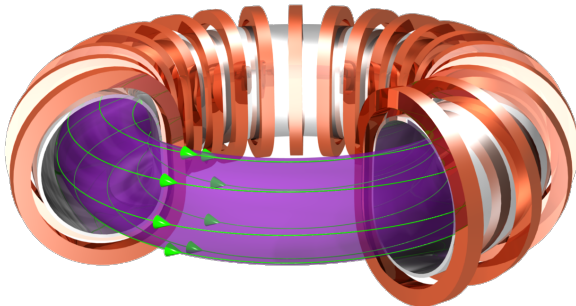


# OptiFun: Optimising Fusion with Functional Programming

Patrik Jansson

Computer Science and Engineering (CSE), Chalmers and U. of Gothenburg

2024-05-17



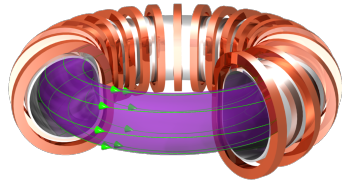
# What is “OptiFun”?

- Chalmers Energy Area of Advance grant (3M SEK) for a collaboration project: *“Optimising Fusion with Functional Programming”*
- 2022–2023: joint work between Computer Science and Physics
- Pls: Prof Patrik Jansson (CSE dept.) + Prof Tünde Fülöp (Physics dept.)

Aim: “... **to combine numeric and symbolic methods** to accelerate first-principles simulations and enable optimisation of fusion confinement designs. ... build a **reliable and versatile toolset** for performance **optimisation** of strongly coupled physical systems **with a large parameter space**, and apply it to explore reliable fusion designs.”

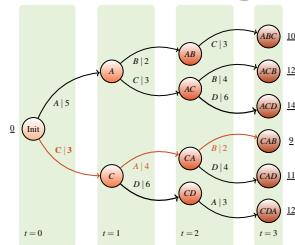
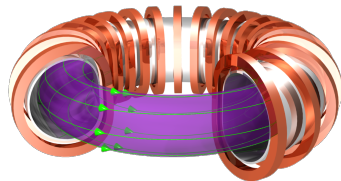
# Applications: fusion energy experiments and climate impact research

- Parameter optimisation of tokamak fusion experiments
  - Several parameters can be adjusted, thus a toolkit is needed to help “tune” the simulations
  - We have published two journal papers based on the results



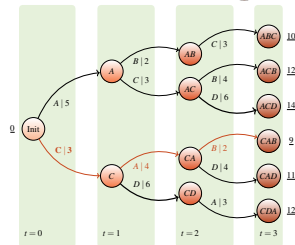
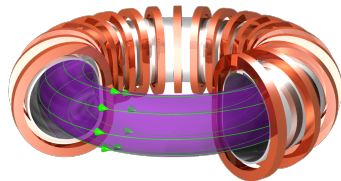
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- Optimal decision making
  - with the Potsdam Institute for Climate Impact Research
  - **The impact of uncertainty on optimal emission policies**, Botta, Jansson, Ionescu. *Earth System Dynamics* (2018)
  - **Responsibility Under Uncertainty: Which Climate Decisions Matter Most?**, Botta et al. incl. Jansson, *Environmental Modeling & Assessment* (2023)



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  - **Responsibility Under Uncertainty: Which Climate Decisions Matter Most?**, Botta et al. incl. Jansson, *Environmental Modeling & Assessment* (2023)
- Very different areas, but common setting:
  - Real experiments are very expensive (or impossible), thus numerical simulations are needed
  - with several input parameters
  - and several objectives (cost, damage, temperature, etc.)



## Setting: black-box function with multiple objectives

- The object of study is an expensive, black-box objective function  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$
- ...and the aim is to find “robust minima” of  $f$ .
- *Expensive* means that each call to  $f$  takes minutes or hours to evaluate.
- *Robust* means that  $f$  should not vary too much near the minima.
- The optimisation framework has to choose points wisely and use the information from each call well.

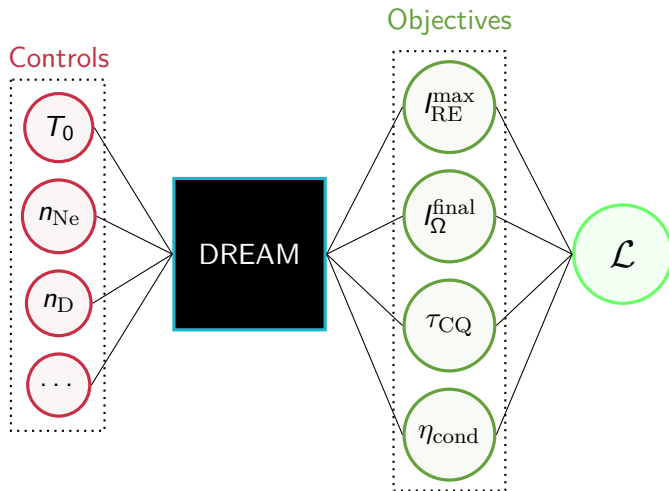
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- Example: two control inputs and two objectives ( $m=n=2$ ): “ $x_1$ =cost” and “ $x_2$ =damage”.
  - The two inputs are some knobs we can turn to change the settings.
  - In the actual physics scenario the inputs are amounts of two gases injected into the fusion reaction chamber.
  - We are given an interval for each input parameter and the task is to find input parameters which give “robust minima”.

# Multi-objective optimization $\Rightarrow$ Alt. 1: Bayesian optimization

- There is rarely a single control point (input vector) that optimises all the objectives.
- Common solution: combine the objectives  $\Rightarrow$  single objective optimization.
- We have published two physics papers based on Bayesian optimization doing this.
  - **Bayesian optimization of massive material injection for disruption mitigation in tokamaks**, Pusztai et al. incl. Jansson & Fülöp, *Journal of Plasma Physics* (2022)
  - **Fluid and kinetic studies of tokamak disruptions using Bayesian optimization**, Ekmark et al. incl. Jansson & Fülöp, *Journal of Plasma Physics* (2024)
  - Several conference presentations.

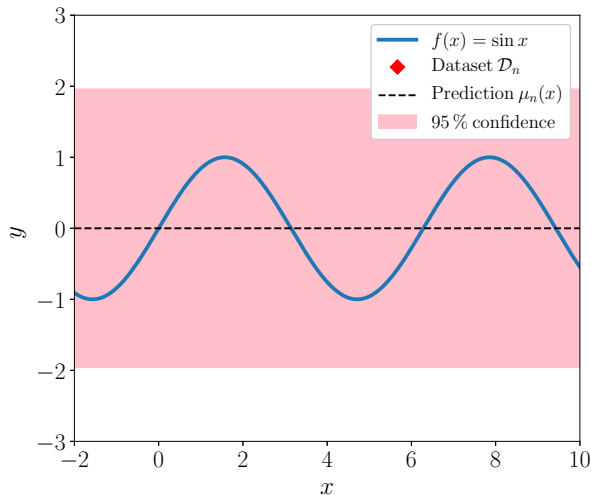
# Black-box optimization: Application to fusion simulations with DREAM



Disruption Runaway Electron Analysis Model (DREAM)

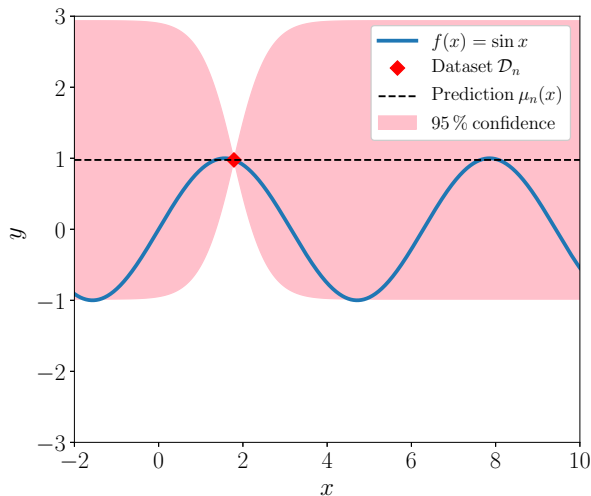
# Bayesian optimization: Step 0

- Global optimization method
- Uses prior belief about  $f$ , e.g. Gaussian Process (GP)
- Updates prior with samples from  $f$  to get posterior that better approximates  $f$



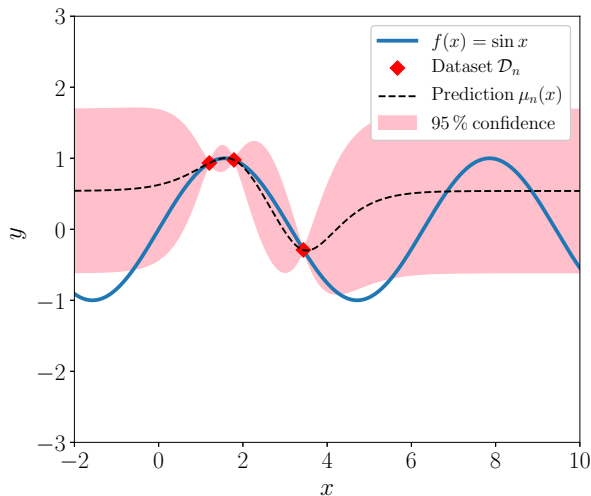
# Bayesian optimization: Step 1

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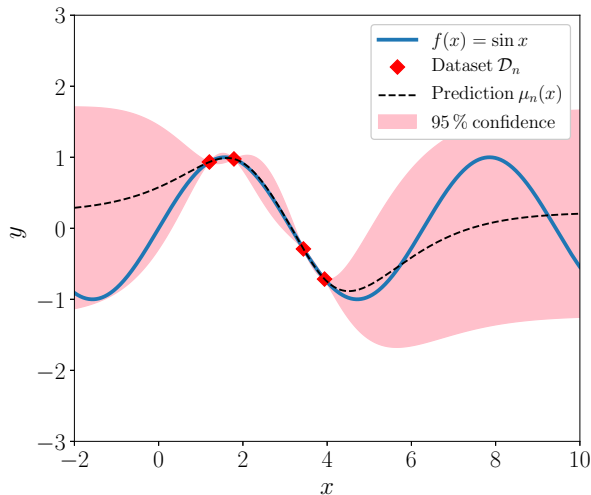
# Bayesian optimization: Step 3

- Global optimization method
- Uses prior belief about  $f$ , e.g. Gaussian Process (GP)
- Updates prior with samples from  $f$  to get posterior that better approximates  $f$



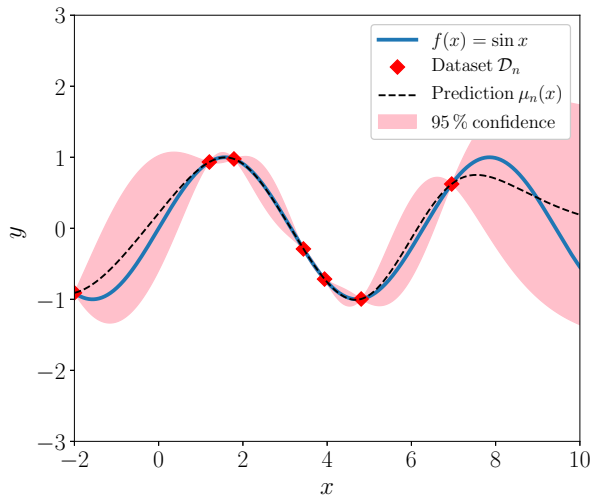
# Bayesian optimization: Step 4

- Global optimization method
- Uses prior belief about  $f$ , e.g. Gaussian Process (GP)
- Updates prior with samples from  $f$  to get posterior that better approximates  $f$
- Balance **exploration** (search broadly) and **exploitation** (focus on promising areas)



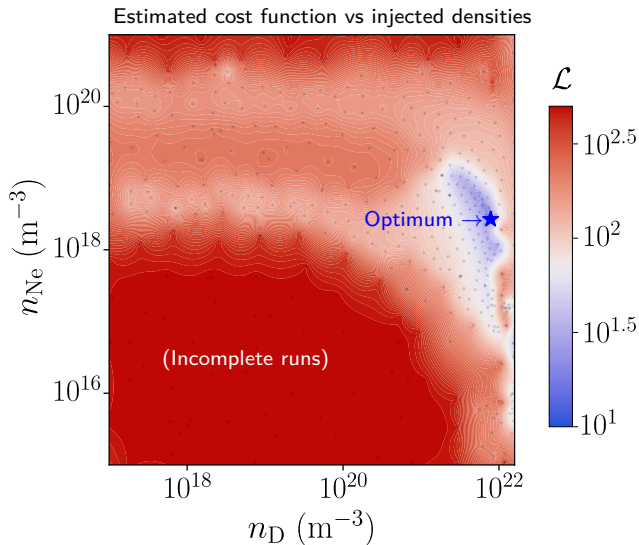
# Bayesian optimization: Step 7

- Global optimization method
- Uses prior belief about  $f$ , e.g. Gaussian Process (GP)
- Updates prior with samples from  $f$  to get posterior that better approximates  $f$
- Balance **exploration** (search broadly) and **exploitation** (focus on promising areas)



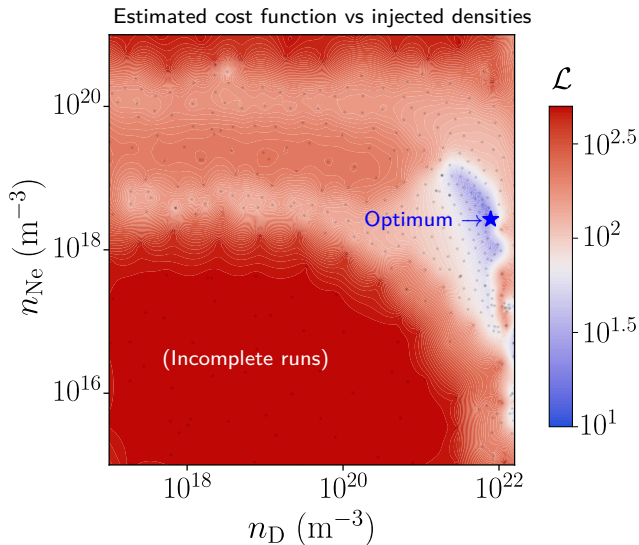
# Results of Bayesian optimization for DREAM

- Injection of neon and deuterium
- **Cost function ( $\mathcal{L}$ ):**
  - Maximum current
  - Heat loss fraction
  - Limits on current quench time
- Blue is good, red is bad



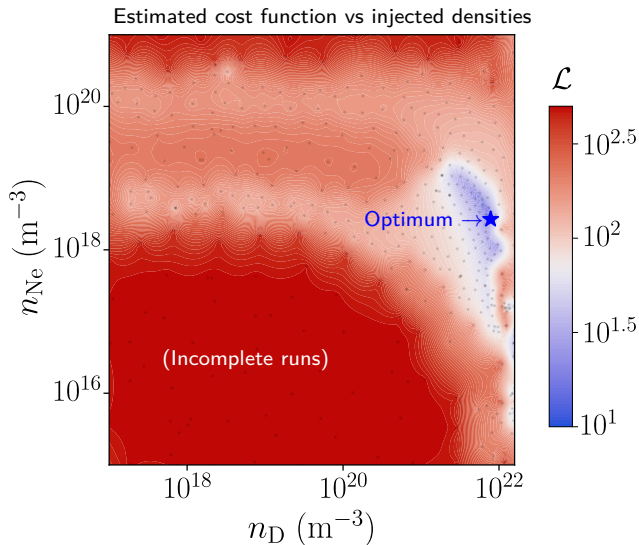
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  - Limits on current quench time
- Blue is good, red is bad
- One optimum found at the star
- but other may be more robust
- or be a better trade-off

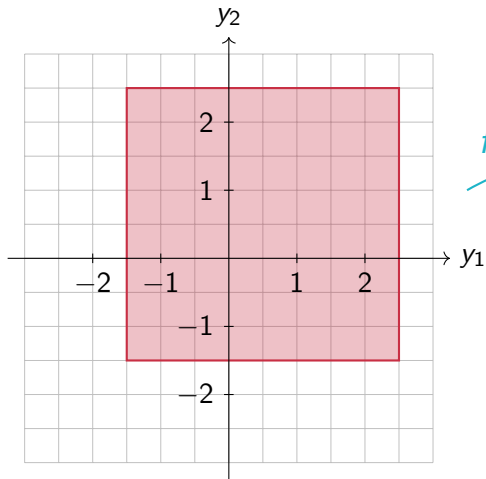


# Multi-objective optimization $\Rightarrow$ multiple optima & trade-offs

- Difficult problem: choose relative weights of the objectives.
- Not only a mathematical, but also an ethical problem (e.g. lives lost vs. cost)
- To solve this part we compute the *Pareto front* of  $f$  and let domain experts decide.
- The Pareto front is a generalisation of optimum and explained in the coming slides.

# Simple example: idealised costs and damages

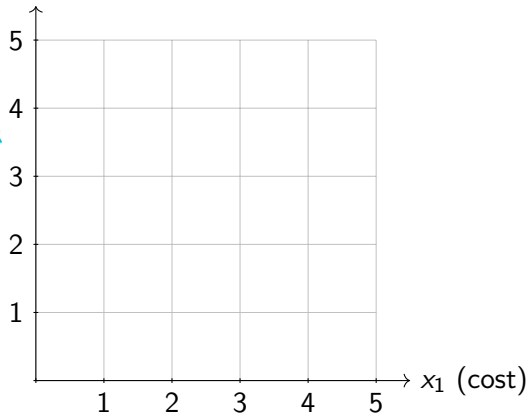
$Y = \text{controls}$



$X = \text{objectives}$

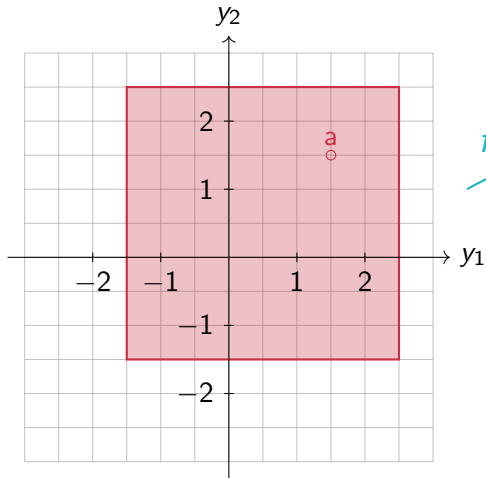
$x_2$  (damage)

$f: Y \rightarrow X$



# Simple example: idealised costs and damages

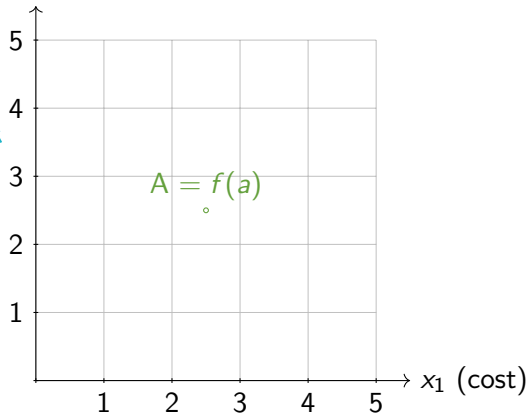
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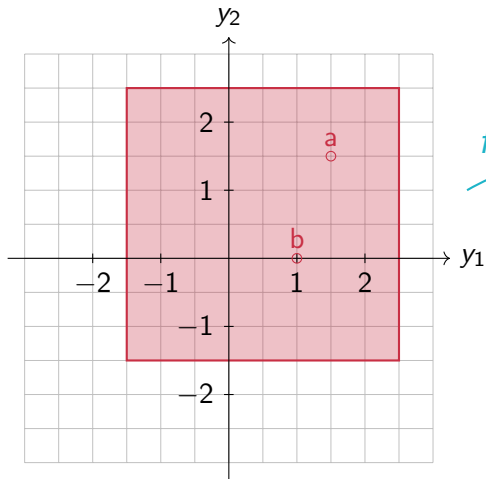
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# Simple example: idealised costs and damages

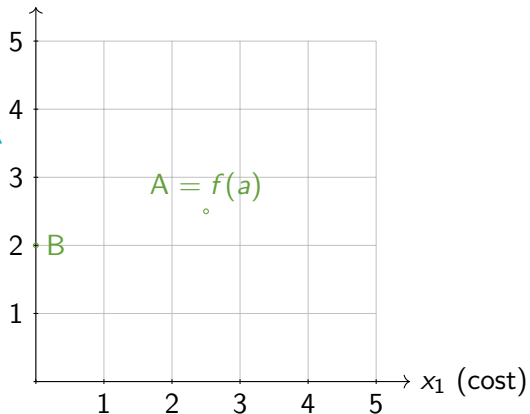
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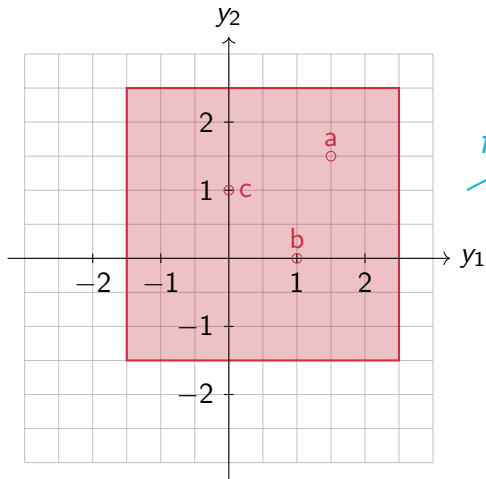
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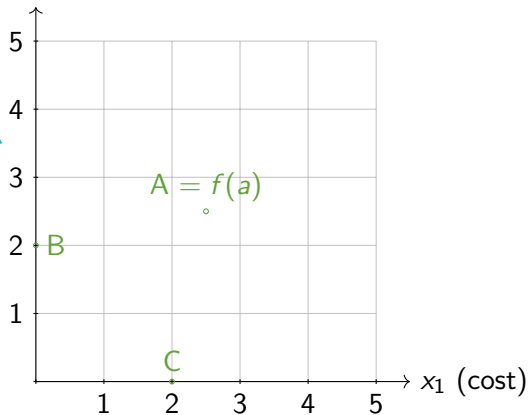
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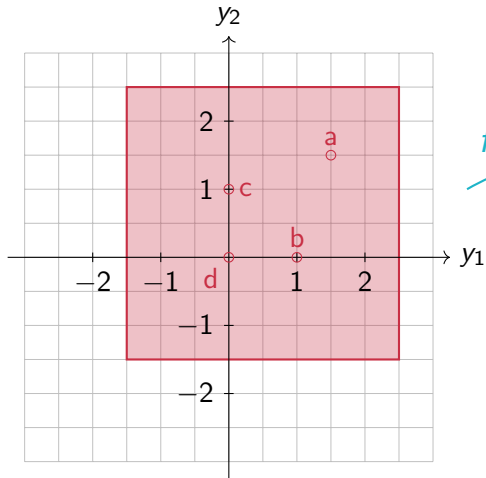
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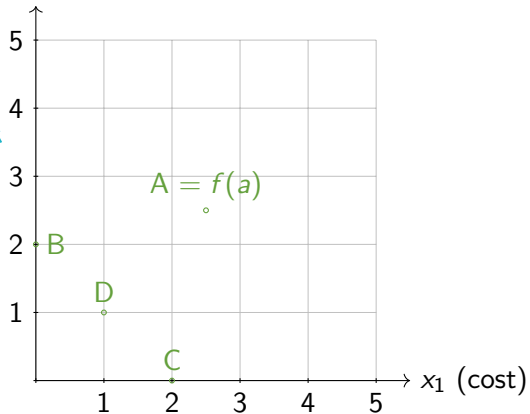
$Y = \text{controls}$



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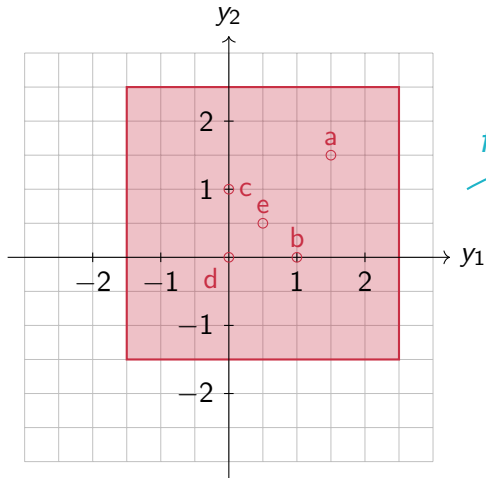
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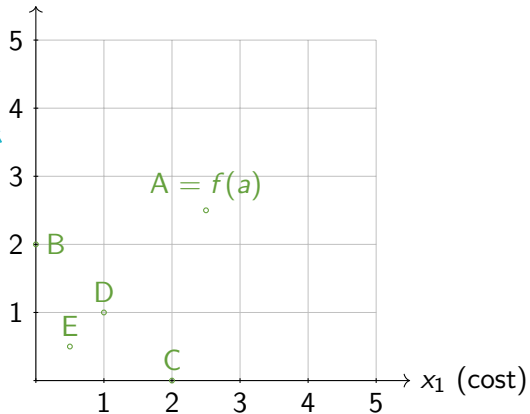
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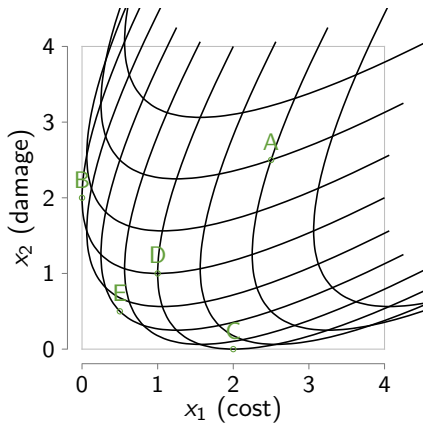
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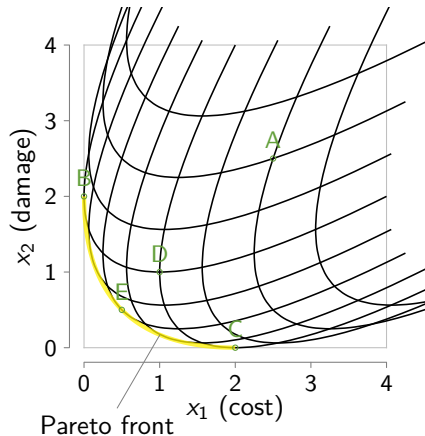
# Objective space (idealised point cloud)



- Each curve keeps  $y_1$  or  $y_2$  fixed and varies the other control continuously.
- The curves shown are for  $y_1 = -1, -0.75, \dots, 1.75, 2$  (same for  $y_2$ ).
- Here the objective function measures cost ( $x_1$ ) and damage ( $x_2$ ).
- They can each reach zero, but not at the same time — there is a trade-off.

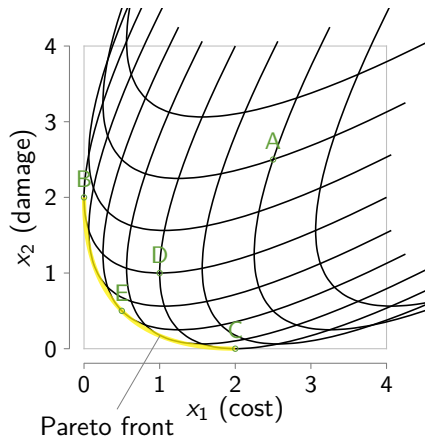
| Point | $y_1$ | $y_2$ | cost | damage | note                   |
|-------|-------|-------|------|--------|------------------------|
| A     | 1.5   | 1.5   | 2.5  | 2.5    | uniformly bad          |
| B     | 1     | 0     | 0    | 2      | minimal cost           |
| C     | 0     | 1     | 2    | 0      | minimal damage         |
| D     | 0     | 0     | 1    | 1      | bad compromise         |
| E     | 0.5   | 0.5   | 0.5  | 0.5    | <b>good compromise</b> |

# Pareto front (“the optima” in objective space)



- Each curve keeps  $y_1$  or  $y_2$  fixed and varies the other control continuously.
- The curves shown are for  $y_1 = -1, -0.75, \dots, 1.75, 2$  (same for  $y_2$ )
- The Pareto front is the set of “optimal points” in objective space.

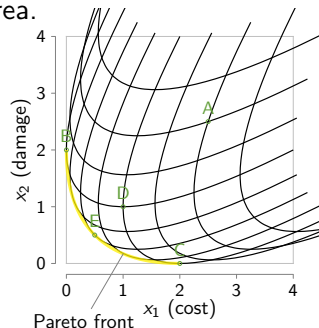
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- The Pareto front is the set of “optimal points” in objective space.
- Aim: Present the Pareto front to the policy maker.
- ...or at least a few alternatives, like B, E, and C.

# Conclusions

- Our framework encapsulates powerful techniques that can be used to find optimal designs in areas where there is a trade-off between objectives.
- We have demonstrated the usefulness through an application in fusion energy research.
- The methodology should be broadly applicable in the energy area.
- Future research directions:
  - Pareto front computation using adaptive mesh refinement
  - Applications to optimal climate decisions



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