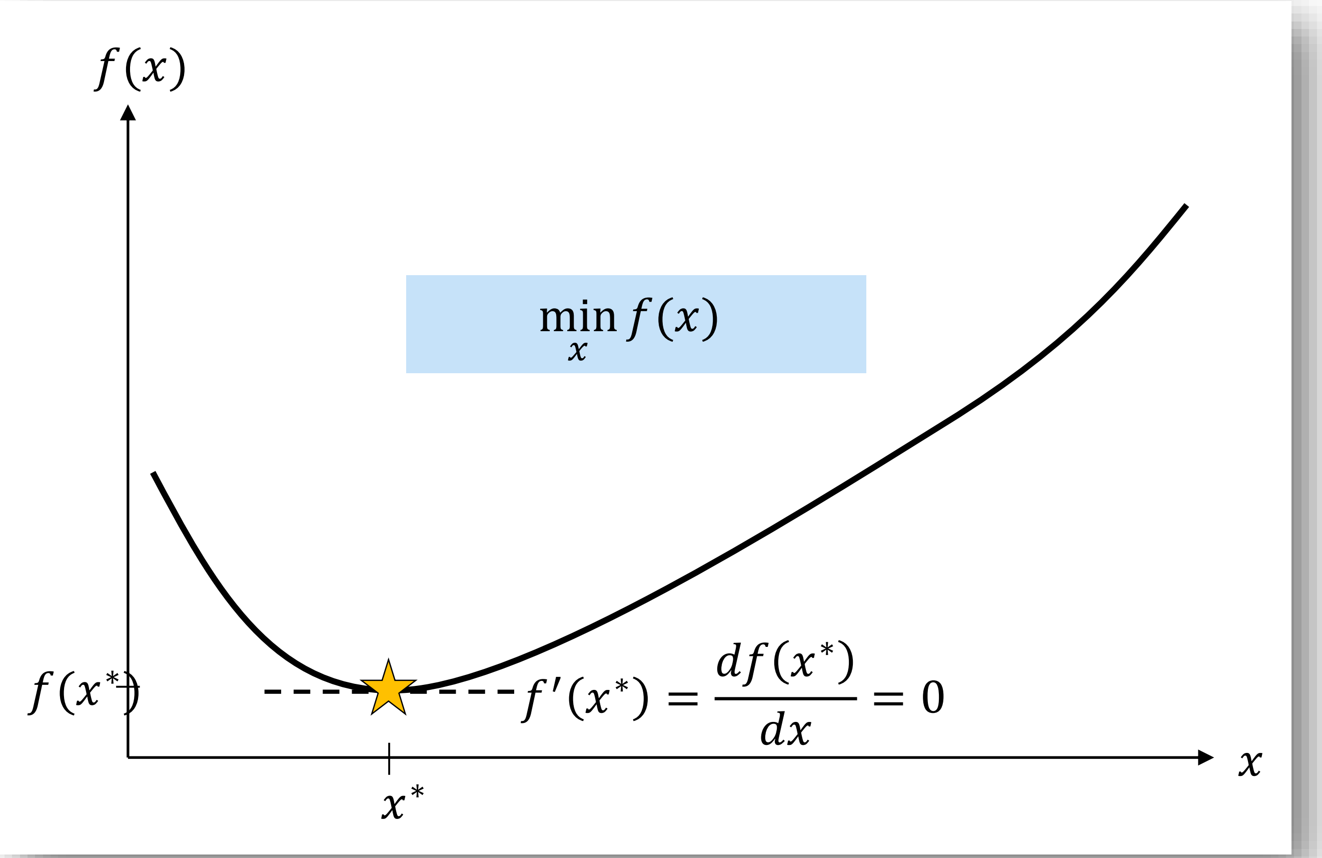
Iterate to approximate root of $f'(x)$

$$x_{n+1} = x_n - \frac{f'(x_n)}{\left(\frac{df'(x_n)}{dx}\right)}$$

$$= x_n - \frac{f'(x_n)}{f''(x_n)}$$

for nonconvex problems: convergence to the global optimum is not guaranteed!

Newton's method for solving unconstrained optimization problems



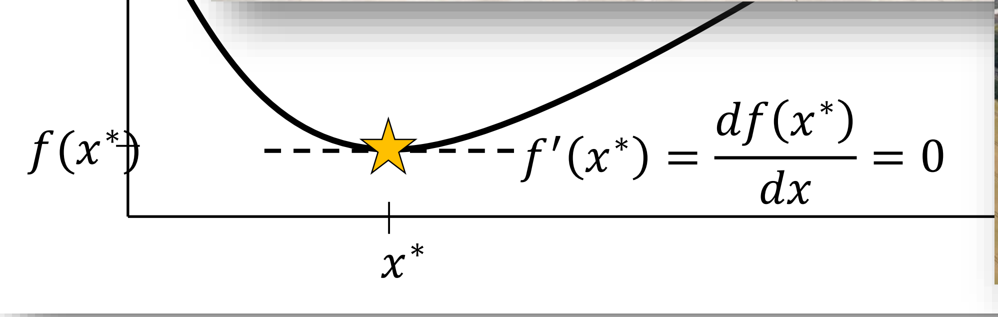
Iterate to approximate root of $f'(x)$

$$x_{n+1} = x_n + \frac{f'(x_n)}{\left(\frac{df'(x_n)}{dx}\right)}$$

$$= x_n + \frac{f'(x_n)}{f''(x_n)}$$

In engineering problems, constraints are the norm, not the exception.

Newton's method for solving unconstrained optimization problems



In engineering problems, constraints are the norm, not the exception.

Solving constraint optimization problems: Method of Lagrange multipliers

Optimization problem		Lagrange formulation
$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$ $$\text{s.t. } h_j(\boldsymbol{x}) = 0, \quad j = 0, \dots, o$$ $$\rightarrow \lambda_j$$	convert	$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_j \lambda_j h_j(\boldsymbol{x})$$ $$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial f(\boldsymbol{x})}{\partial x_i} - \sum_j \lambda_j \frac{\partial h_j(\boldsymbol{x})}{\partial x_i} = 0, \quad i = 0, \dots, m$$ $$\frac{\partial \mathcal{L}}{\partial \lambda_j} = -h_j(\boldsymbol{x}) = 0, \quad j = 0, \dots, o$$

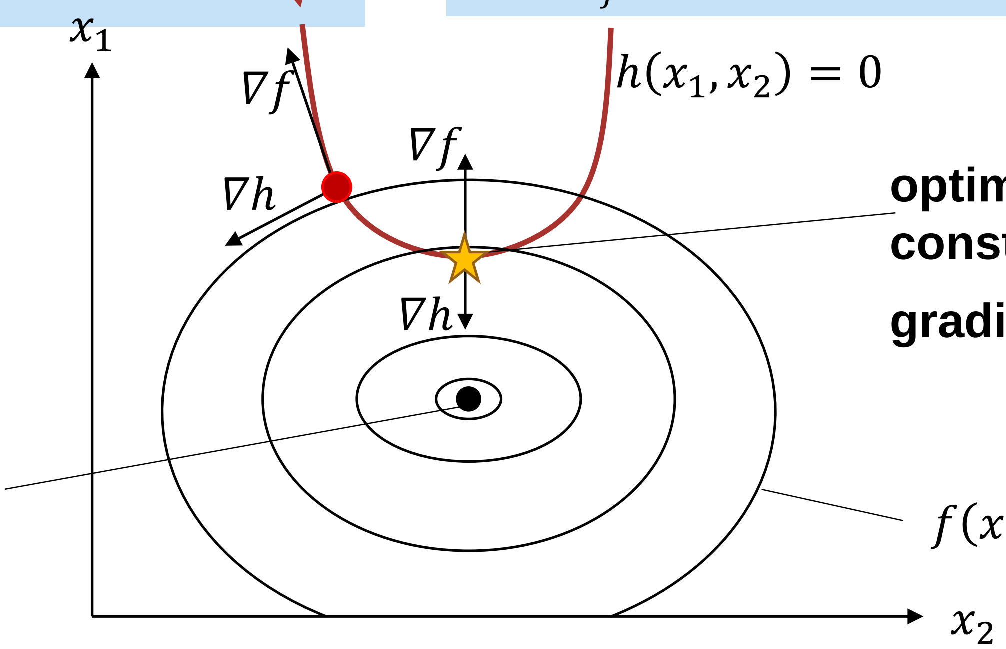
Approach

1. for each constraint j introduce a **Lagrange multiplicator** λ_j
2. formulate the **Lagrange function** $\mathcal{L}$:
   extend the objective function by the product of Lagrange-multiplicator λ_j and its constraint h_j
3. calculate **partial derivatives of the Lagrange function**
   with respect to variables x_i and Lagrange-multiplicators λ_j
4. set the partial derivatives to 0 and **solve the equation system**

Why does this work?

Idea behind the method of Lagrange multipliers

Optimization problem		Lagrange formulation
$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$ $$\text{s.t.}\;\; h_j(\boldsymbol{x}) = 0, \;\; j = 0, \dots, o$$ $$\rightarrow \lambda_j$$	convert	$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_j \lambda_j \, h_j(\boldsymbol{x})$$ $$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial f(\boldsymbol{x})}{\partial x_i} - \sum_j \lambda_j \frac{\partial h_j(\boldsymbol{x})}{\partial x_i} = 0, \qquad i = 0, \dots, m$$ $$\frac{\partial \mathcal{L}}{\partial \lambda_j} = -h_j(\boldsymbol{x}) = 0, \qquad j = 0, \dots, o$$



optimum of constrained problem:

gradients ∇f and ∇h are parallel

optimum of unconstrained problem

After this lecture, you are able to…

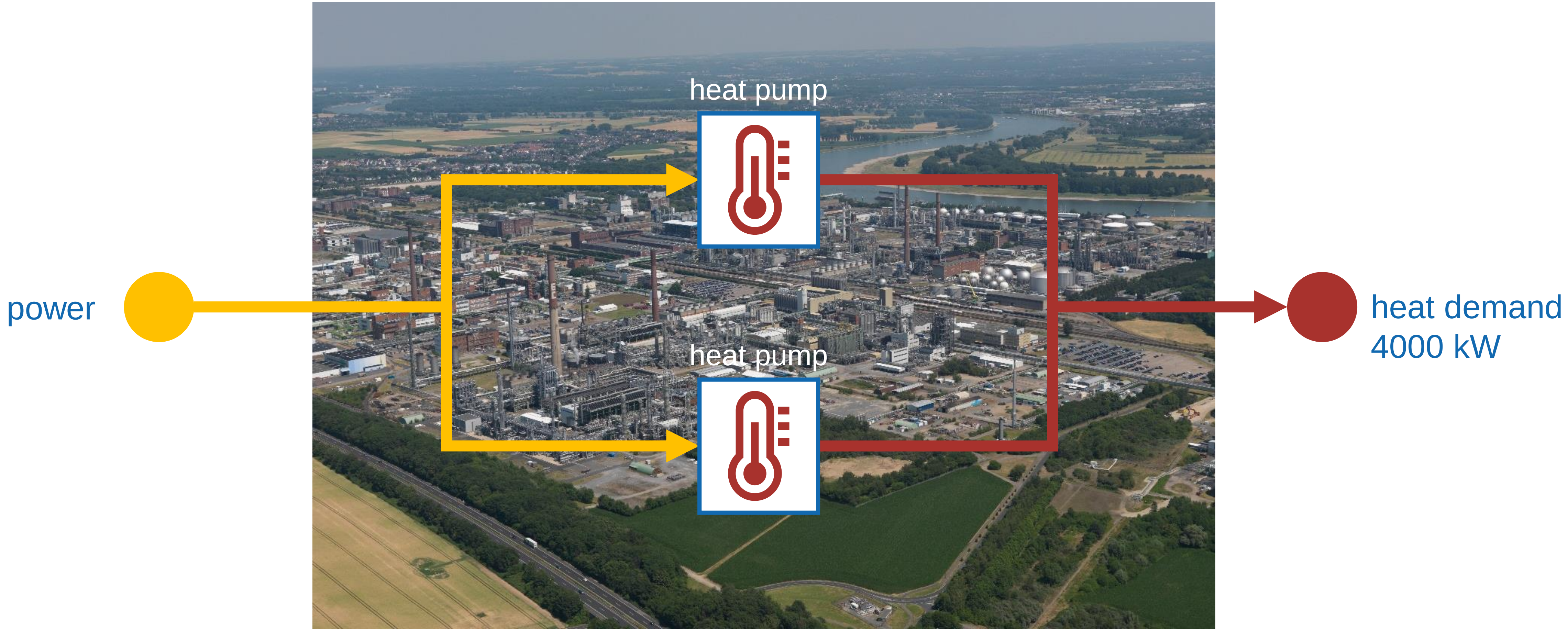
✓ identify basic **elements of an optimization problem**.

✓ distinguish **linear problems** (LP) and **nonlinear problems** (NLP).

✓ use basic **solution methods** for both LPs and NLPs.

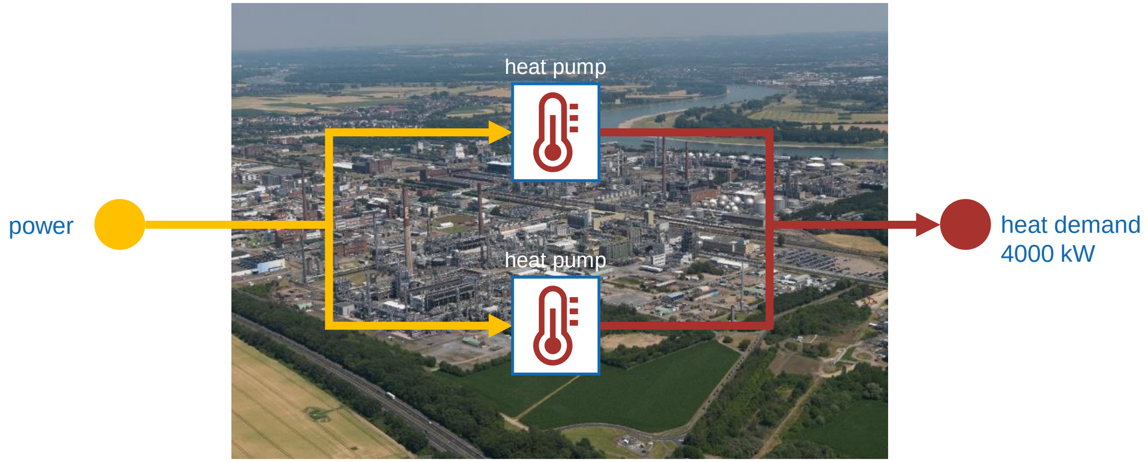
- formulate simple **energy system optimization problems (LP and NLP)**

Example: Optimal operation of two heat pumps



Source: INEOS Köln GmbH

Example: Optimal operation of two heat pumps



heat pumps consume electricity to produce heat

$$P_{HP1} = f(\dot{Q}_{HP1})$$
$$P_{HP2} = f(\dot{Q}_{HP2})$$

heat demand needs to be satisfied

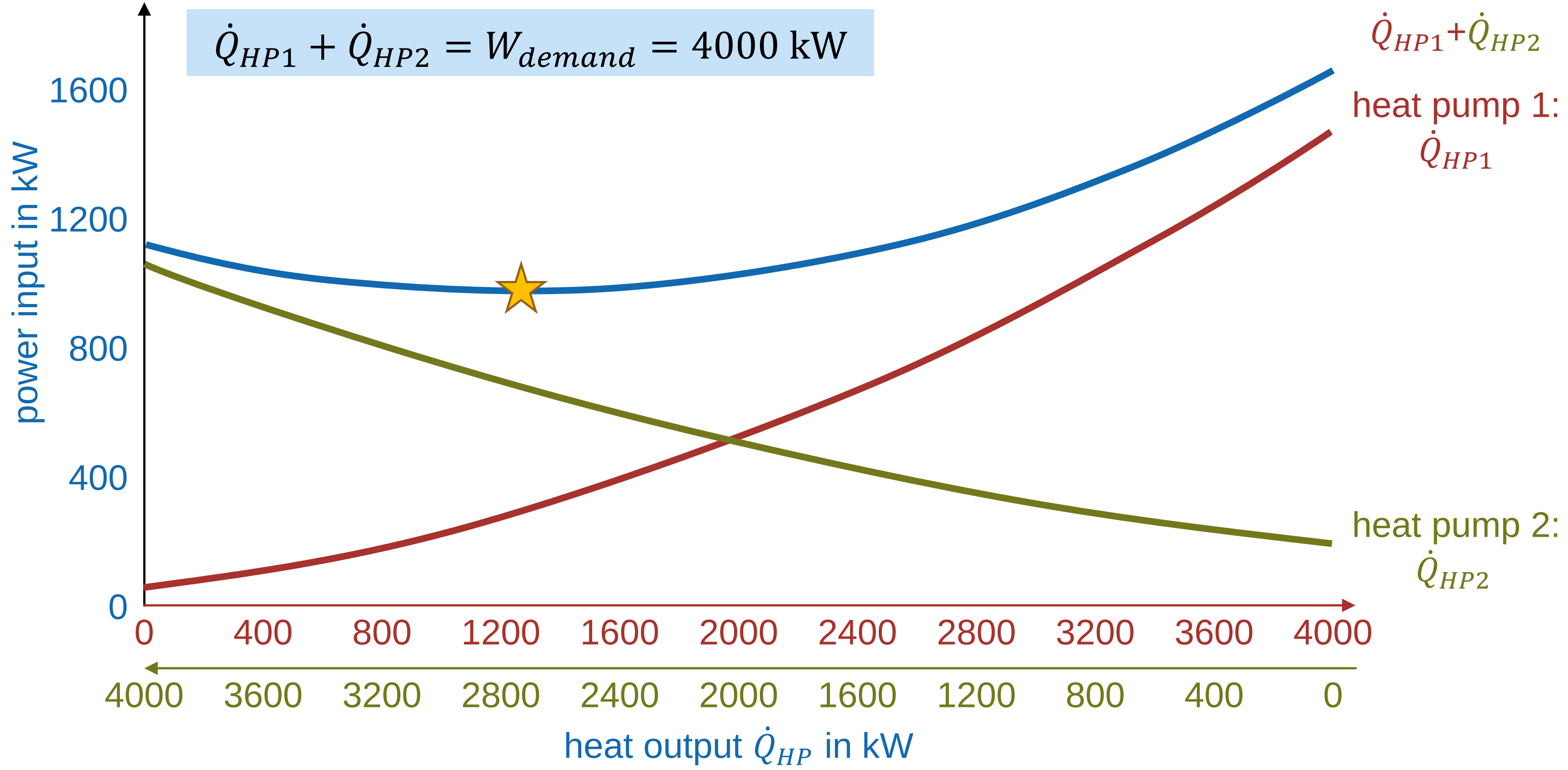
$$\dot{Q}_{HP1} + \dot{Q}_{HP2} - \dot{Q}_{demand} = 0$$

minimize overall electricity consumption

$$\min_{\dot{Q}_{HP1},\dot{Q}_{HP2}} P_{tot} = P_{HP1}(\dot{Q}_{HP1}) + P_{HP2}(\dot{Q}_{HP2})$$

variable
parameter

Example: Optimal operation of two heat pumps
Solution by inspection



Example: Optimal operation of two heat pumps
Method of Lagrange multipliers

$$\min_{\dot{Q}_{HP1},\dot{Q}_{HP2}} \quad P_{tot} = P_{HP1}\,(\dot{Q}_{HP1}) + P_{HP2}\,(\dot{Q}_{HP2})$$

$$\text{s.t.} \qquad \dot{Q}_{HP1} + \dot{Q}_{HP2} - \dot{Q}_{demand} = 0$$

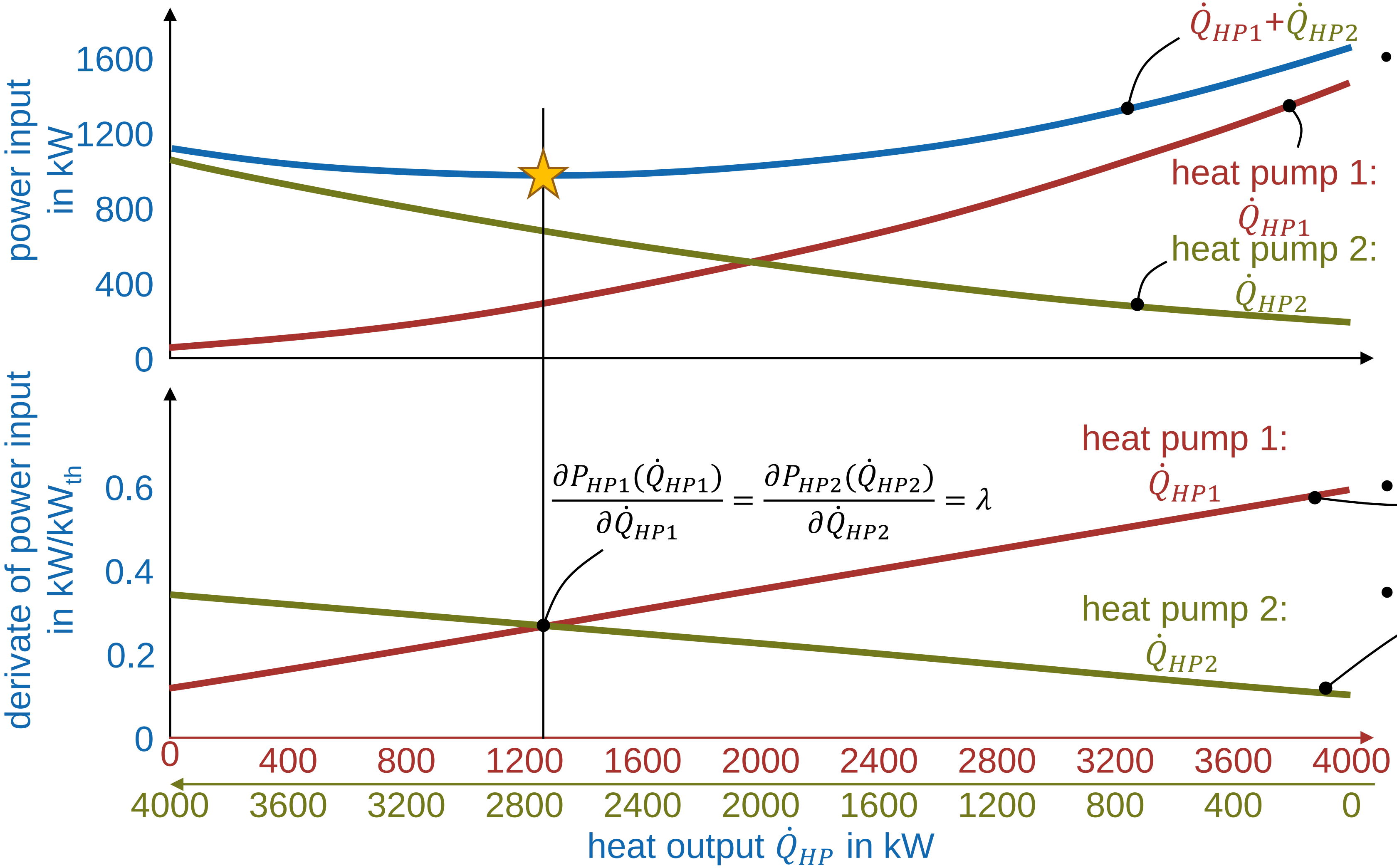
$$\mathcal{L}(\dot{Q}_{HP1}, \dot{Q}_{HP2}, \lambda) = P_{HP1}(\dot{Q}_{HP1}) + P_{HP2}(\dot{Q}_{HP2}) - \lambda(\dot{Q}_{HP1} + \dot{Q}_{HP2} - \dot{Q}_{demand})$$

- $\dfrac{\partial \mathcal{L}}{\partial \dot{Q}_{HP1}} = \dfrac{\partial P_{HP1}(\dot{Q}_{HP1})}{\partial \dot{Q}_{HP1}} - \lambda = 0$
- $\dfrac{\partial \mathcal{L}}{\partial \dot{Q}_{HP2}} = \dfrac{\partial P_{HP2}(\dot{Q}_{HP2})}{\partial \dot{Q}_{HP2}} - \lambda = 0$

Lagrange multiplier λ is called the „shadow price“ (price of an additional unit in the objective function)

- $\dfrac{\partial \mathcal{L}}{\partial \lambda} = \dot{Q}_{HP1} + \dot{Q}_{HP2} - \dot{Q}_{demand} = 0$

Example: Optimal operation of two heat pumps



- $\frac{\partial \mathcal{L}}{\partial \lambda} = \dot{Q}_{HP1} + \dot{Q}_{HP2} - \dot{Q}_{demand} = 0$ ✓
- $\frac{\partial \mathcal{L}}{\partial \dot{Q}_{HP1}} = \frac{\partial P_{HP1}(\dot{Q}_{HP1})}{\partial \dot{Q}_{HP1}} - \lambda = 0$
- $\frac{\partial \mathcal{L}}{\partial \dot{Q}_{HP2}} = \frac{\partial P_{HP2}(\dot{Q}_{HP2})}{\partial \dot{Q}_{HP2}} - \lambda = 0$ ✓

Optimization problem classes

variables

continuous

equations

linear

linear program (LP)

Always converges to a global optimum
If it exists ☺

nonlinear

nonlinear program (NLP)

- Newton/Lagrange
  - Convergence only for convex problems guaranteed
  - Otherwise, only local optima
  - Global optimization method are available but computationally expensive

today

After this lecture, you are able to…

- ✓ identify basic **elements of an optimization problem**.
- ✓ distinguish **linear problems** (LP) and **nonlinear problems** (NLP).
- ✓ use basic **solution methods** for both LPs and NLPs.
- ✓ formulate simple **energy system optimization problems (LP and NLP)**.