University of Central Lancashire
UCLan

CO3519
Artificial Intelligence

Dimensionality and objective functions
Example scenarios
Correlating data (intro/discussion)

Where opportunity creates success

Module structure

Upon successful completion of this module, a student will be able to:

1) Explain the theoretical underpinnings of algorithms and techniques specific to artificial intelligence;
2) Critically evaluate the principles and algorithms of artificial intelligence;
3) Analyse and evaluate the theoretical foundations of artificial intelligence and computing;
4) Implement artificial intelligence algorithms.

uncertainty quantification

optimization

reasoning and learning

agents and decisions

knowledge representation

modelling

game theory

Module structure

On the field of **modelling**, we will:

- Discuss the use of models in optimization and decision support;
- Apply optimization algorithms to model parameterization;
- Assess model quality by validation and testing.

uncertainty quantification

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reasoning and learning

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Dimensionality and objective functions

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23rd November 2021

Specification of an MCO decision problem

Three elements need to be specified to facilitate multicriteria decision support:

1) The **parameter space**: What is it that can be varied and is in direct control (or to be assumed as being under direct control) of the decision maker? What quantities define that which is possible in the scenario?

   The permitted range (+ any applicable constraints) need to be stated.

2) The **objective space**: What are our criteria? If numerical optimization with scipy is to be used, best expressed as minimization objectives.

3) The **objective function** – if all criteria are minimization objectives, this can be called a multicriteria **cost function**.

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2) The **objective space**: What are our criteria? If numerical optimization with scipy is to be used, best expressed as minimization objectives.

3) The **objective function** – if all criteria are minimization objectives, this can be called a multicriteria **cost function**: This must *actually be implemented **as a function***, in the sense that the term has in programming.

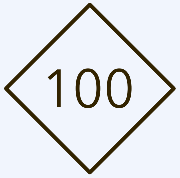
Specification of an MCO decision problem

In general, all objectives **y** (taken together) are a function of all parameters **x** (taken together); or, equivalently, each objective y_i is a function of the whole list or vector of parameters $\mathbf{x} = [x_0, \dots x_{m-1}]$.

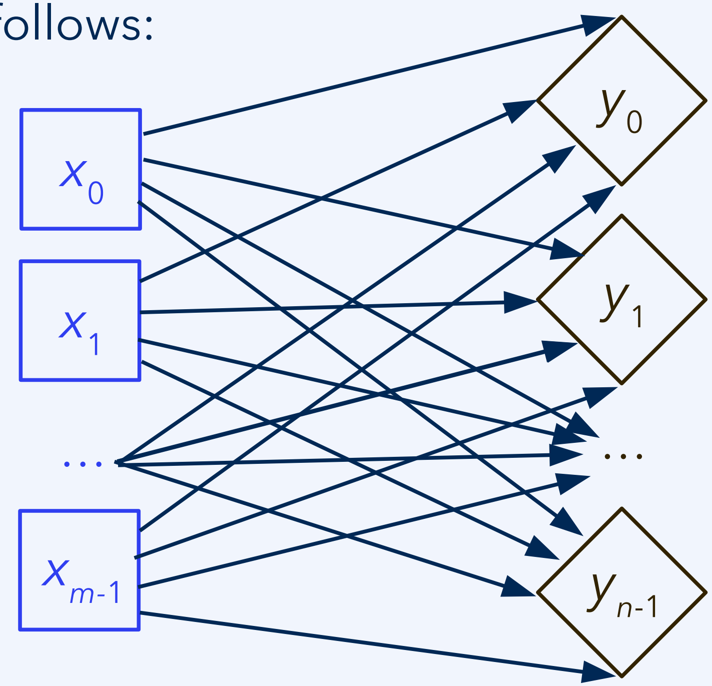
As an **influence diagram**, this would look as follows:

rectangles represent **decisions (parameters)**

circles or ellipses repre-sent **unknown quantities**



diamonds contain **objective outcomes**



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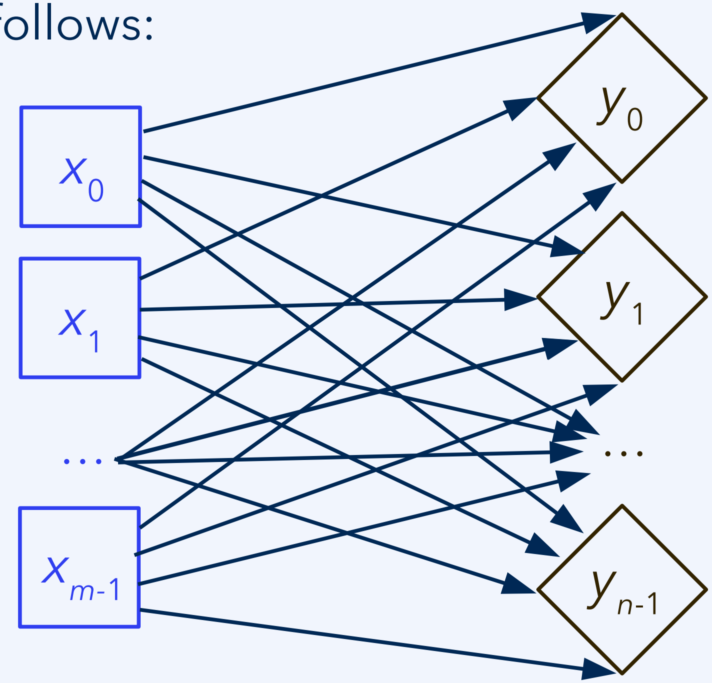

Required functional dependencies:

- $y_0(x_0, x_1, \ldots, x_{m-1})$
- $y_1(x_0, x_1, \ldots, x_{m-1})$
- …
- $y_{n-1}(x_0, x_1, \ldots, x_{m-1})$

A model for each of these will be needed.

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Observation

Directly combining all variables complicates the process of constructing the objective function, often unnecessarily. It can help to introduce **intermediate quantities**, simplifying the structure of the problem so that no longer "all depends on all."

Specification of an MCO decision problem

It is convenient to implement the cost function according to this template:

```
def cost_function(x):
    [body of the cost function]
    return y
```

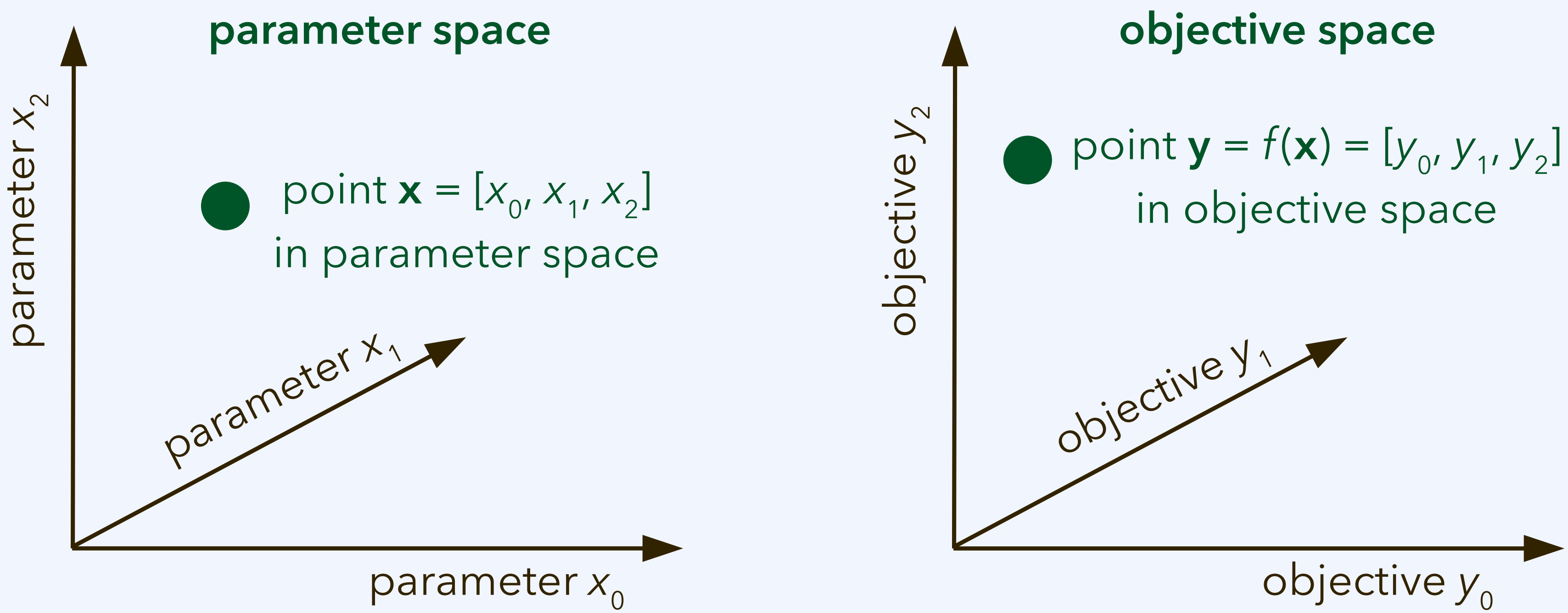
Therein, **x** is a list with *m* elements, x[0] to x[m-1]: The parameter values.

The return value **y** is a list with *n* elements, y[0] to y[n-1]: The outcomes.

This function must be an implementation of an algorithm that determines the outcomes for the optimization objectives for any given permitted parameters.

Then it can be passed on to scipy, *e.g.*, using the wrappers from our notebooks.

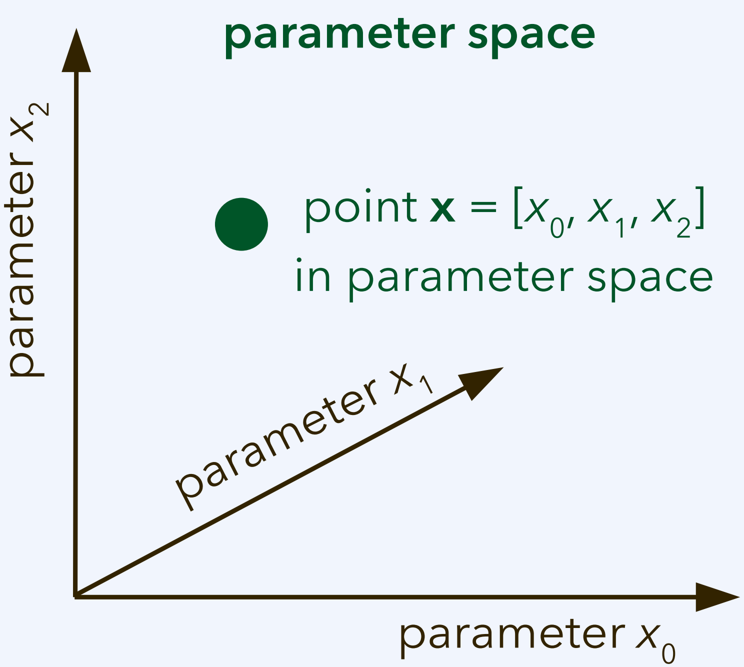
Specification of a MCO decision problem



In general, there can be any number m of parameters (m-dimensional parameter space) and any number n of objectives (n-dimensional objective space).

The optimization problem is defined by a function f that maps a list of parameters x = [x_0, …, x_{m-1}] to the outcome for the objectives **y** = f(**x**) = [y_0, …, y_{n-1}].

Dimensionality



first direction: $\mathbf{e}_1 = [1, 0, 0]$

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third direction: $\mathbf{e}_3 = [0, 0, 1]$

In general, there can be any number *m* of parameters (*m*-dimensional parameter space) and any number *n* of objectives (*n*-dimensional objective space).

By **dimension** of a space or set we mean the **number of independent directions** in which it is possible to move while remaining in the respective space or set.

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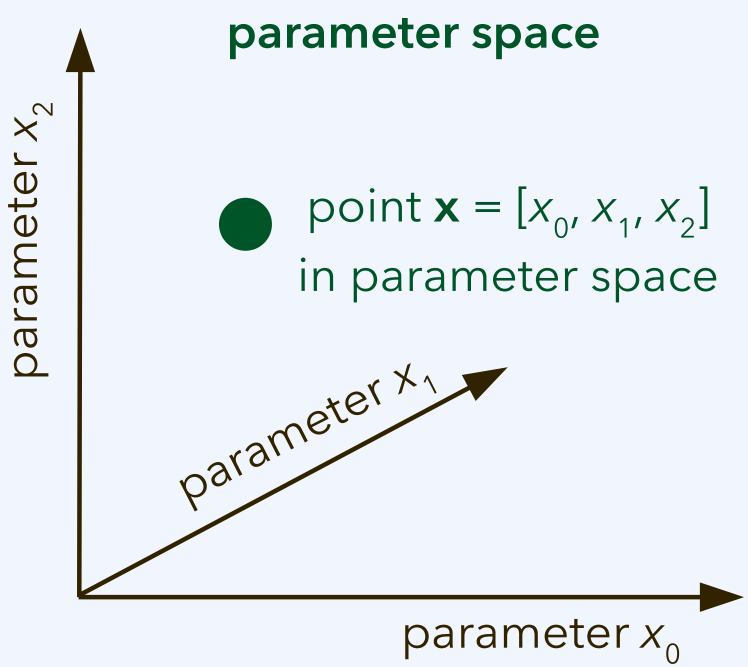

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Any fourth direction (mathematically, a vector) would be **linearly dependent** on the above; *i.e.*, it can be constructed as a **linear combination**:

$$[4, 3, 2] = 4\mathbf{e}_1 + 3\mathbf{e}_2 + 2\mathbf{e}_3$$

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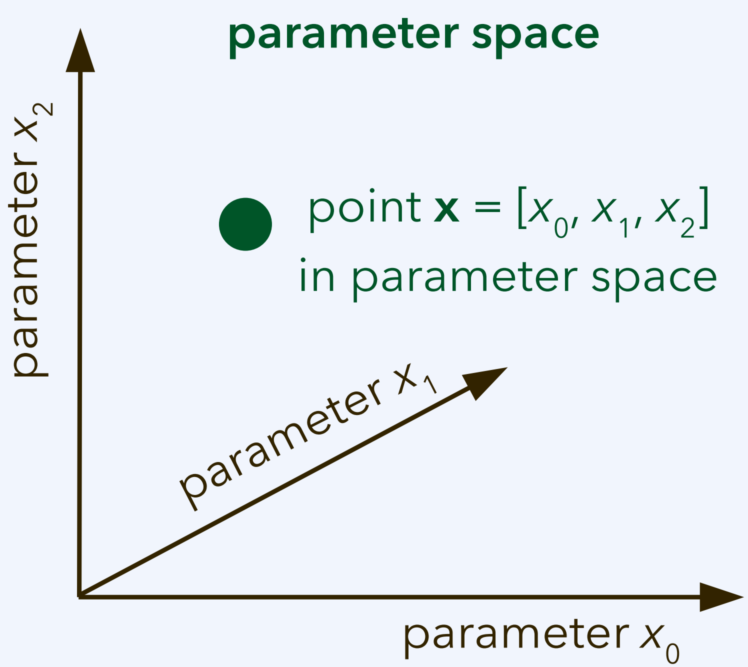

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Another way of obtaining the **dimension of a finite object** is to **rescale** it by a factor c (*e.g.*, double all lengths, $c = 2$) and evaluate how its total size changes.

If the dimension of the object is m, its size will change by the factor c^m. For example, a cube increases its volume by factor 8 if all lengths double ($c = 2$).

Dimensionality in multicriteria optimization

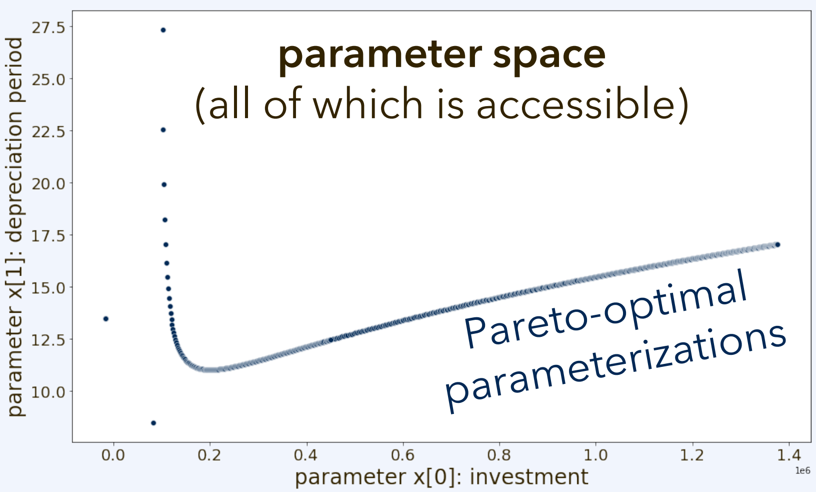
In general, a function has a **domain** and a **range** (also called **codomain**).

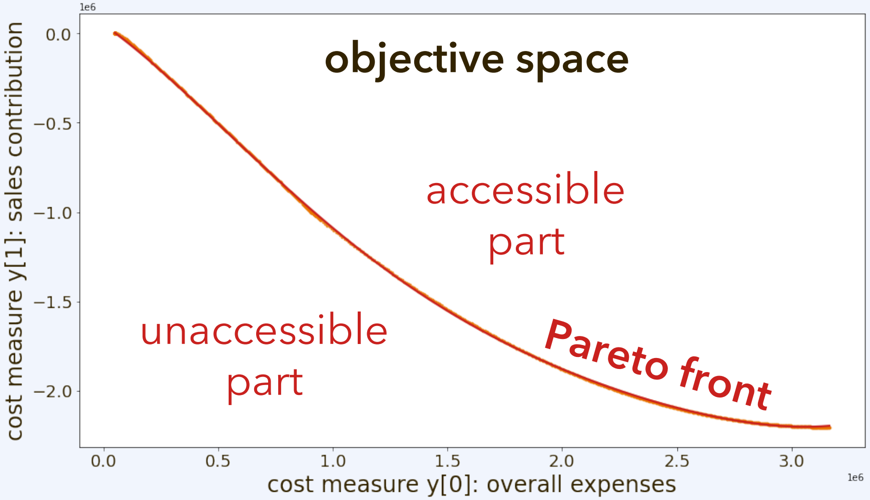
Any element of the domain is a valid argument. The function value (or return value) must be an element of the range.

$$\mathbf{y} = f(\mathbf{x})$$

with $\mathbf{x} = [x_0, x_1, \ldots, x_{m-1}]$
and $\mathbf{y} = [y_0, y_1, \ldots, y_{n-1}]$

In our case, the **parameter space** is the domain and the **objective space** is the range/codomain.





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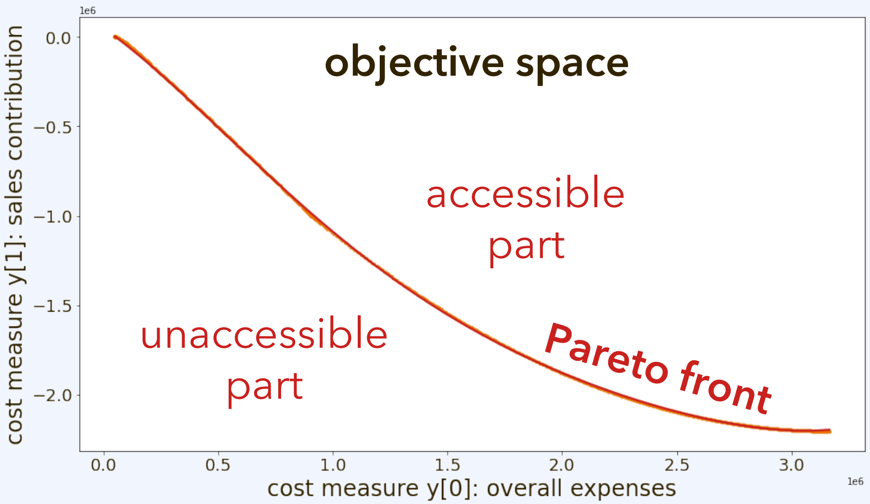
In our case, the **parameter space** is the domain and the **objective space** is the range/codomain.

The **image** of a function is that **part of the range** (codomain) consisting of the actually occurring function values, *i.e.*, those that are obtained as $f(\mathbf{x})$ for some $\mathbf{x}$ from the domain.

In our case, the image is the **accessible part of objective space**.



Dimensionality in multicriteria optimization

What dimension do the spaces and sets have in multicriteria optimization?

- The dimension of the **parameter space**, defined by m independently variable parameters $x_0, \ldots, x_{m-1}$, is exactly m, by construction.
- The **objective space**, defined over n criteria $y_0, \ldots, y_{n-1}$, has dimension n.
- The **accessible part of objective space** (*i.e.*, image of the objective function) cannot be higher-dimensional than the objective space as such. Therefore, its dimension q must satisfy $q \leq n$. However, the image of a continuous function cannot be greater than that of its domain. Therefore, $q \leq m$.

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- The **Pareto front** in objective space must be lower-dimensional than objective space itself, due to the domination criterion; therefore, $p \leq n-1$ for its dimension p. But it must also all be accessible; therefore, $p \leq q \leq m$.
- The dimension $p' \leq m$ of the **Pareto-optimal region in parameter space** must be at least the same as that of the Pareto front; hence, $p \leq p' \leq m$.

Example scenarios

Example scenario #1a (Tutorial 1.2 problem)

Here, the accessible part of objective space was one-dimensional ($q = 1$).
There was no "Pareto front," but a single optimal point ($p' = p = 0$).

Three parameters ($m = 3$):

- investment $i = x_0$
- depreciation period $d = x_1$
- production volume $p = x_2$

One optimization criterion ($n = 1$):

- total expected balance per year y

  (inverted for minimization)

Example scenario #1a (T1.2): Visualization

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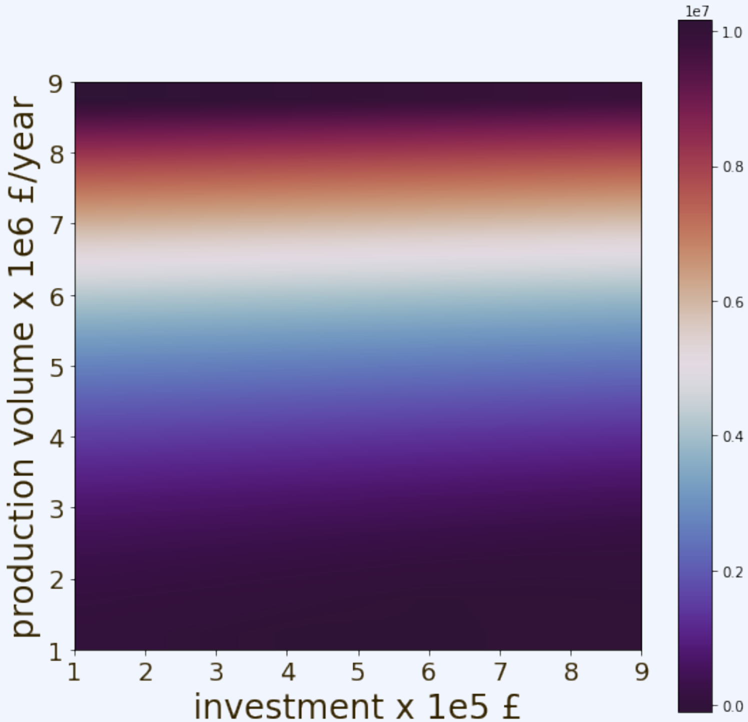

Visualization of the scenario by Anzhi Wang (with $d = 12$ fixed)

Example scenario #1b (industrial investment)

Here, the accessible part of objective space is two-dimensional ($q = 2$).
The set of Pareto-optimal choices and Pareto front are both 1D ($p' = p = 1$).

Two parameters ($m = 2$):

- investment $i = x_0$
- depreciation period $d = x_1$

Two optimization criteria ($n = 2$):

- expenses y_0
- contribution from sales y_1 (that is, $-1\times$ the income from sales)

Example scenario #1b: Visualization

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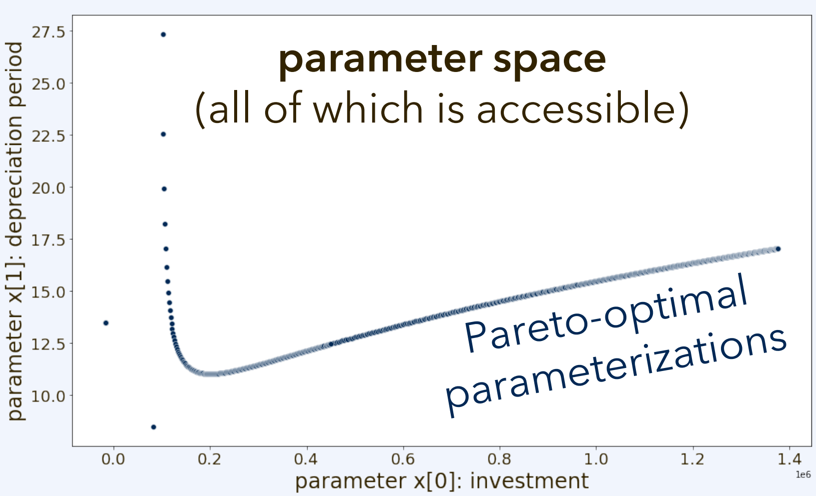
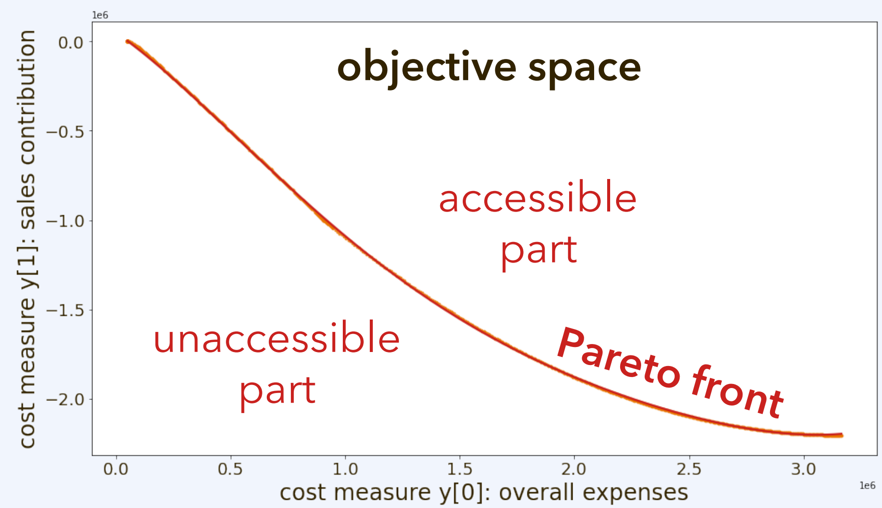
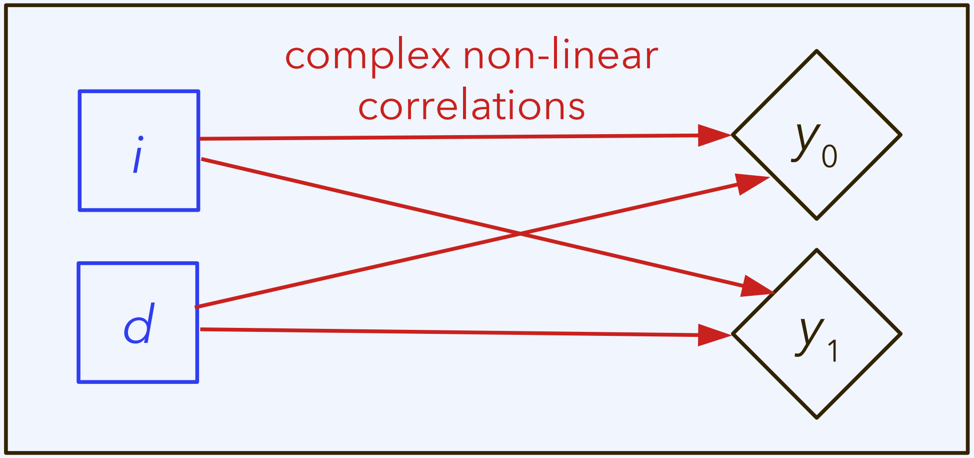
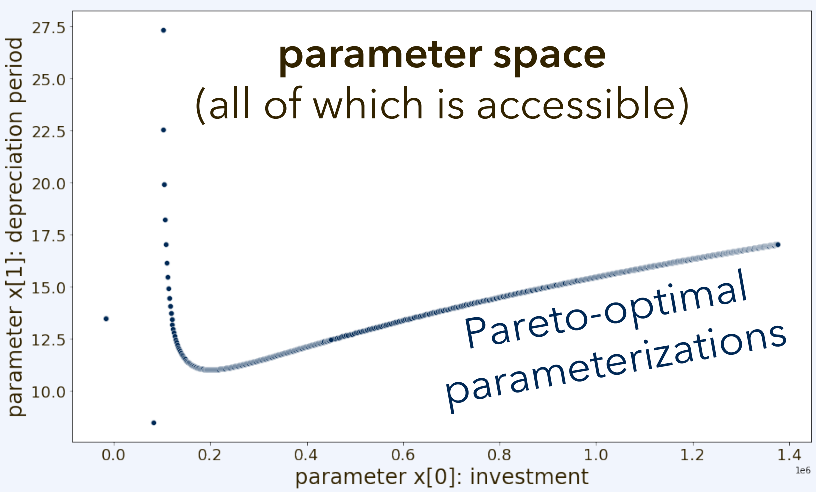
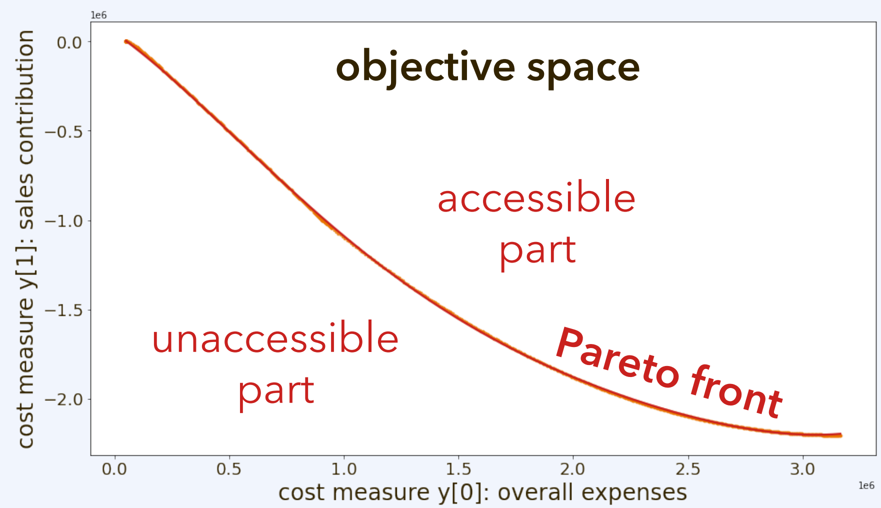




Example scenario #1b: Influence diagram







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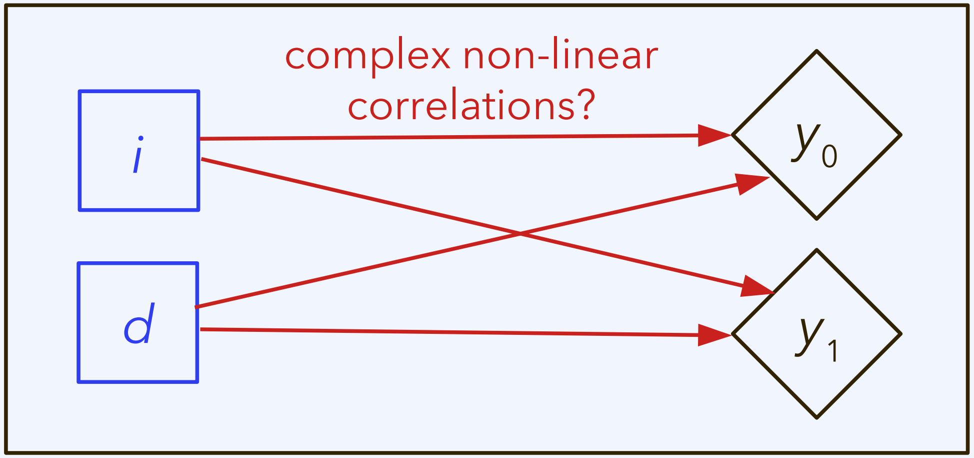
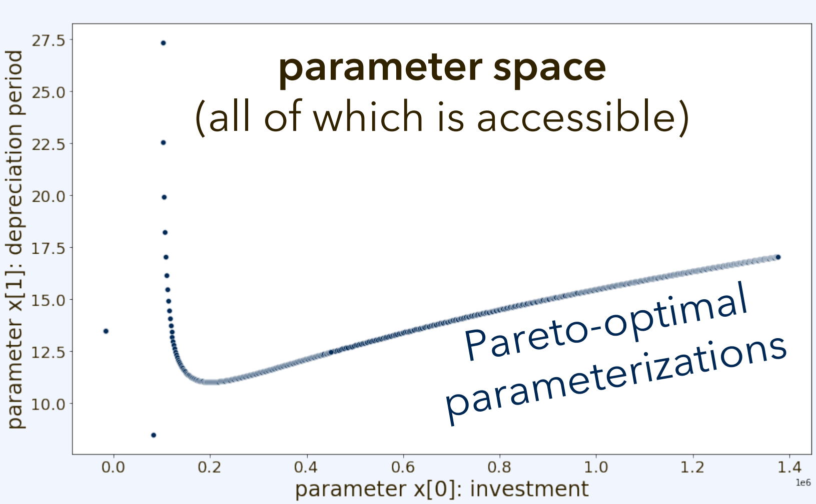
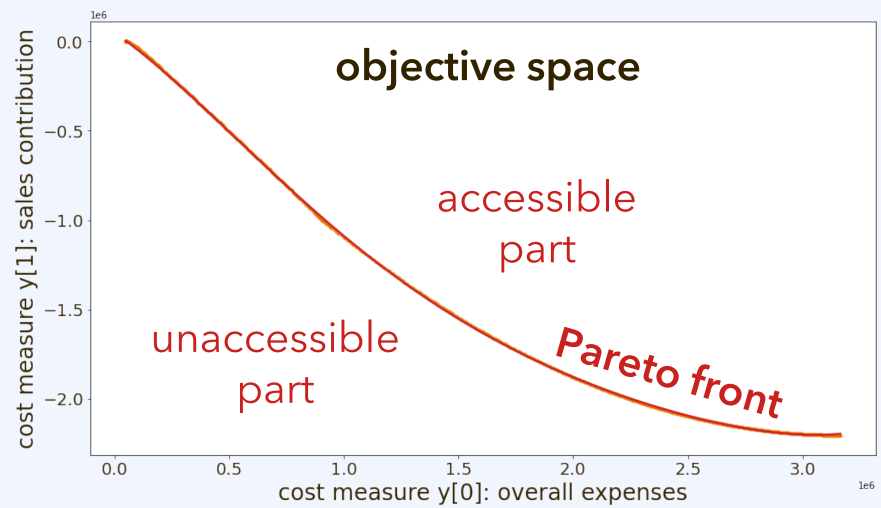


Really?

Check the implementation





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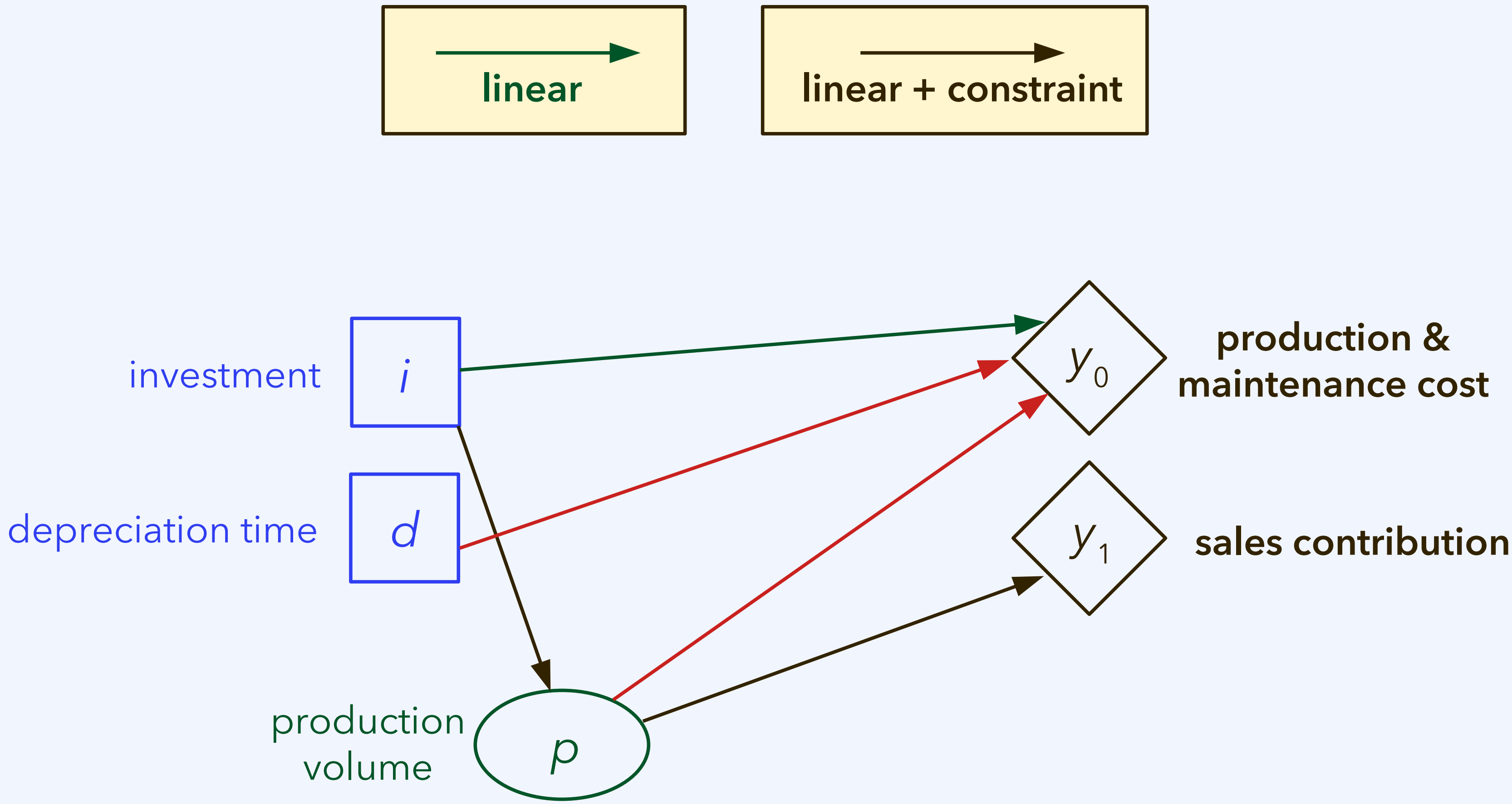
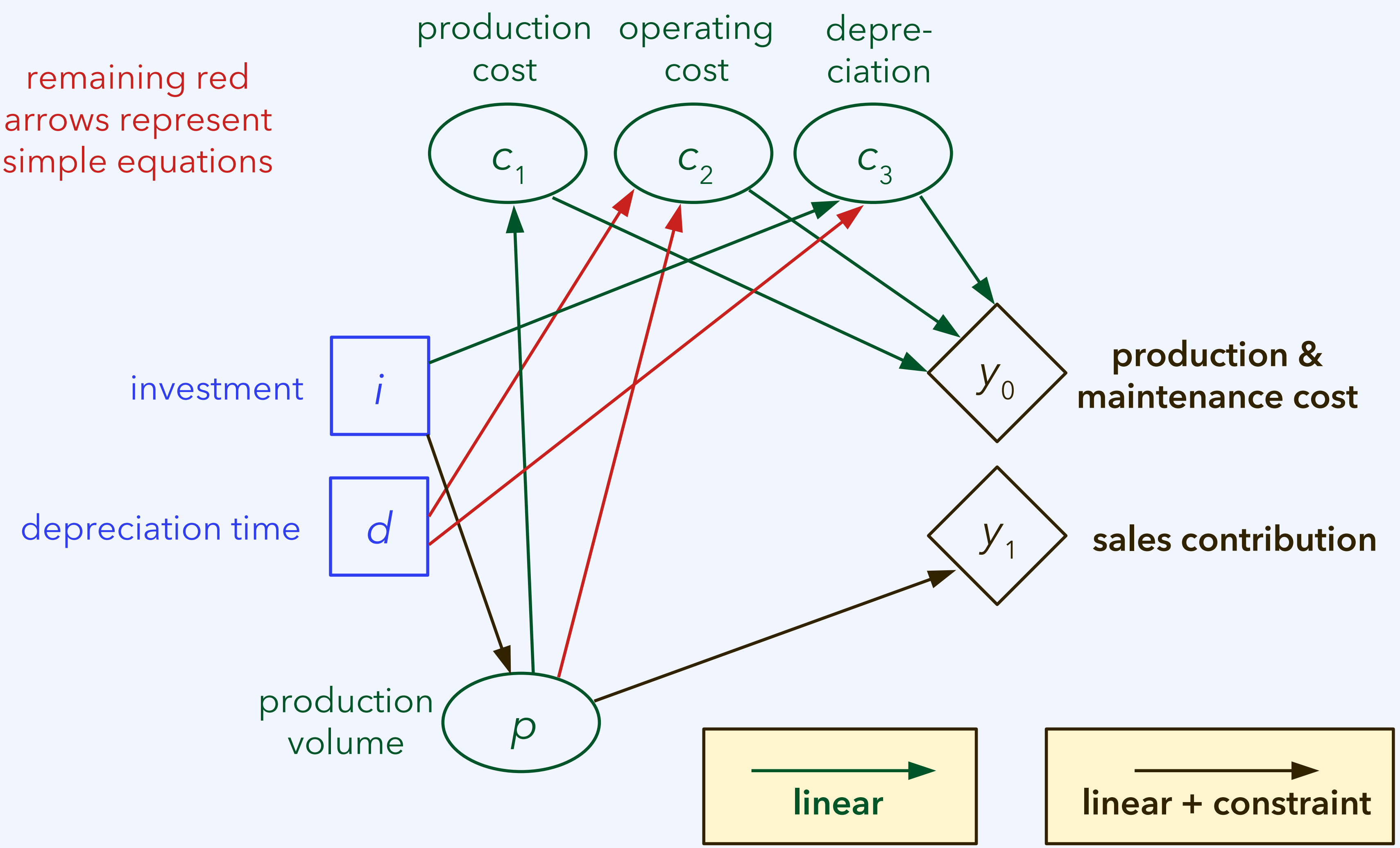


Example scenario #1b: Influence diagram

remaining red arrows represent simple equations



Example scenario #2 (Caribbean)

Government might support a one-time investment into the university, of the order of 40 million sol., if the Grand Council can agree on a convincing plan how to spend it. You would like to present such a plan to the Grand Council.

Example parameters:

x_0, x_1, and x_2) **Fractions of the one-time investment** going into A, B, and C. The share going into D is then given by $1 - x_0 - x_1 - x_2$.

3D parameter space, constraints: $0 \leq x_0, x_1, x_2$ as well as $x_0 + x_1 + x_2 \leq 1$.

Example minimization objectives (**3D objective space**):

y0) Decrease in research strength within five years, measured by citations to papers from our institution in the fifth year, compared to last year.

y1) Others' share in the real-estate sector five years from now, measured by the fraction of tenants within the city *not* living on our property.

y2) Number of votes in the Grand Council against the plan.

Example scenario #2 (Caribbean)

The accessible part of objective space was three-dimensional ($q = 3$).
The Pareto front was two-dimensional ($p = 2$).
The set of Pareto-optimal parameterizations was two-dimensional ($p' = 2$).

Example parameters (3D parameter space, $m = 3$):

- x_0, x_1, and x_2) Fractions of the one-time investment going into A, B, and C.
  The share going into D is then given by $1 - x_0 - x_1 - x_2$.
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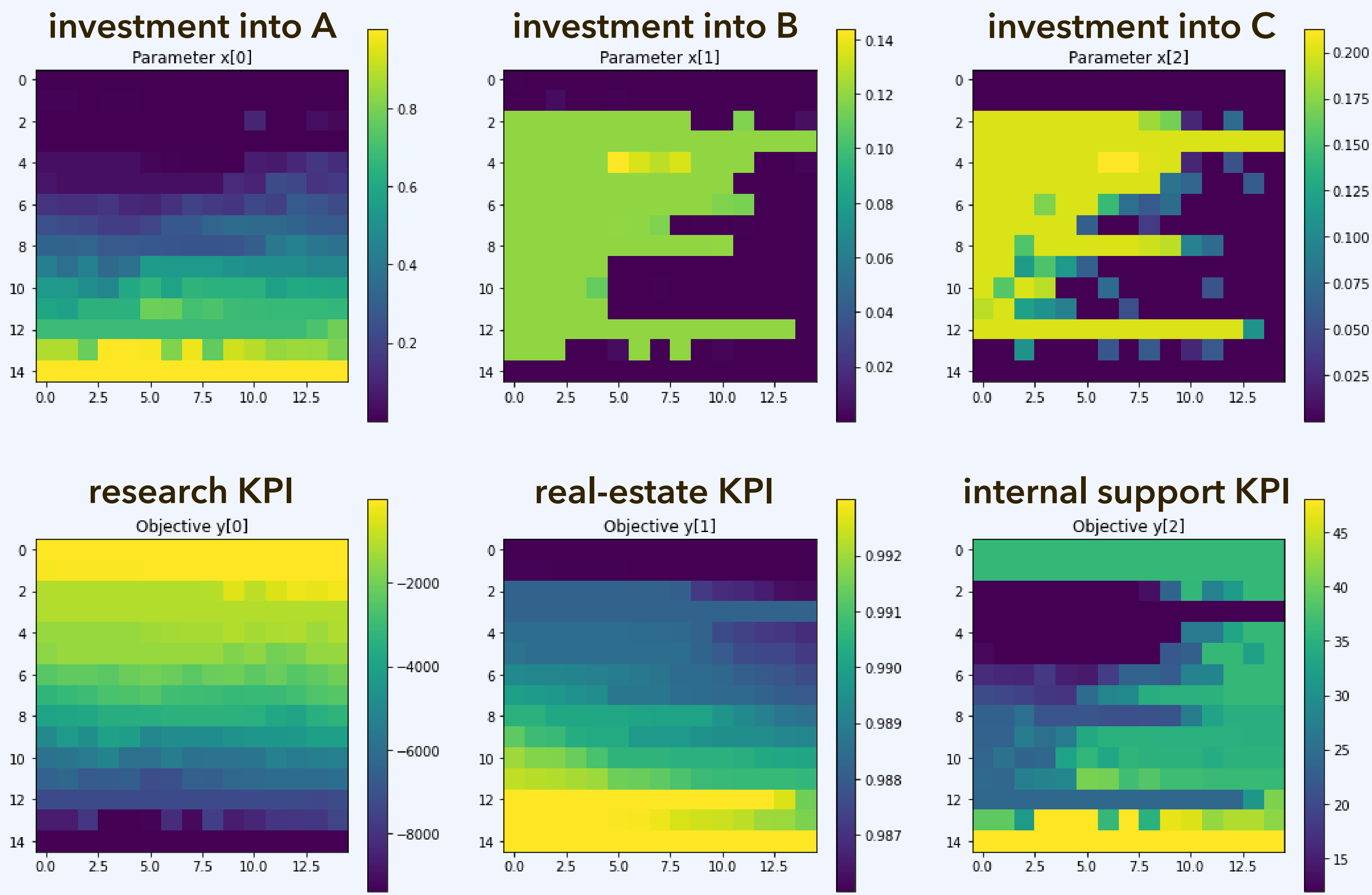
Example scenario #2 (Caribbean): Visualization



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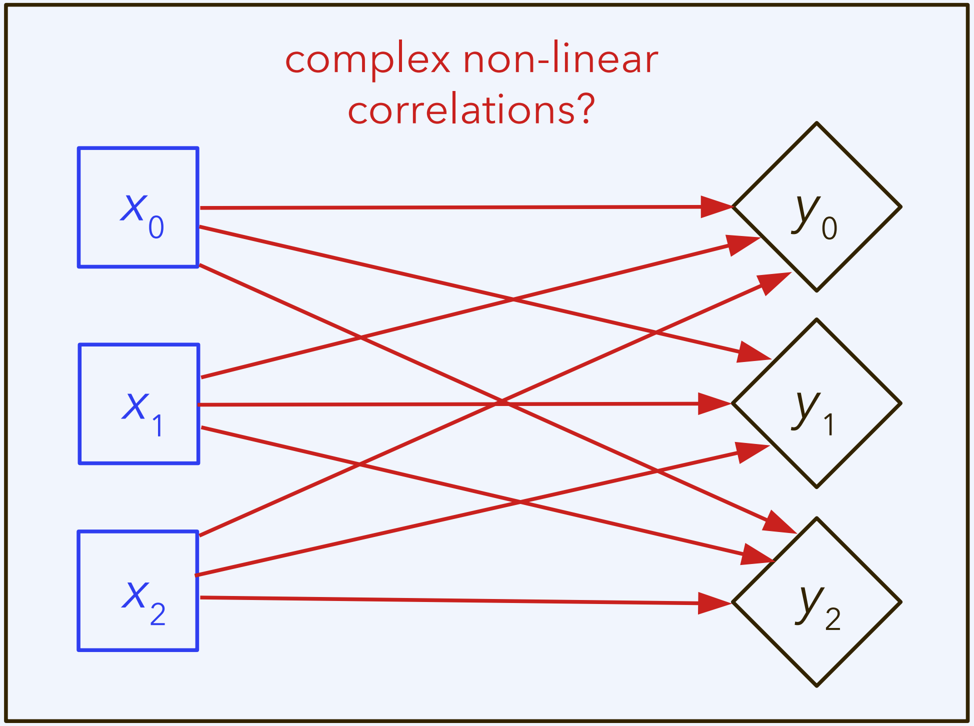

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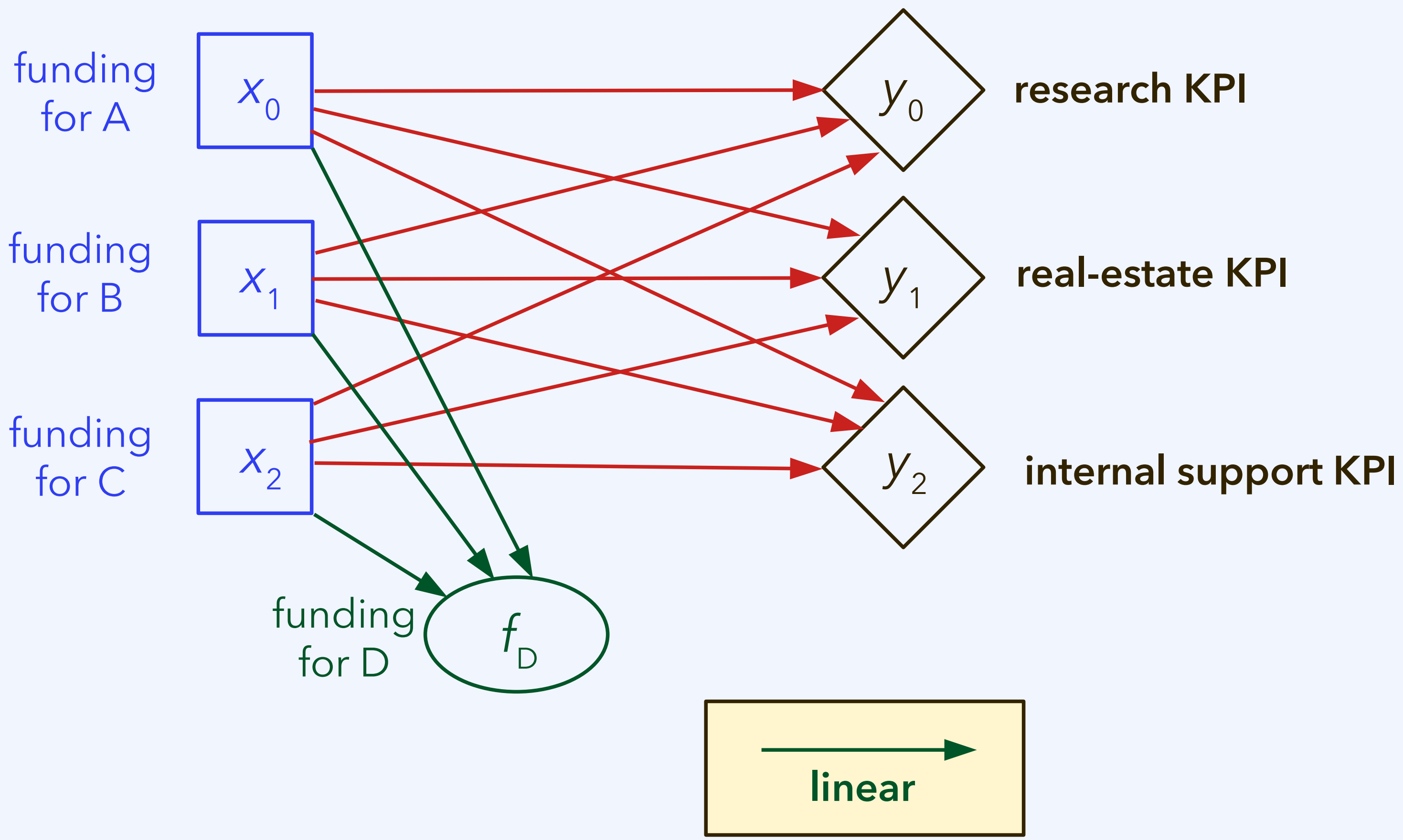

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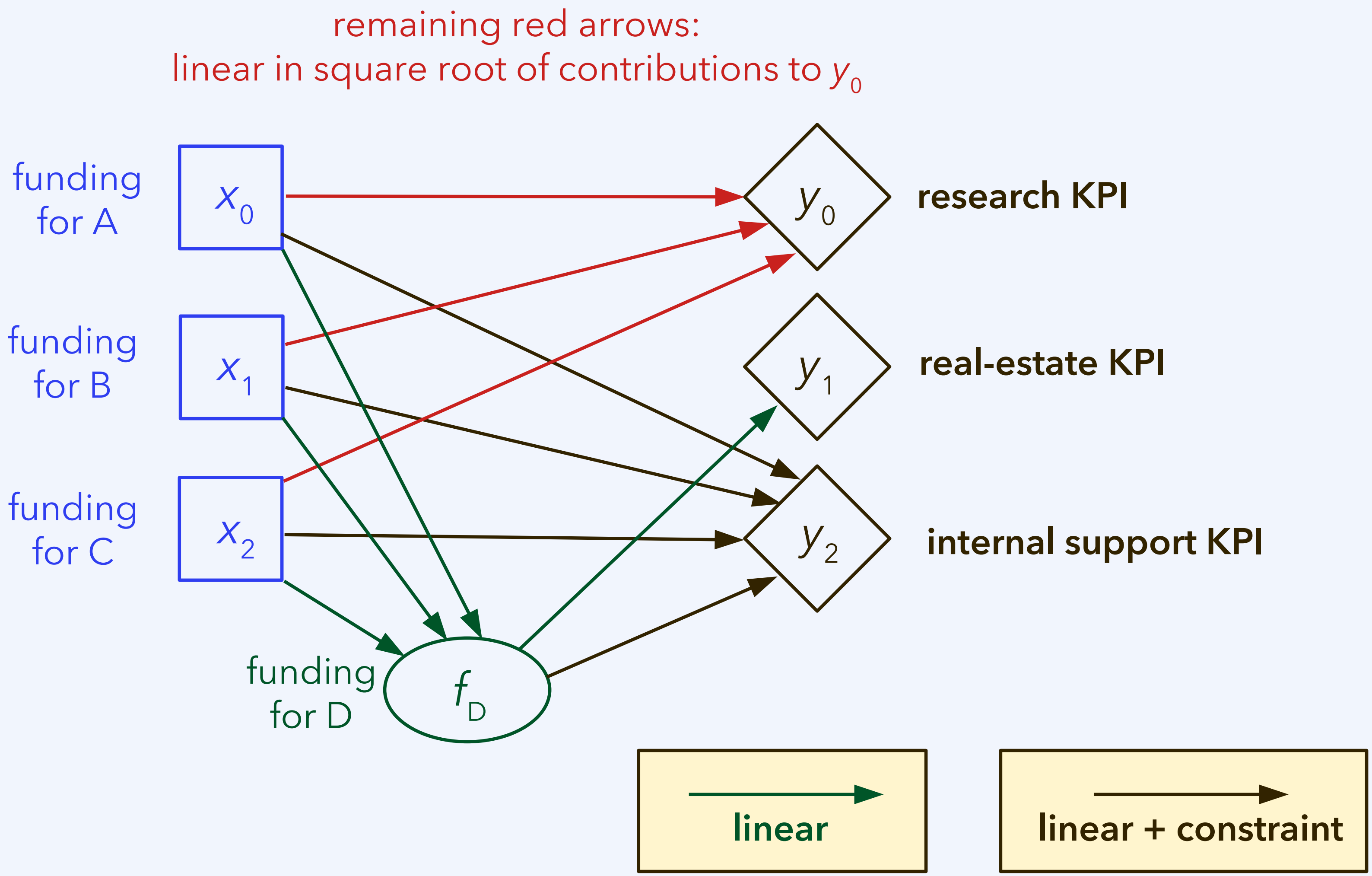


Example #3 from research practice

The considered problem was from model optimization. The task was to parameterize models that accurately reflect physical behaviour.

Four model parameters, $m = 4$.

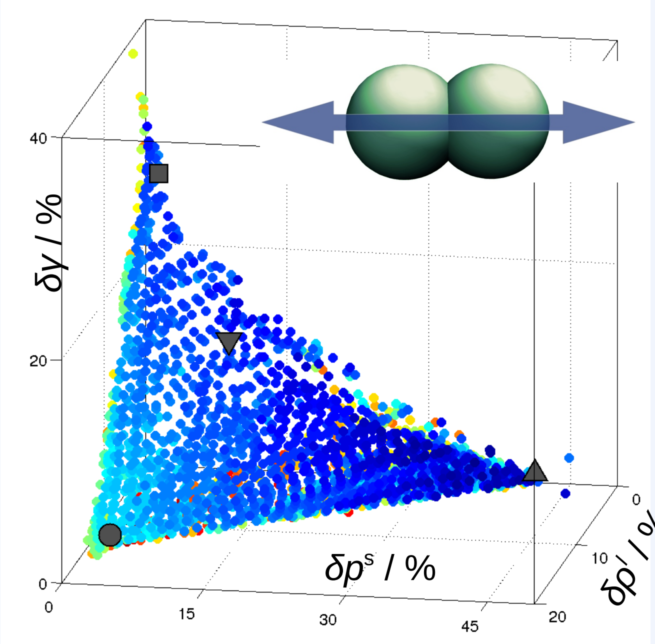
Three criteria (quantifying accuracy of predictions for three kinds of properties), $n = 3$.

Dimension of image of the objective function (accessible part of objective space), $q = 3$.

Dimension of the Pareto front, $p = 2$.

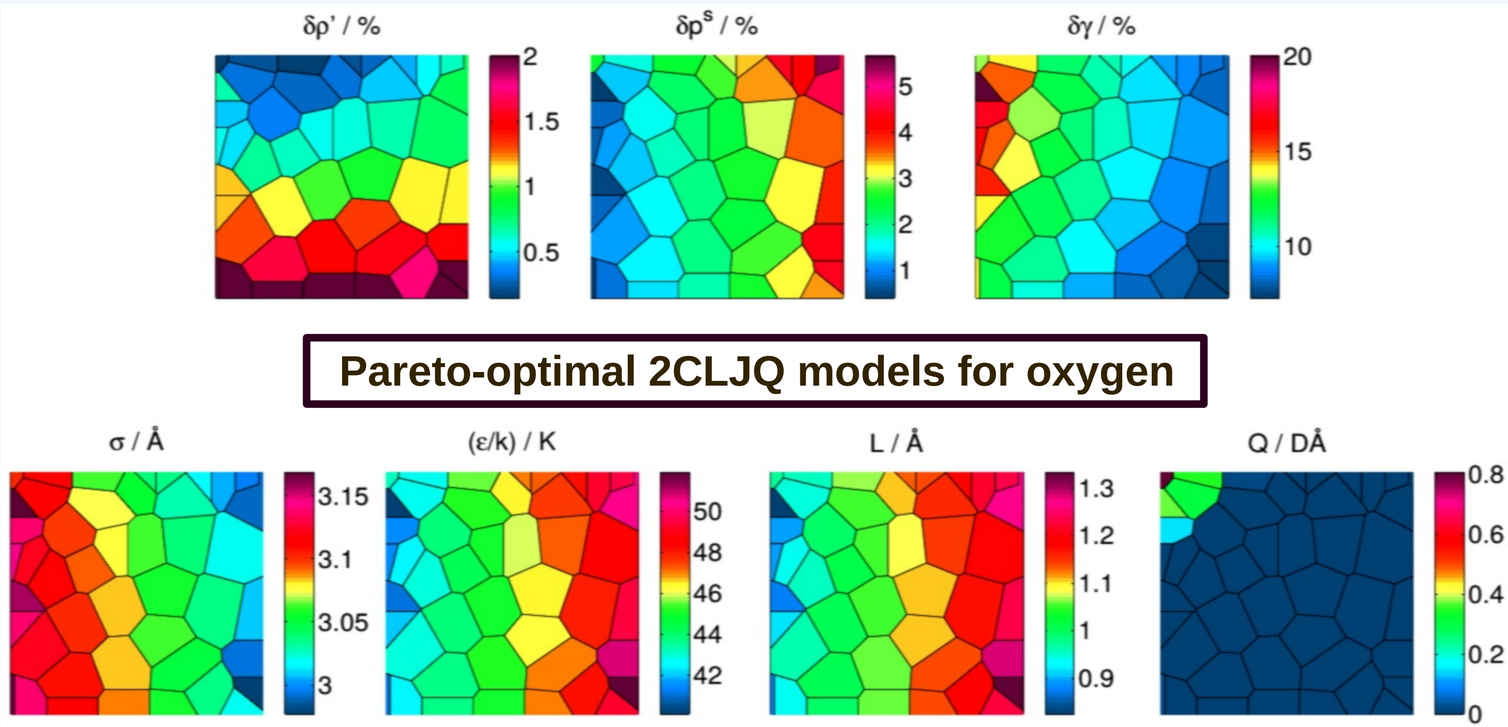
Dimension of Pareto-optimal part of parameter space: $p' = 2$.

2CLJQ molecular models of low-molecular fluids: Objective space and Pareto front



Example #3 from research practice: Visualization

Self-organized patch plots[1] visualizing the Pareto front and the Pareto-optimal models:



objective space

parameter space

[1]K. Stöbener, P. Klein, M. Horsch, K. Küfer, H. Hasse, *Fluid Phase Equilib.* 411, 33 – 42, **2016**.

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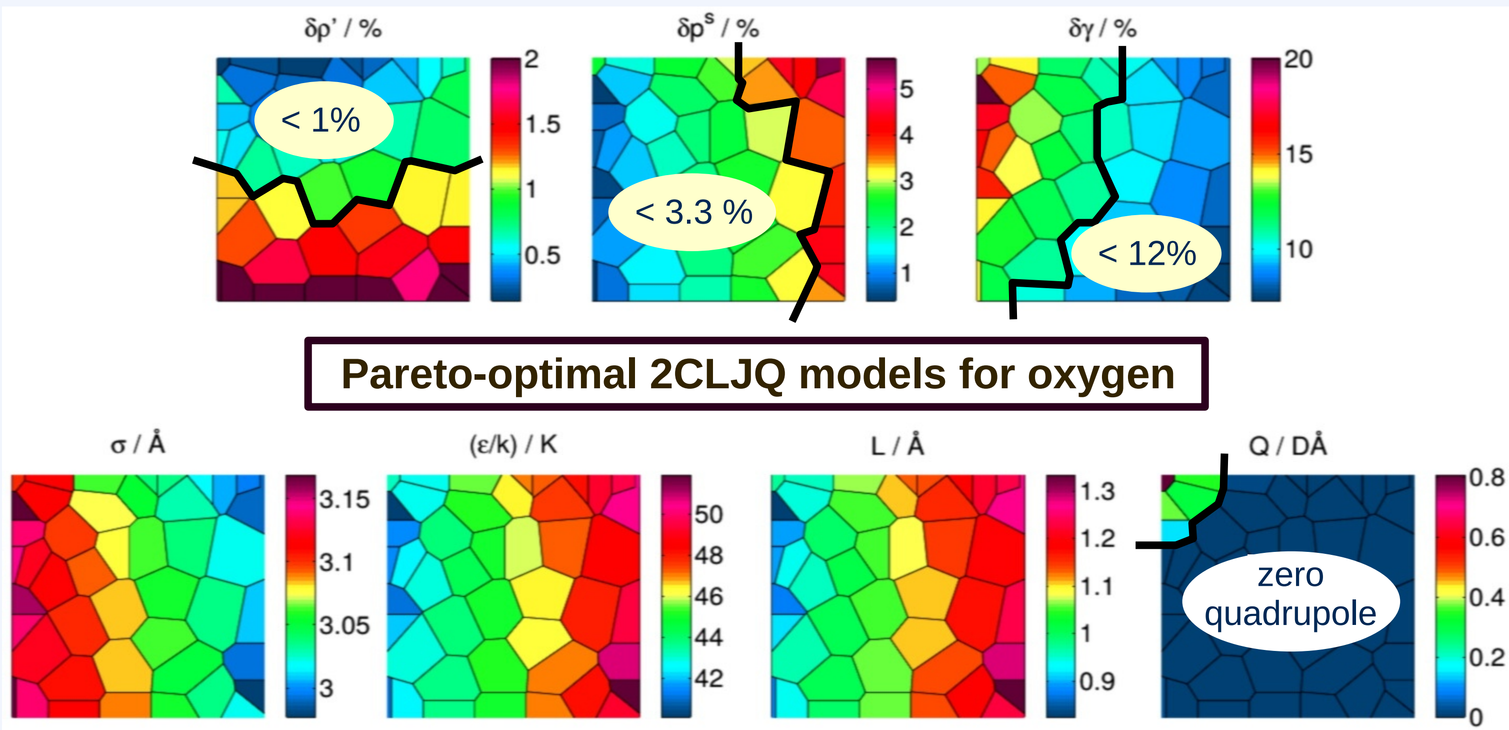

objective space

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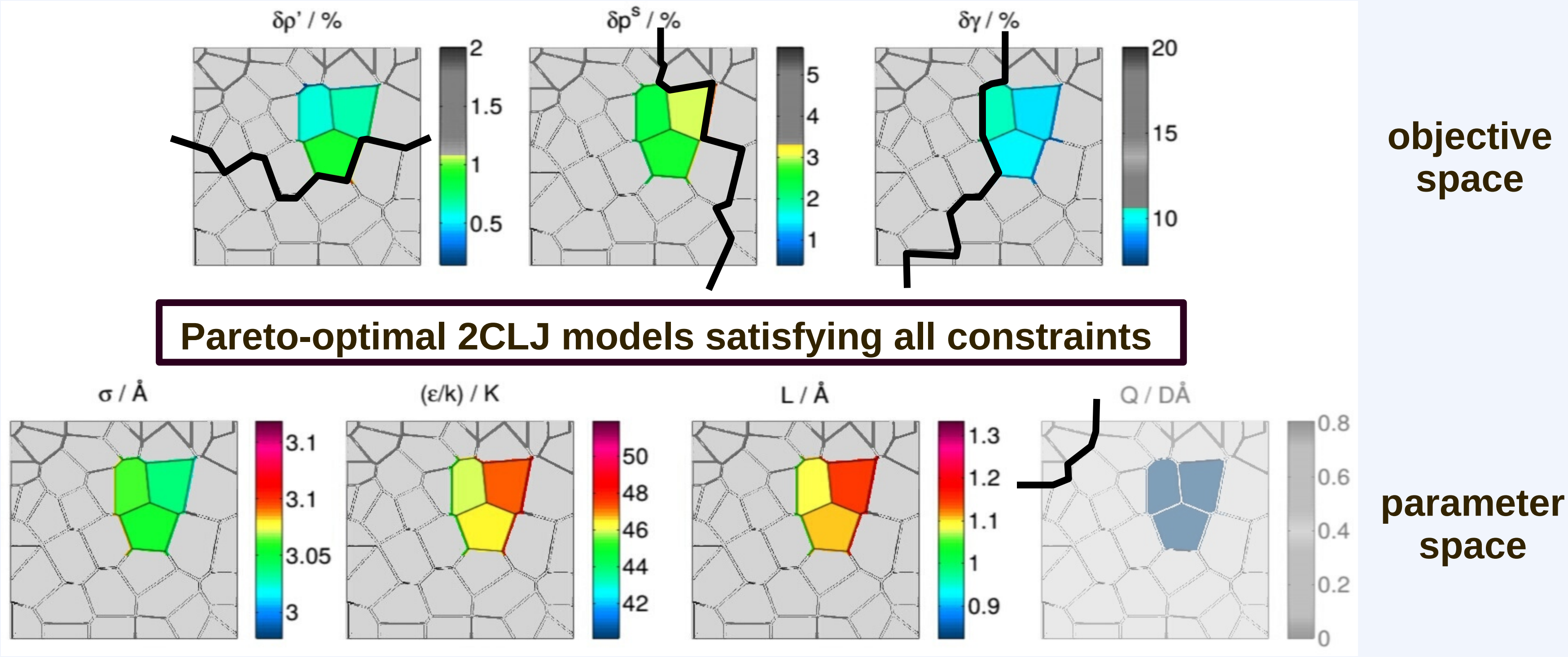

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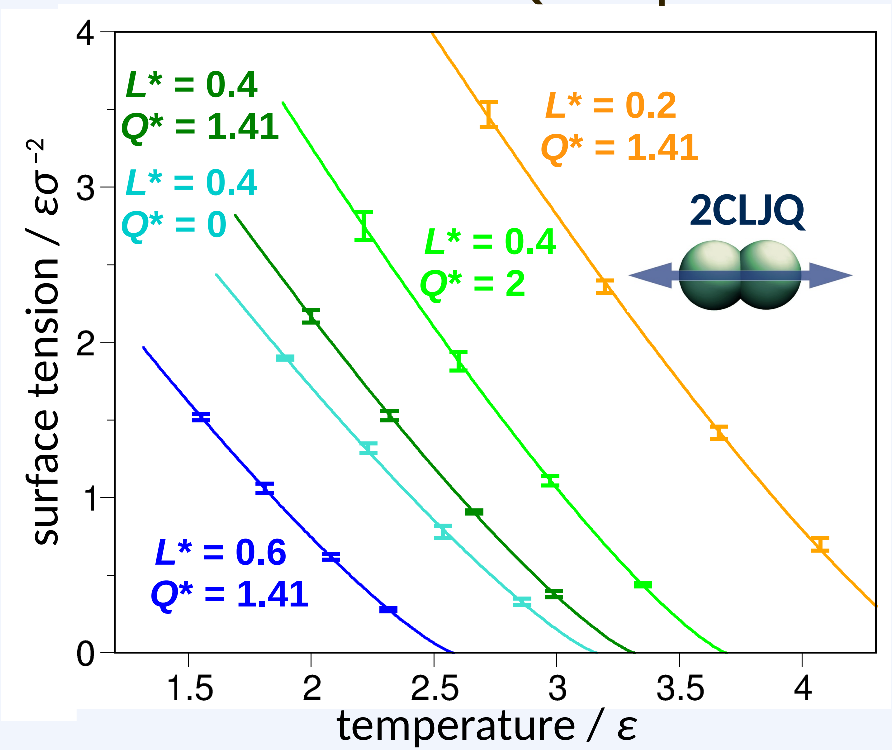
Example #3: Underlying model (non-linear)

2 LJ Centres + Quadrupole



- Systematic exploration of the physically relevant part of the model parameter space
- Correlation of the 2LJCQ surface tension by critical-scaling expressions

Discussion

What problems are you finding when constructing a model cost function?

What is most challenging at specifying parameters and objectives?

What should we focus on in our discussion of modelling?

Correlating data (intro/discussion)

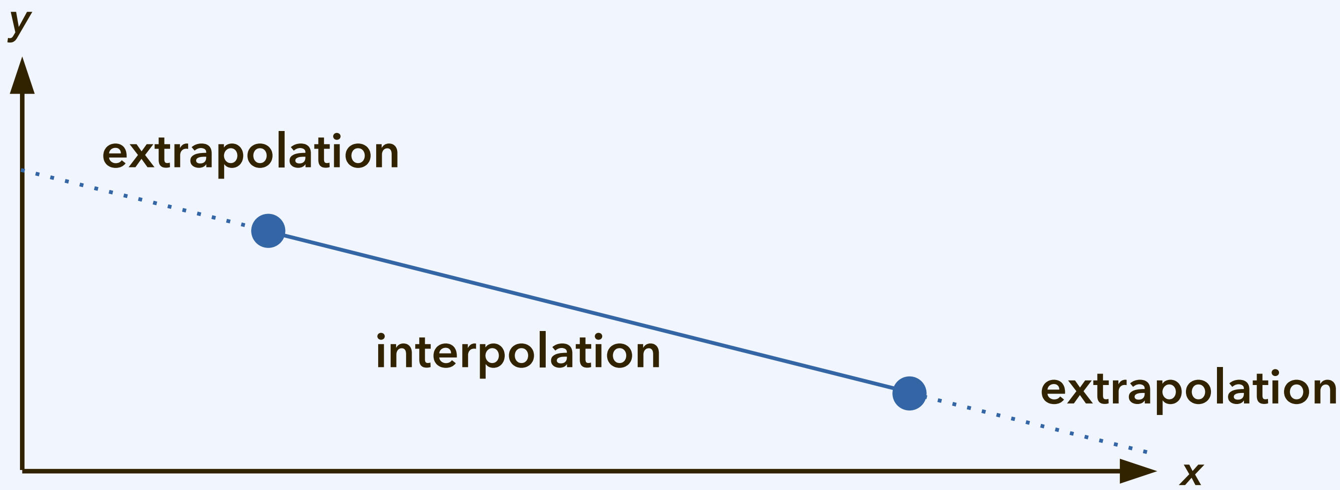
CO3519

23rd November 2021

Linear regression

Any two points define the equation of a line, $y = mx + b$.

Two unknowns, exactly two data points by which the unknowns are eliminated.

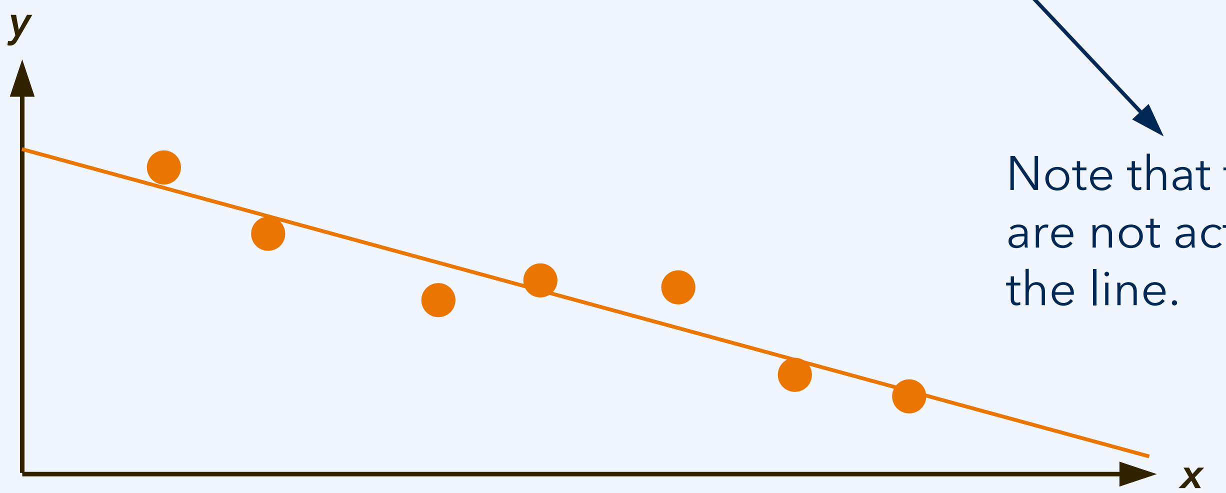


This permits both **interpolation** and **extrapolation**. But how reliable are they?

Linear regression

However, it is also possible to linearly correlate larger data sets.

Two unknowns, many more data points: Apparently overspecified.



Note that the points are not actually on the line.

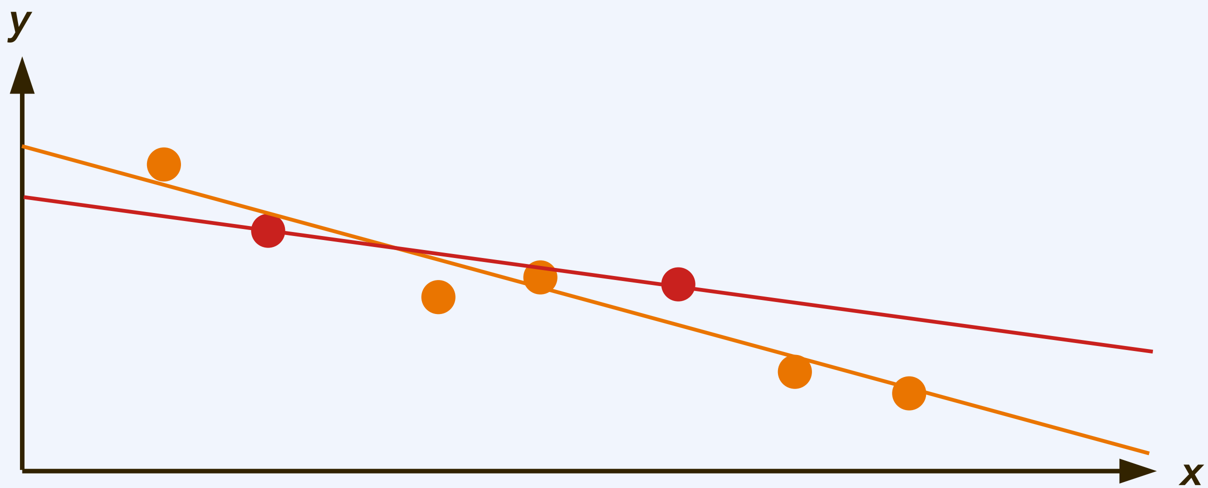
Determining a linear regression (*i.e.*, fit to data) is an **optimization problem**.

Usually the mean square deviation between the line and the data is minimized.

Regression and reliability: Discussion

The red line is exact for the two data points from which it was determined.
The orange line is inexact for all data points.

Why would we still rather prefer to rely on the orange line?



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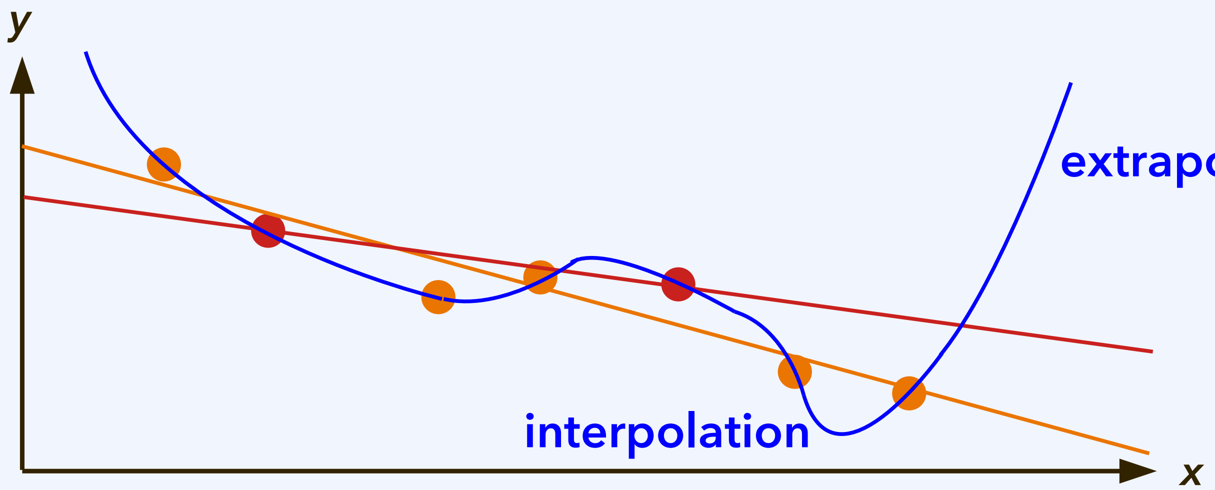

The blue line is exact for all data points.

Would we rely on it for interpolation and/or extrapolation? If no, why not?

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CO3519
Artificial Intelligence

Dimensionality and objective functions
Example scenarios
Correlating data (intro/discussion)

Where opportunity creates success