

# Learning for Decision-Making under Uncertainty

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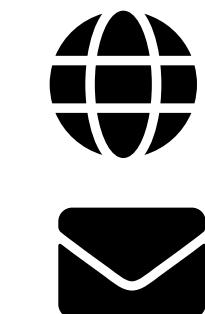
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Center for Statistics and Machine Learning



PRINCETON  
UNIVERSITY

**Bartolomeo Stellato – MIP Workshop, May 25 2023**



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# It is hard to make decisions under uncertainty

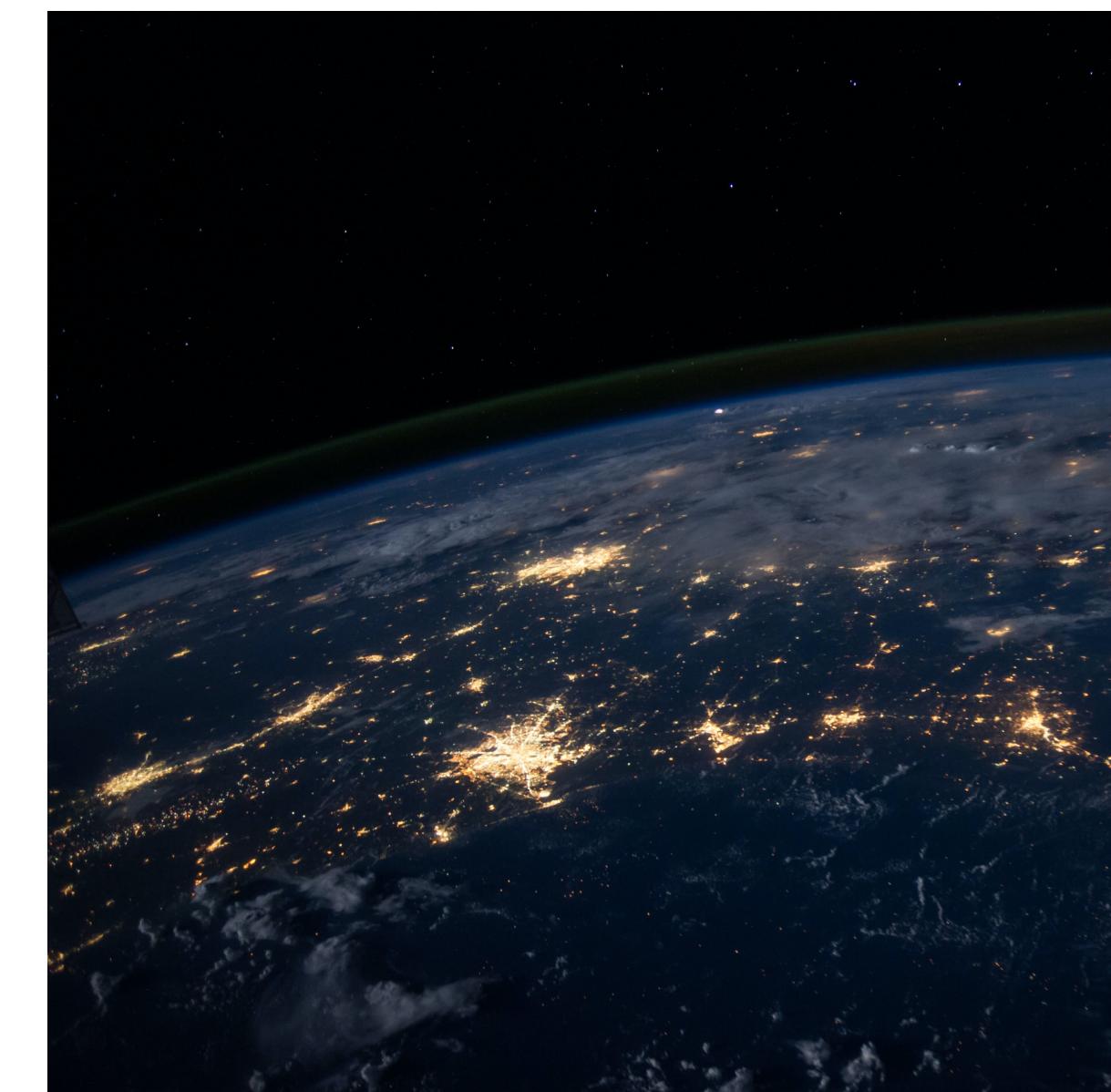
Transportation



Finance



Energy



# It is hard to make decisions under uncertainty

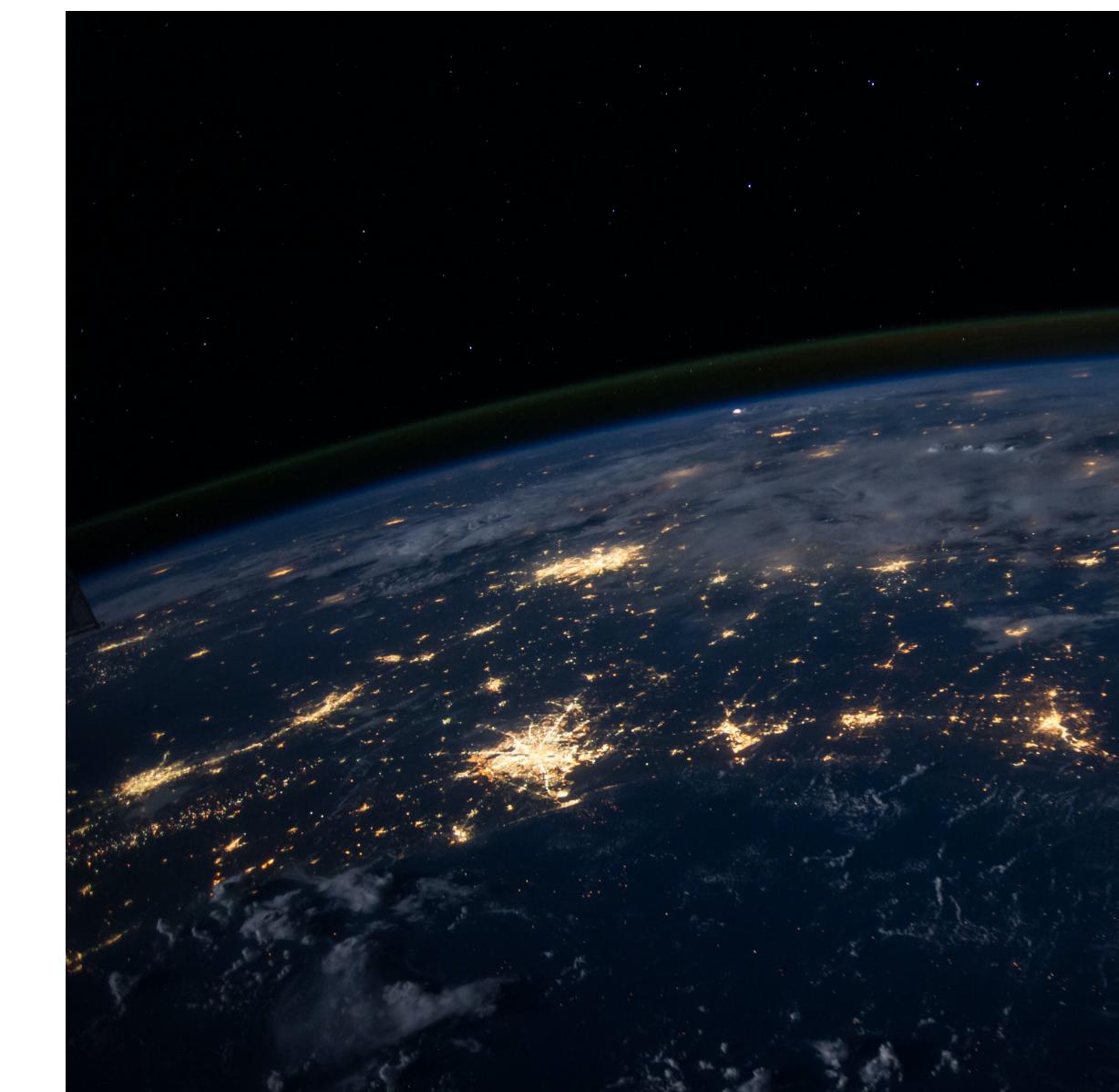
Transportation



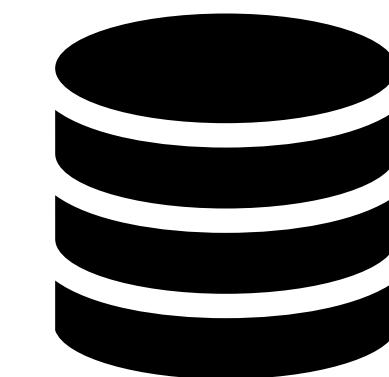
Finance



Energy



But we have data!



# Problem setup with uncertain constraints

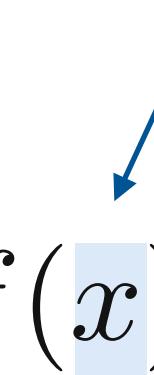
# Problem setup with uncertain constraints

minimize       $f(x)$   
subject to     $g(u, x) \leq 0$

# Problem setup with uncertain constraints

optimization  
variable

minimize       $f(x)$   
subject to      $g(u, x) \leq 0$



# Problem setup with uncertain constraints

optimization  
variable

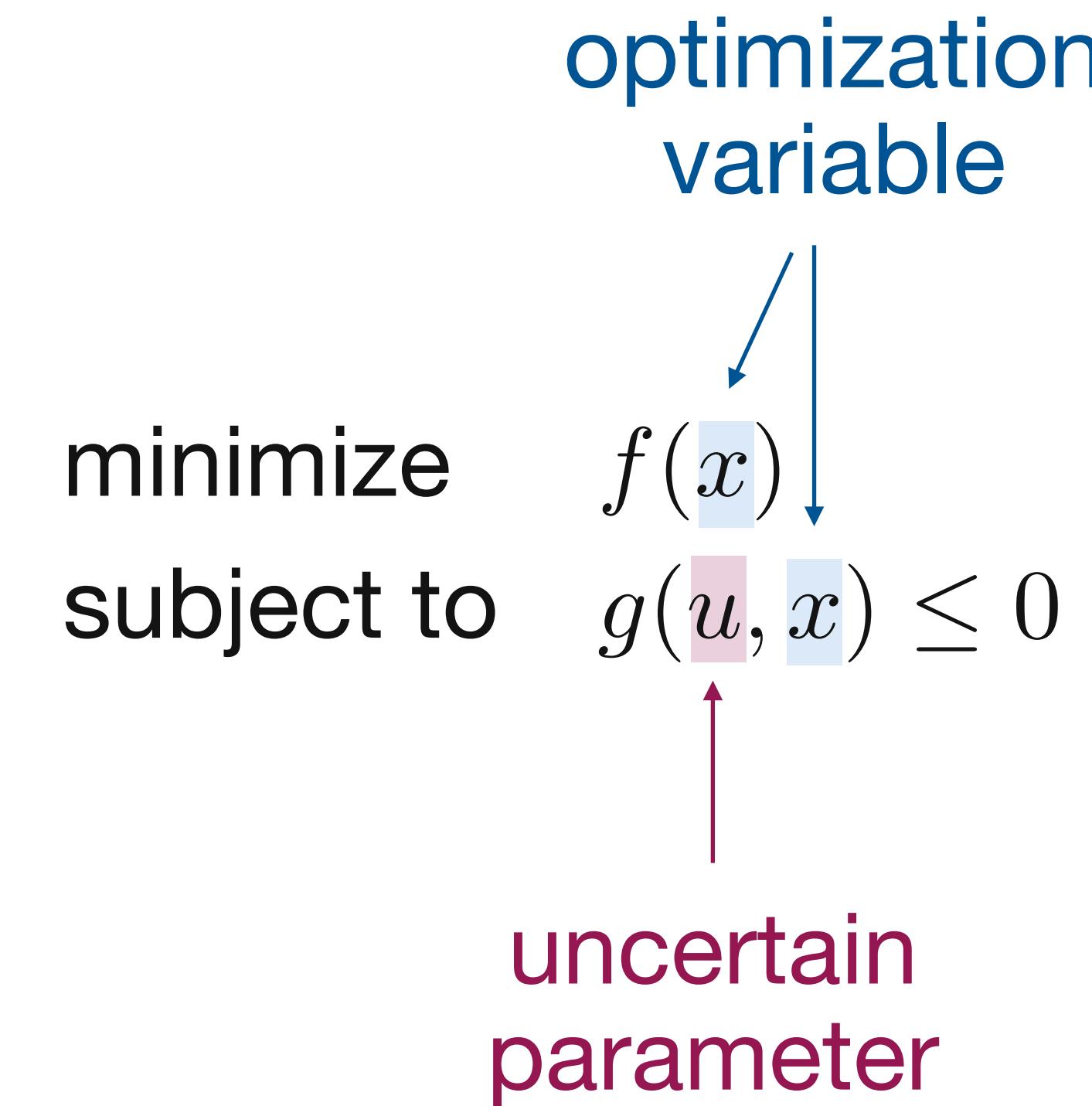
minimize       $f(x)$

subject to      $g(u, x) \leq 0$

uncertain  
parameter

The diagram illustrates a constrained optimization problem. It features two main components: 'optimization variable' and 'uncertain parameter'. The 'optimization variable' is represented by a blue box containing the symbol 'x'. The 'uncertain parameter' is represented by a pink box containing the symbol 'u'. Arrows point from each of these boxes to their respective components in the mathematical expressions. Specifically, the blue arrow points from the 'optimization variable' to the 'x' in the function  $f(x)$ . The pink arrow points from the 'uncertain parameter' to the 'u' in the constraint  $g(u, x) \leq 0$ .

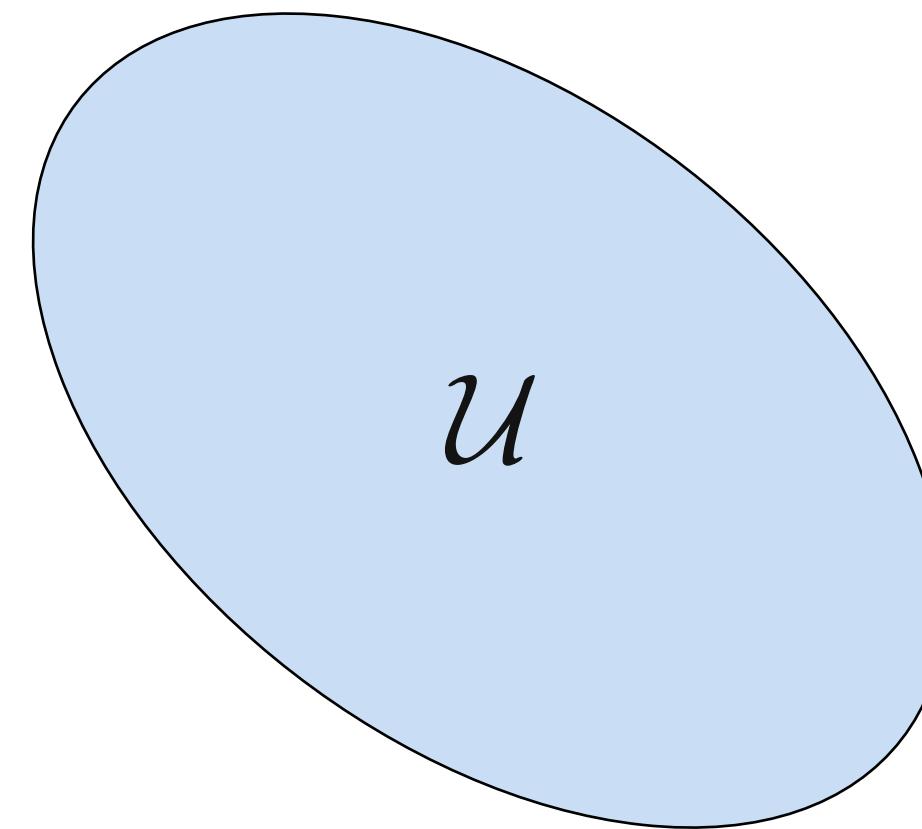
# Problem setup with uncertain constraints



We want to guarantee constraint satisfaction

# Robust optimization recipe

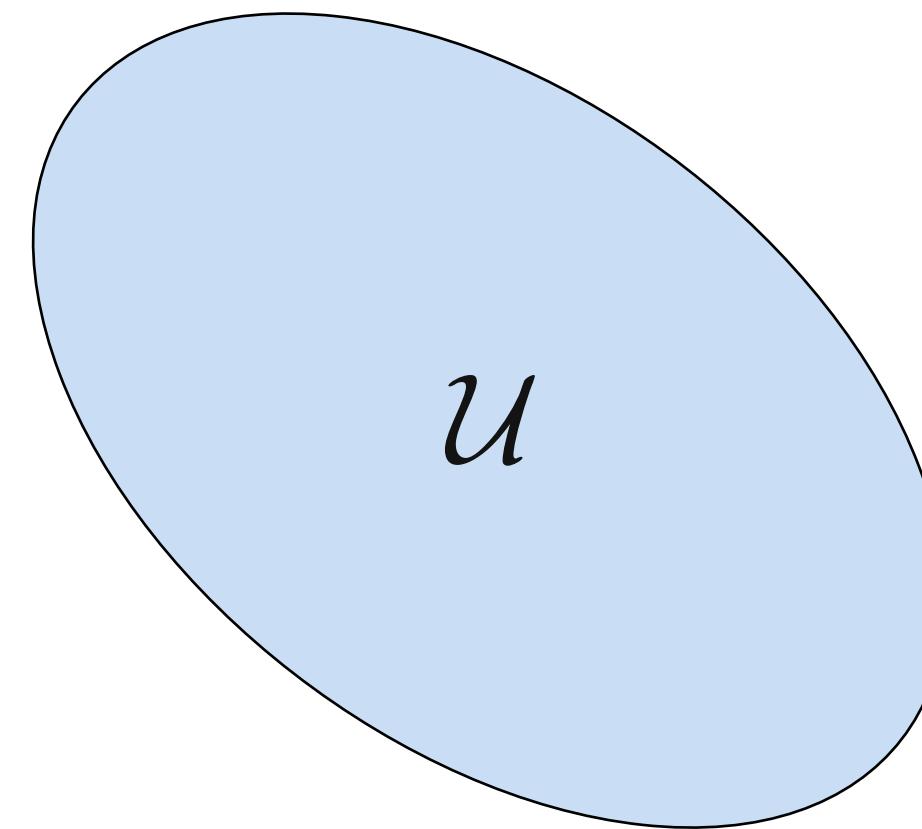
1. Pick uncertainty set  $\mathcal{U}$
2. Ensure constraint satisfaction  $\forall u \in \mathcal{U}$



minimize  $f(x)$   
subject to  $g(u, x) \leq 0, \quad \forall u \in \mathcal{U}$

# Robust optimization recipe

1. Pick uncertainty set  $\mathcal{U}$
2. Ensure constraint satisfaction  $\forall u \in \mathcal{U}$



$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && g(u, x) \leq 0, \quad \forall u \in \mathcal{U} \end{aligned}$$

How do we pick the uncertainty set?

# Picking the uncertainty set is difficult

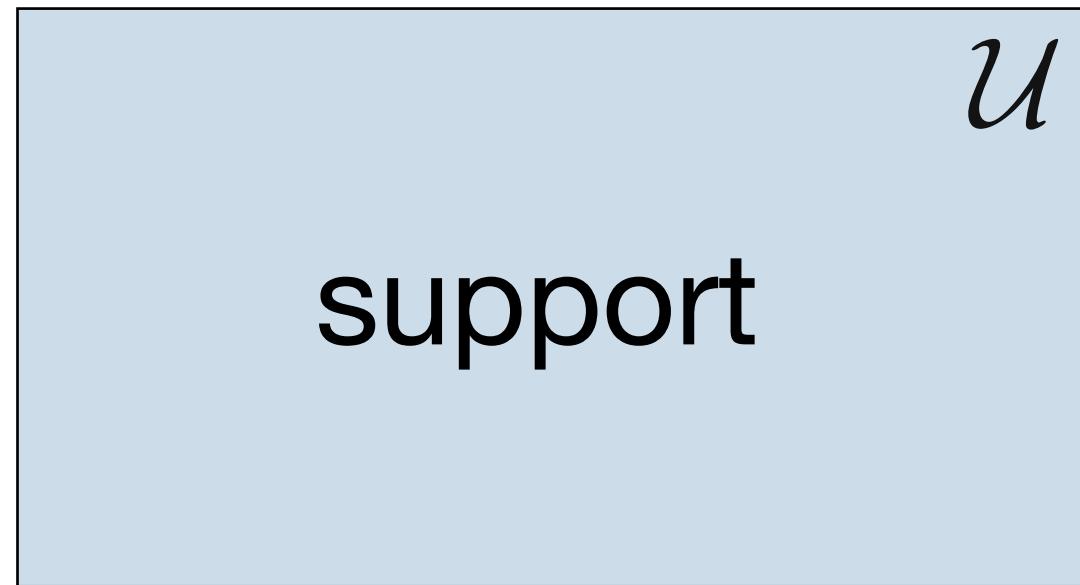
Worst-case approach



✗ Very conservative

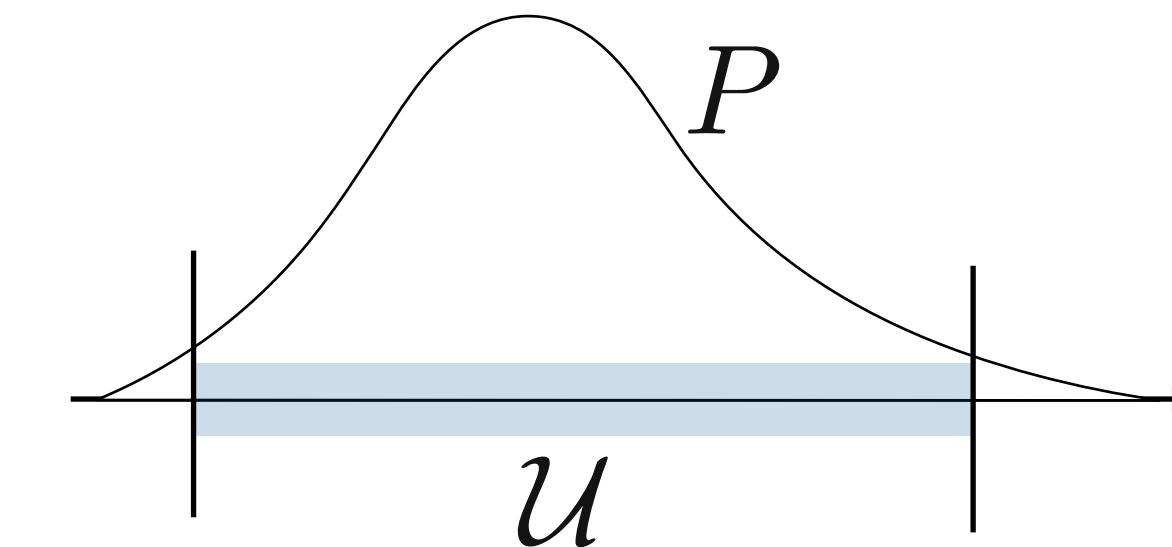
# Picking the uncertainty set is difficult

Worst-case approach



✗ Very conservative

Probabilistic approach



✗ nobody knows  $P$

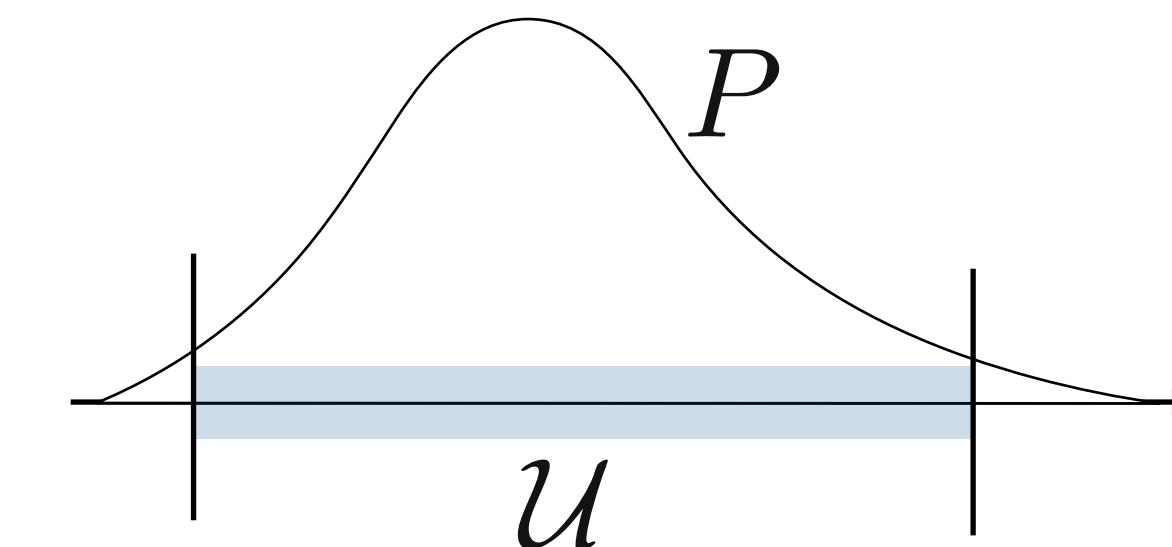
# Picking the uncertainty set is difficult

## Worst-case approach



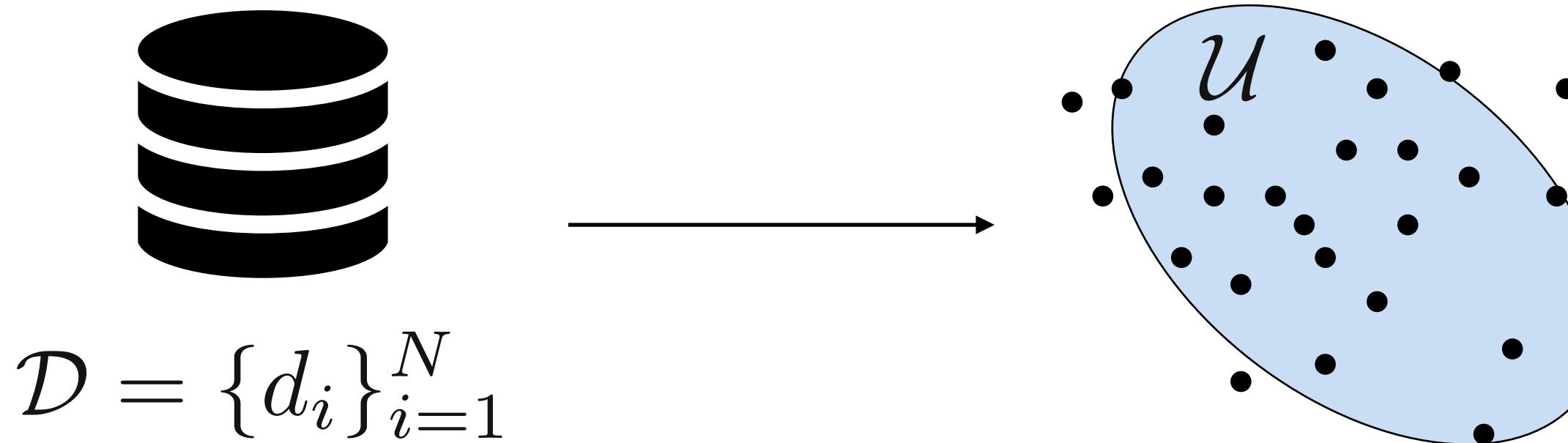
✗ Very conservative

## Probabilistic approach



✗ nobody knows  $P$

## Can we use data?

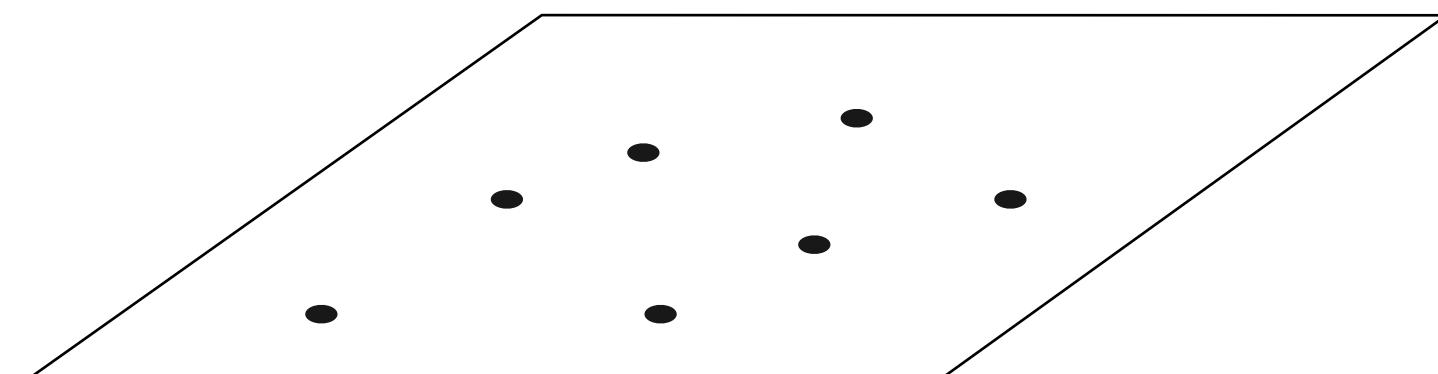


# Estimating true distribution from data

## Data-Driven Distributionally Robust Optimization

Data

$$\mathcal{D} = \{d_i\}_{i=1}^N$$



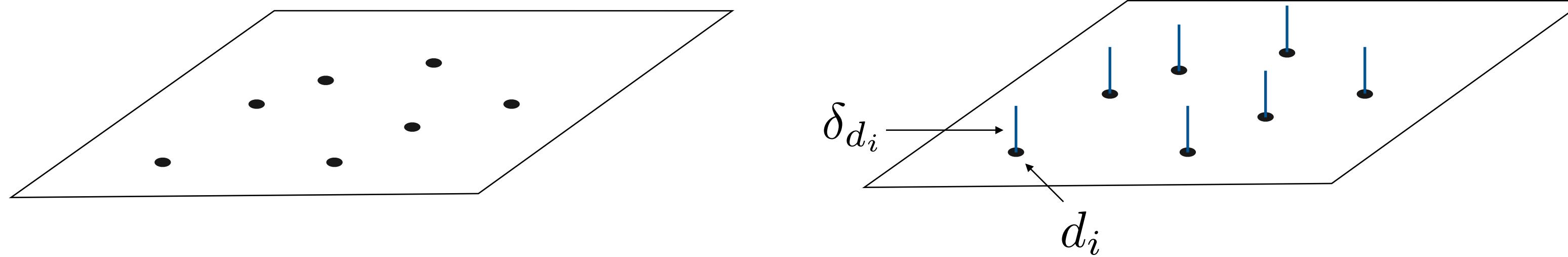
# Estimating true distribution from data

## Data-Driven Distributionally Robust Optimization

### Empirical Distribution

Data  
 $\mathcal{D} = \{d_i\}_{i=1}^N$

$$\hat{\mathbf{P}}^N = \frac{1}{N} \sum_{i=1}^N \delta_{d_i}$$



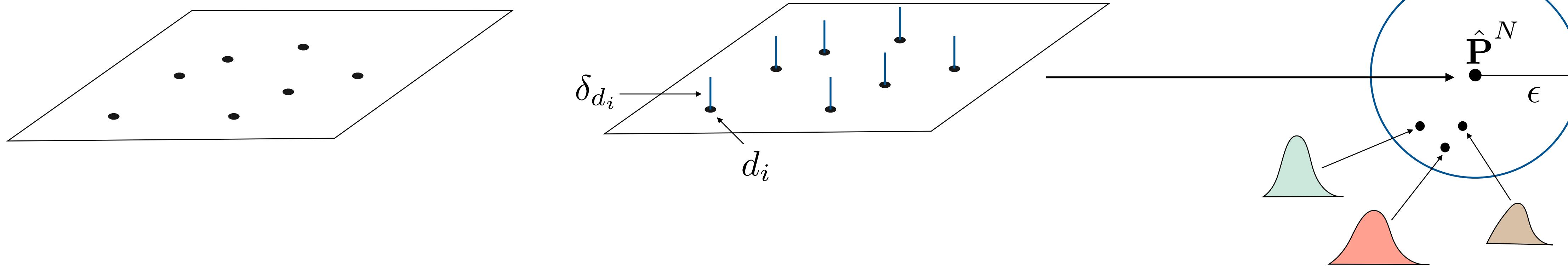
# Estimating true distribution from data

## Data-Driven Distributionally Robust Optimization

**Data**  
 $\mathcal{D} = \{d_i\}_{i=1}^N$

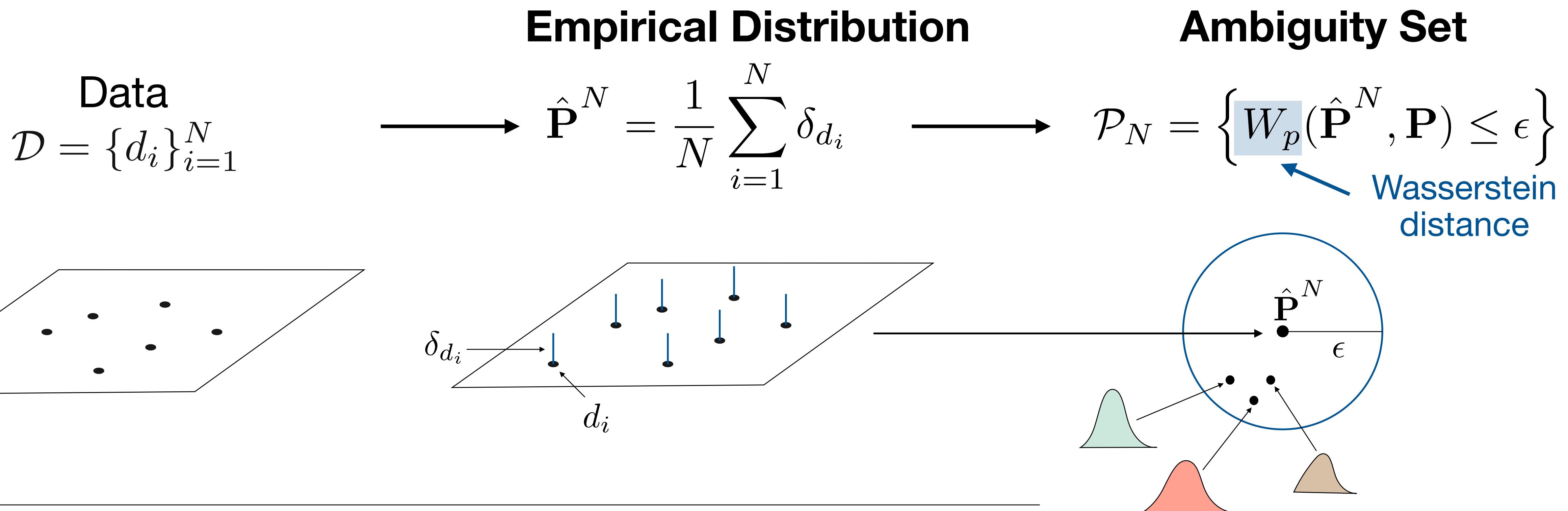
**Empirical Distribution**  
 $\hat{\mathbf{P}}^N = \frac{1}{N} \sum_{i=1}^N \delta_{d_i}$

**Ambiguity Set**  
 $\mathcal{P}_N = \left\{ W_p(\hat{\mathbf{P}}^N, \mathbf{P}) \leq \epsilon \right\}$

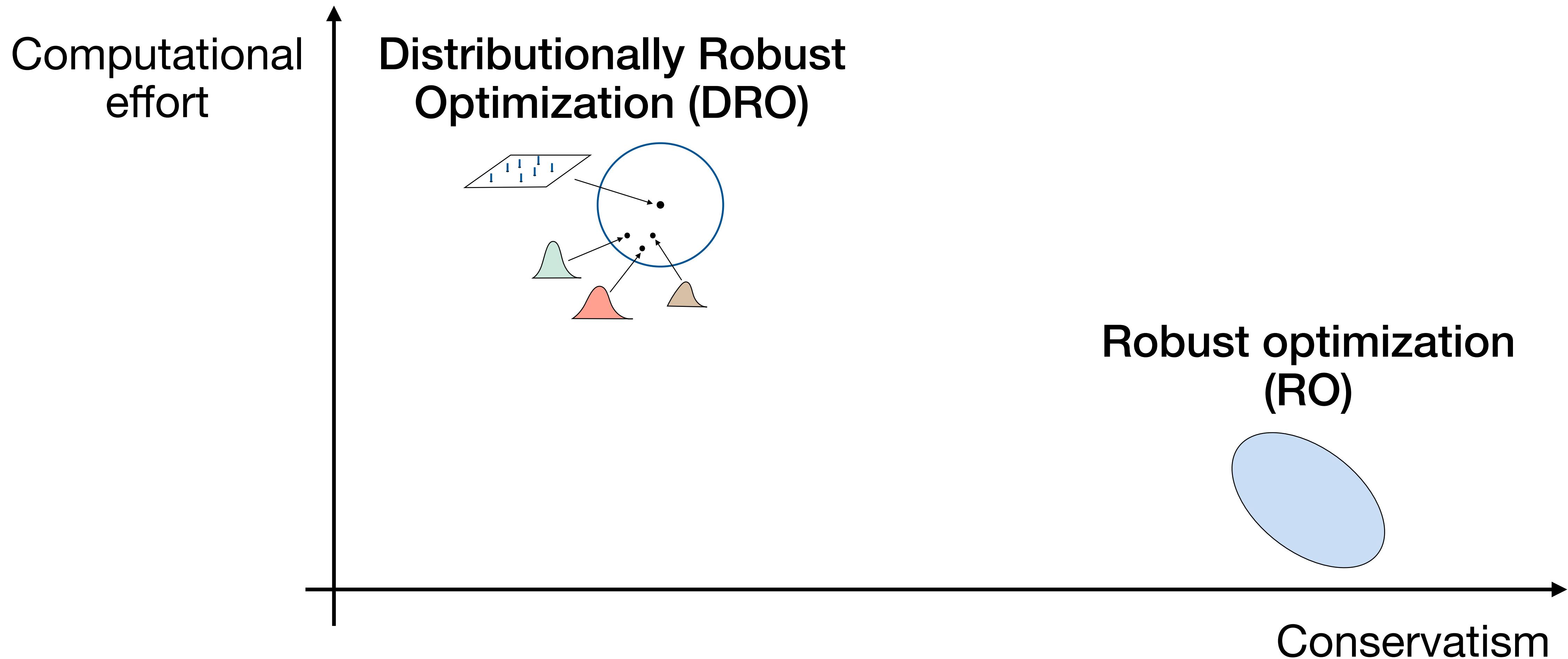


# Estimating true distribution from data

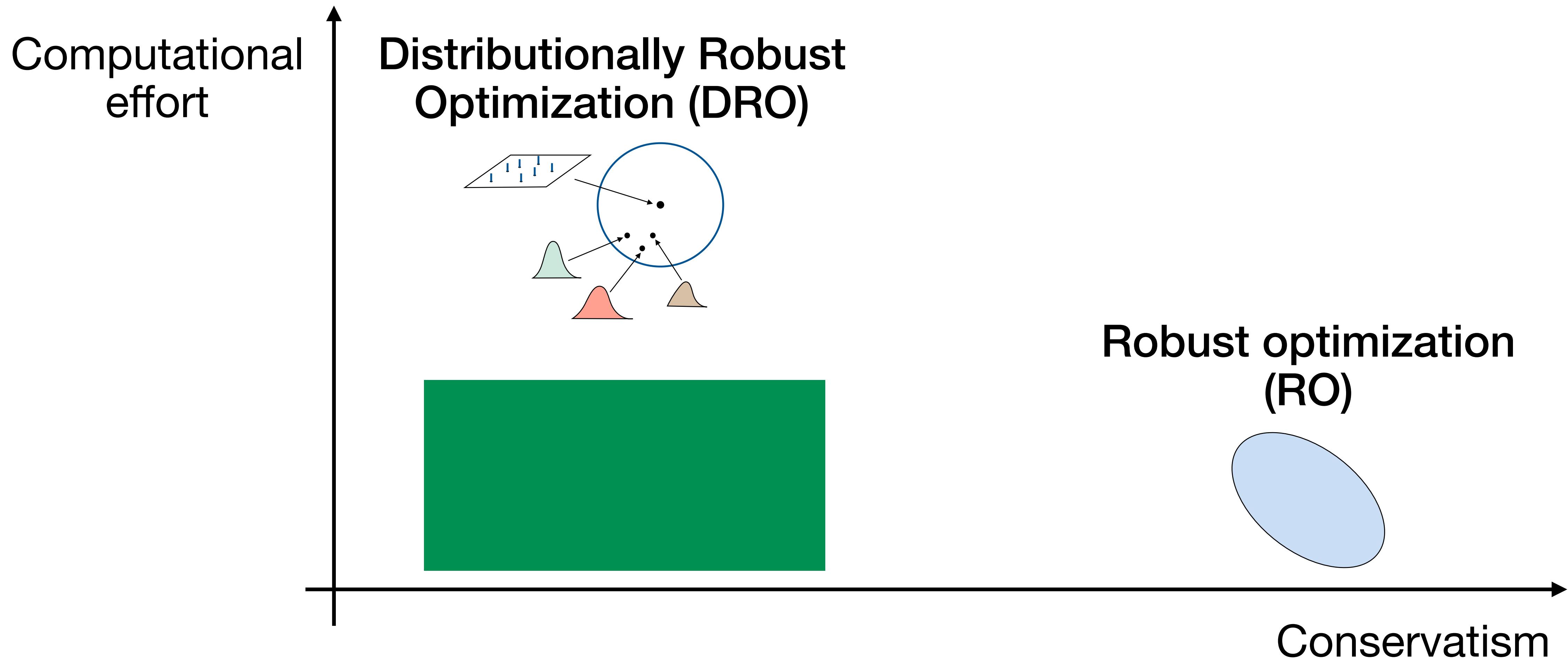
## Data-Driven Distributionally Robust Optimization



# Robust vs Distributionally Robust Optimization

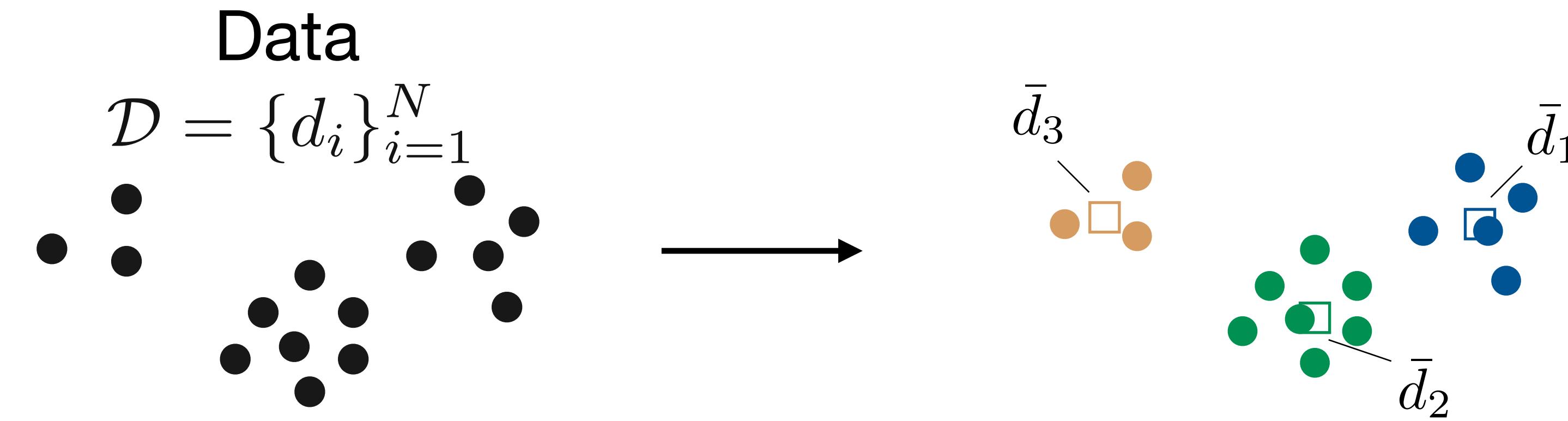


# Robust vs Distributionally Robust Optimization

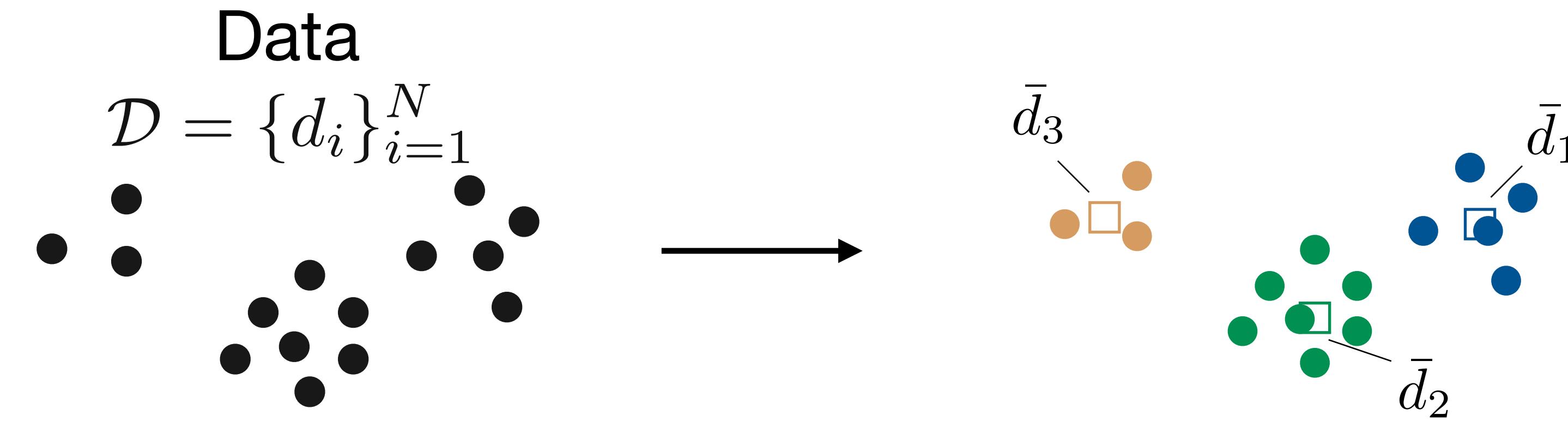


Can we get the  
best of both worlds?

# Clustering reduces dimensionality

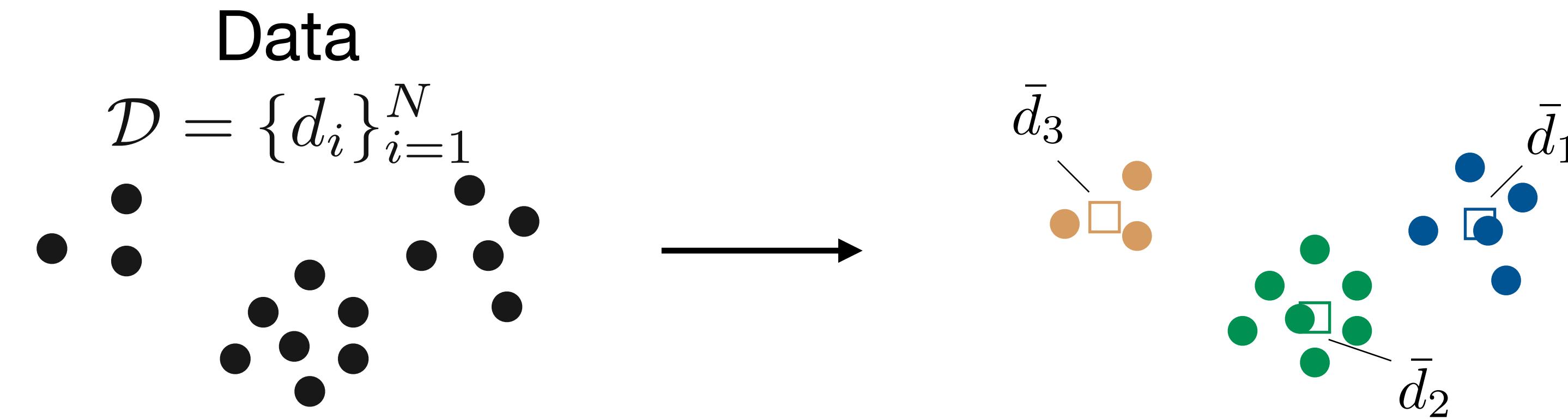


# Clustering reduces dimensionality



minimize 
$$\sum_{k=1}^K \sum_{i \in C_k} \|d_i - \bar{d}_k\|^2$$

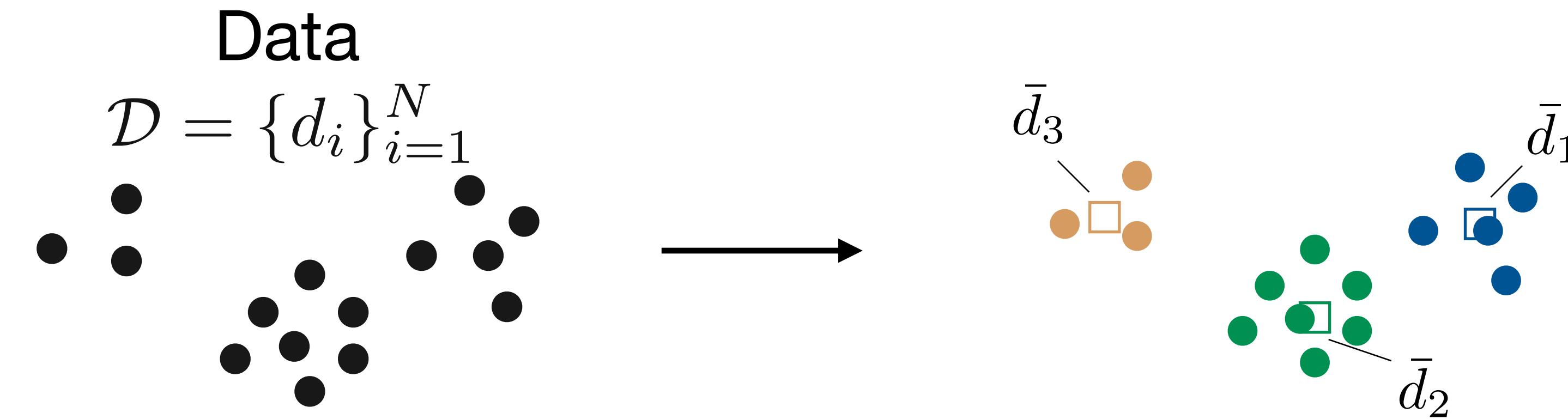
# Clustering reduces dimensionality



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cluster centers

# Clustering reduces dimensionality



minimize 
$$\sum_{k=1}^K \sum_{i \in C_k} \|d_i - \bar{d}_k\|^2$$

cluster centers

Main idea  
Use cluster centers  
instead of original data

# Probabilistic guarantees

concave  
function


$$\mathbf{E}(g(u, x)) \leq 0$$

# Probabilistic guarantees

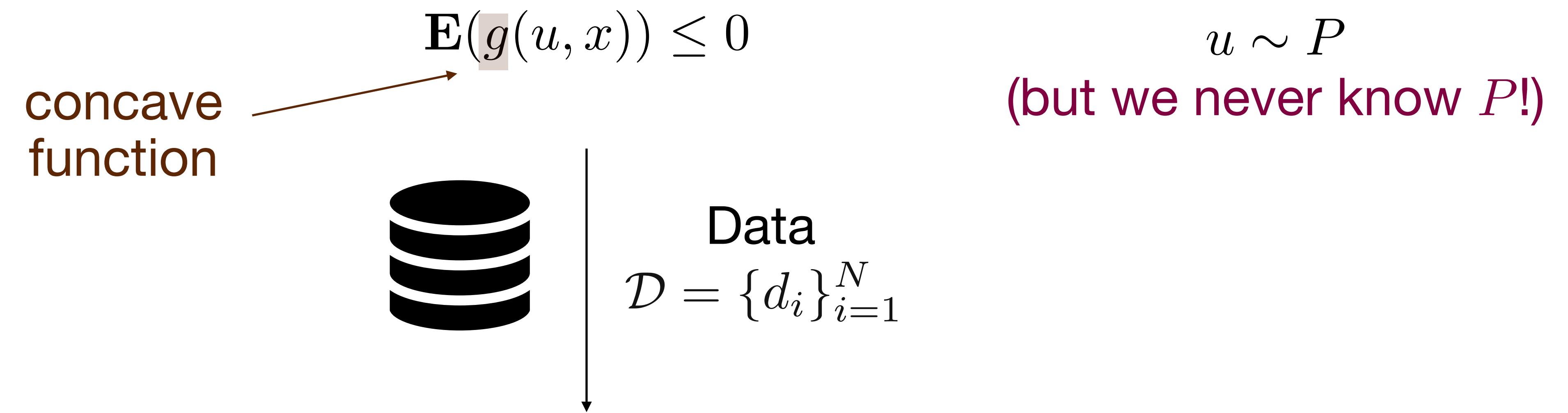
$$\mathbf{E}(g(u, x)) \leq 0$$

concave  
function

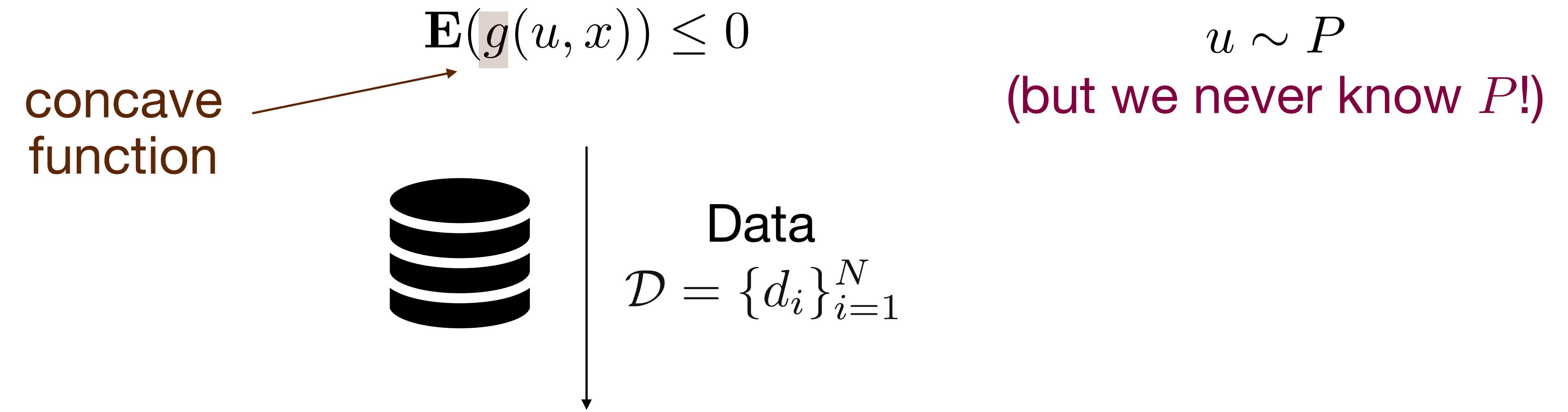
$u \sim P$   
(but we never know  $P$ !)



# Probabilistic guarantees



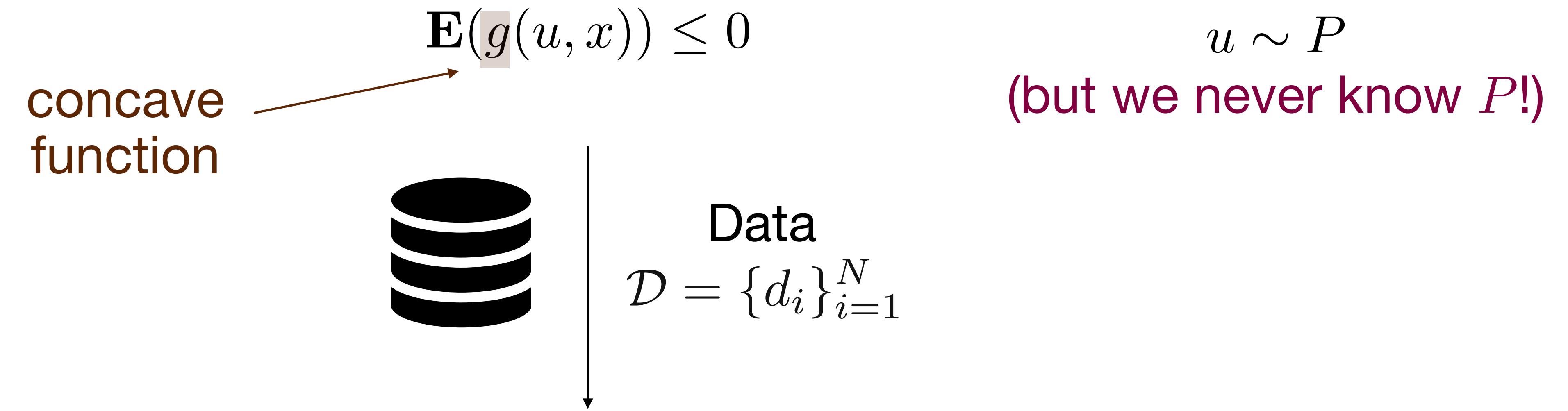
# Probabilistic guarantees



Data-driven probabilistic guarantees

$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

# Probabilistic guarantees



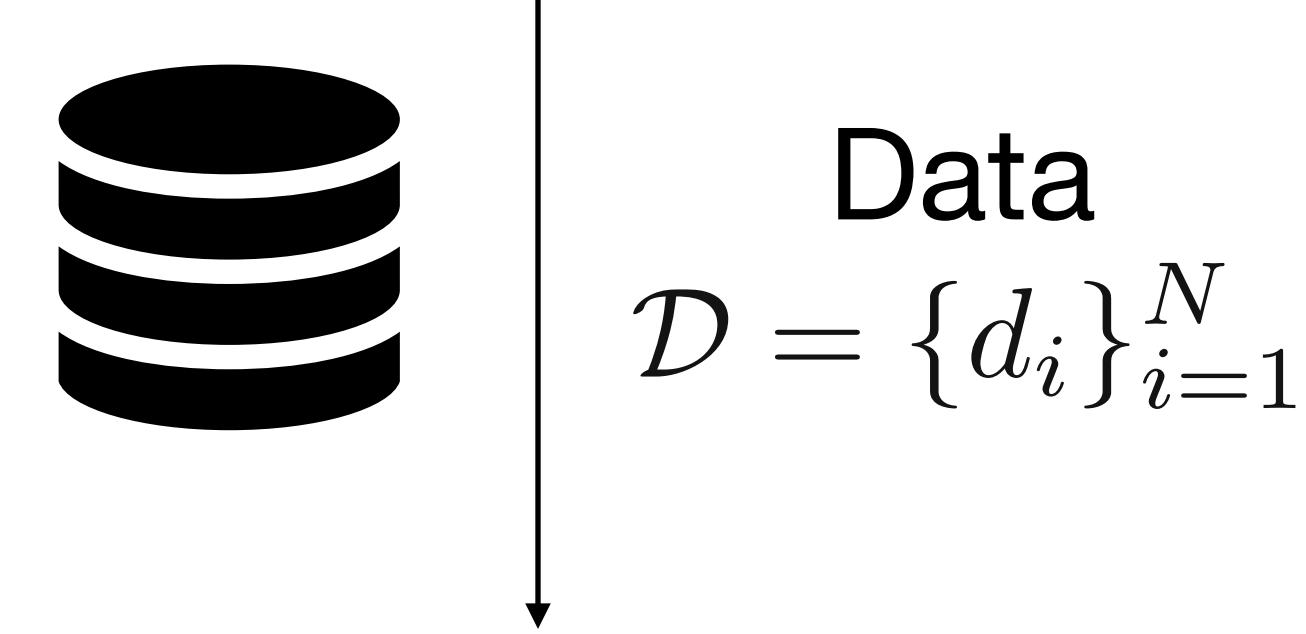
Data-driven probabilistic guarantees

Product Distribution  $\longrightarrow \mathbf{P}^N(\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$

# Probabilistic guarantees

$$\text{concave function} \quad \xrightarrow{\quad} \quad \mathbf{E}(g(u, x)) \leq 0$$

$u \sim P$   
*(but we never know  $P$ !)*



## Data-driven probabilistic guarantees

$$\text{Product Distribution} \quad \longrightarrow \quad \mathbf{P}^N(\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

↑  
data-driven solution

# Probabilistic guarantees

$$\mathbf{E}(g(u, x)) \leq 0$$

concave function

$u \sim P$   
(but we never know  $P$ !)



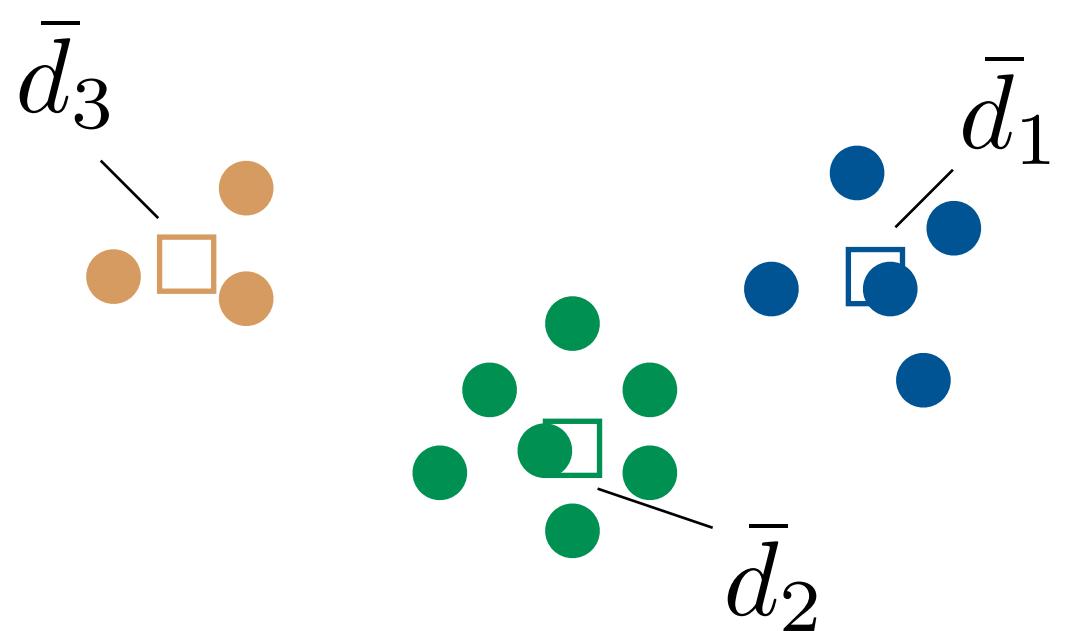
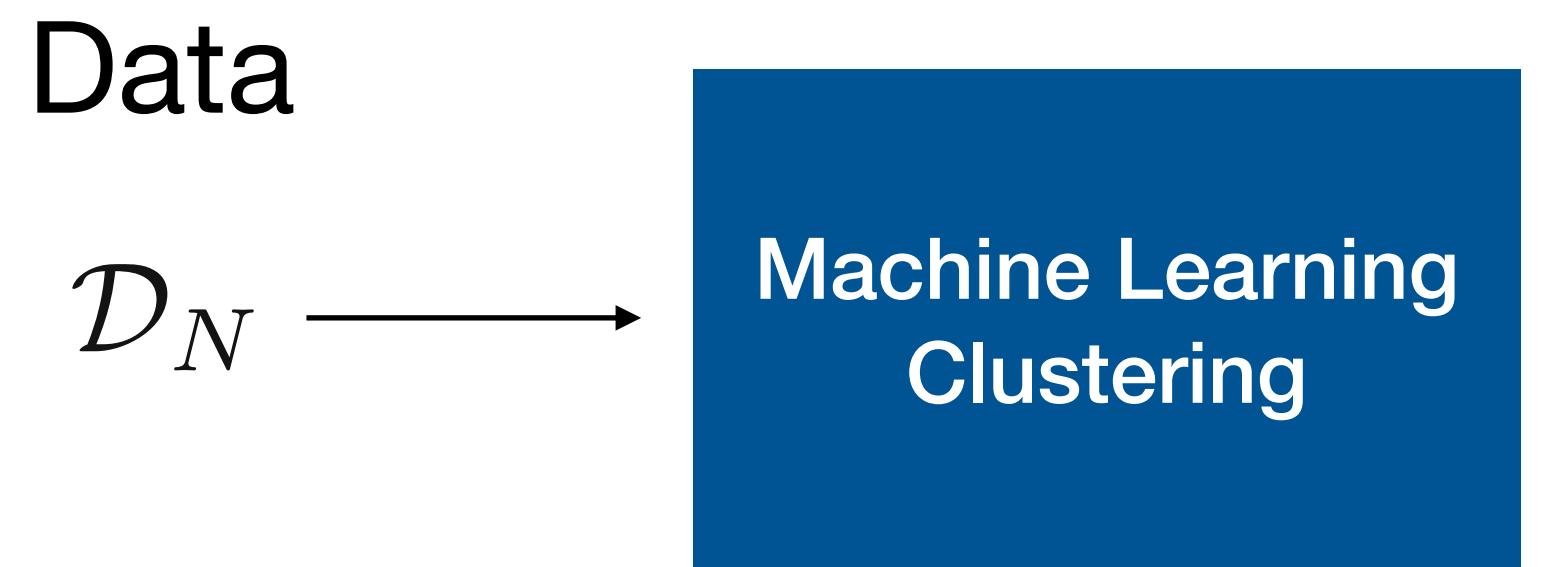
## Data-driven probabilistic guarantees

Product Distribution  $\longrightarrow \mathbf{P}^N(\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta \longleftarrow$  probability of constraint satisfaction

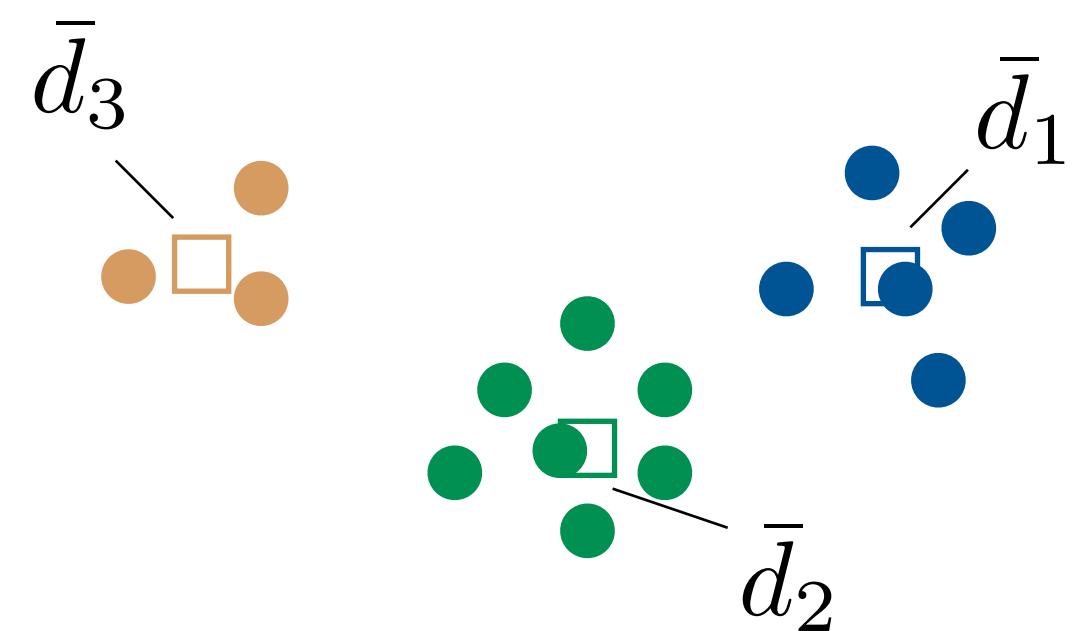
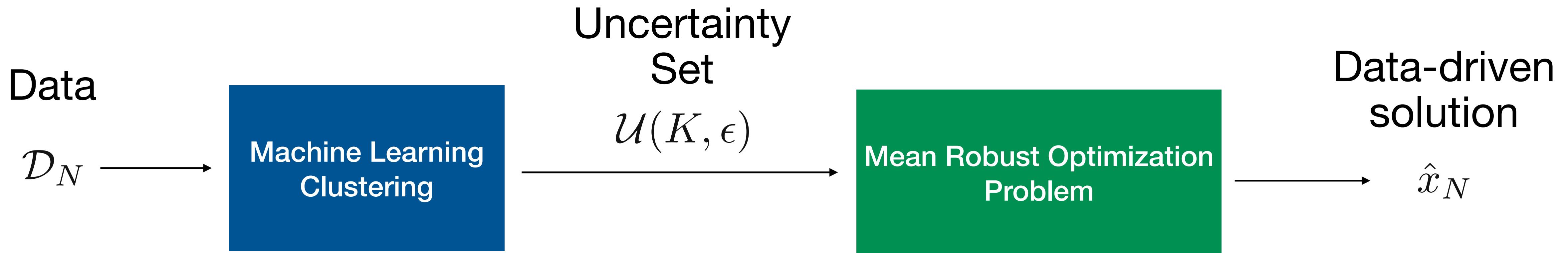
data-driven solution

# Mean Robust Optimization

# Mean Robust Optimization (MRO)

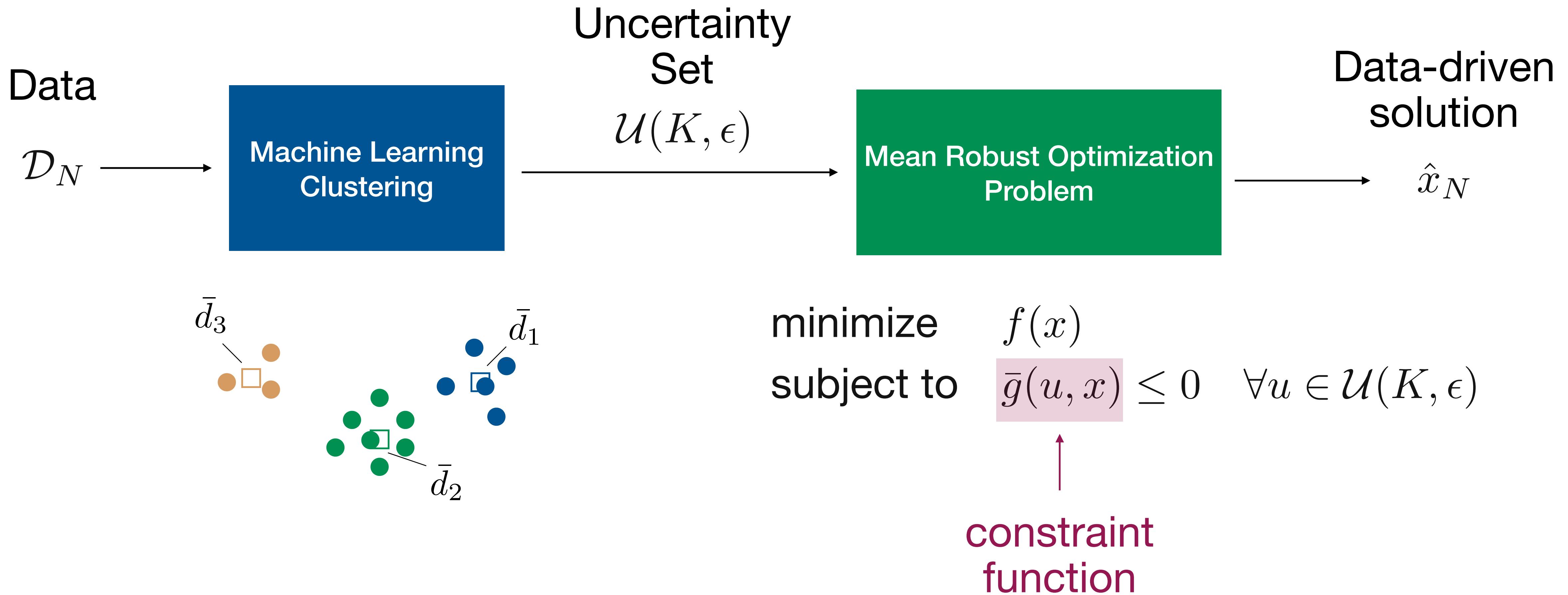


# Mean Robust Optimization (MRO)

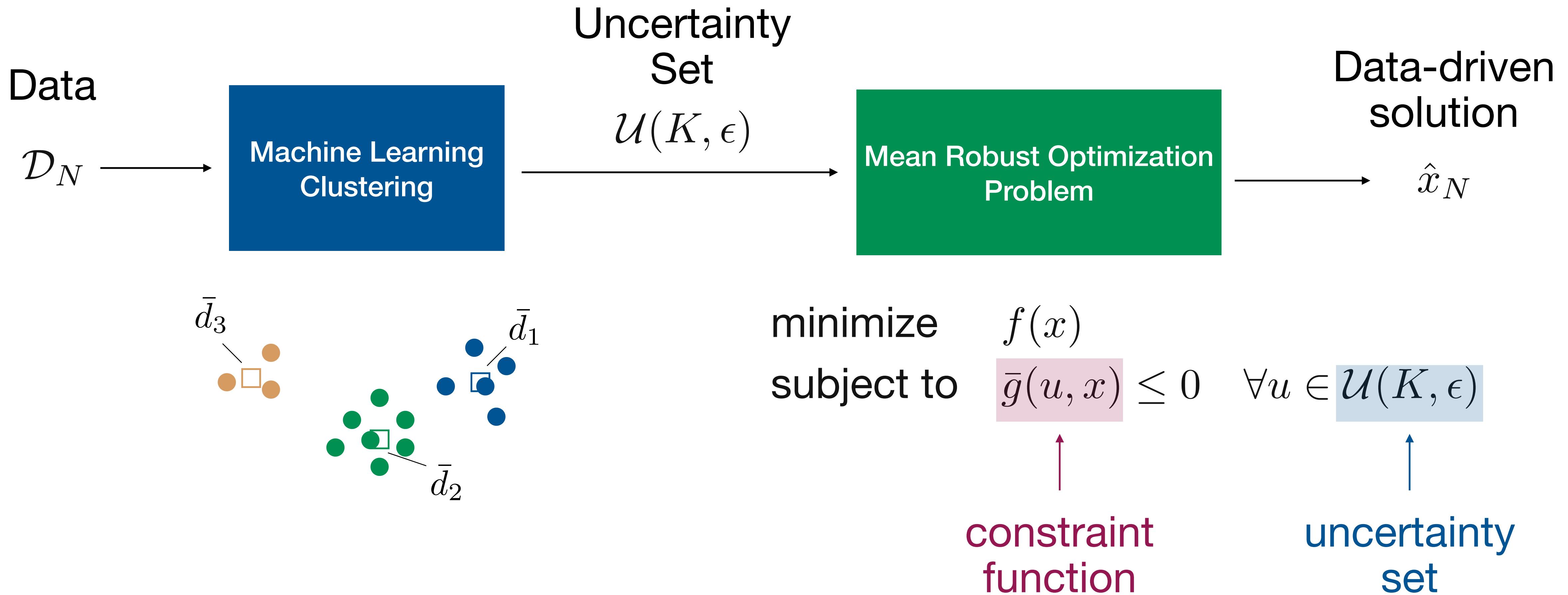


$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & \bar{g}(u, x) \leq 0 \quad \forall u \in \mathcal{U}(K, \epsilon) \end{array}$$

# Mean Robust Optimization (MRO)

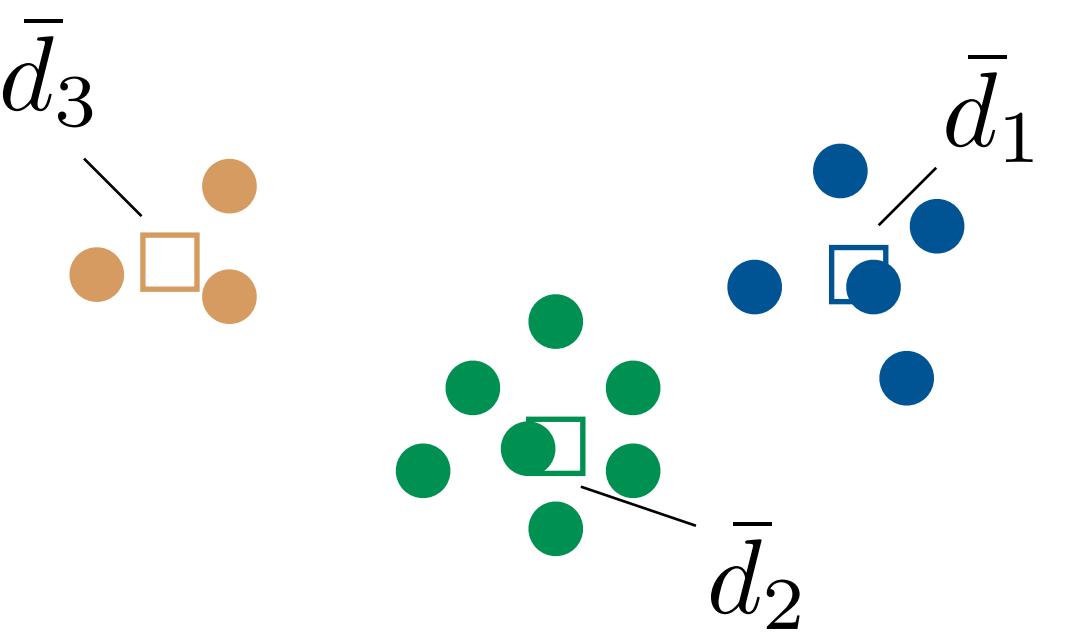


# Mean Robust Optimization (MRO)



# Uncertainty set

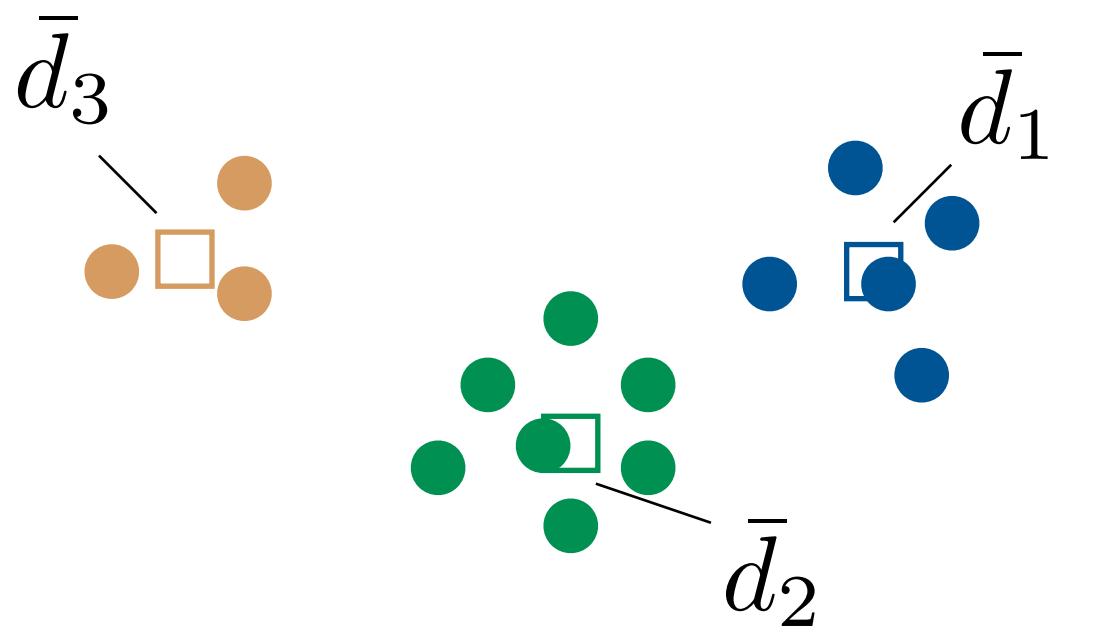
$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$



# Uncertainty set

$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

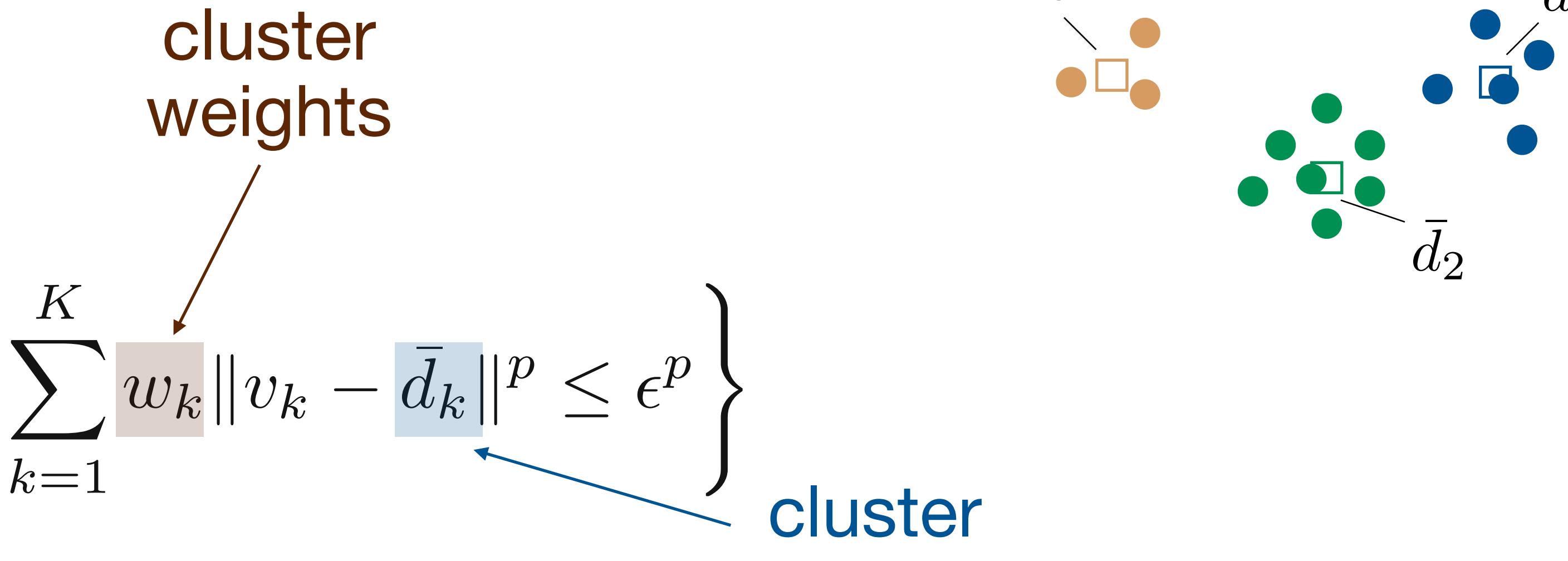
cluster  
weights



# Uncertainty set

$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

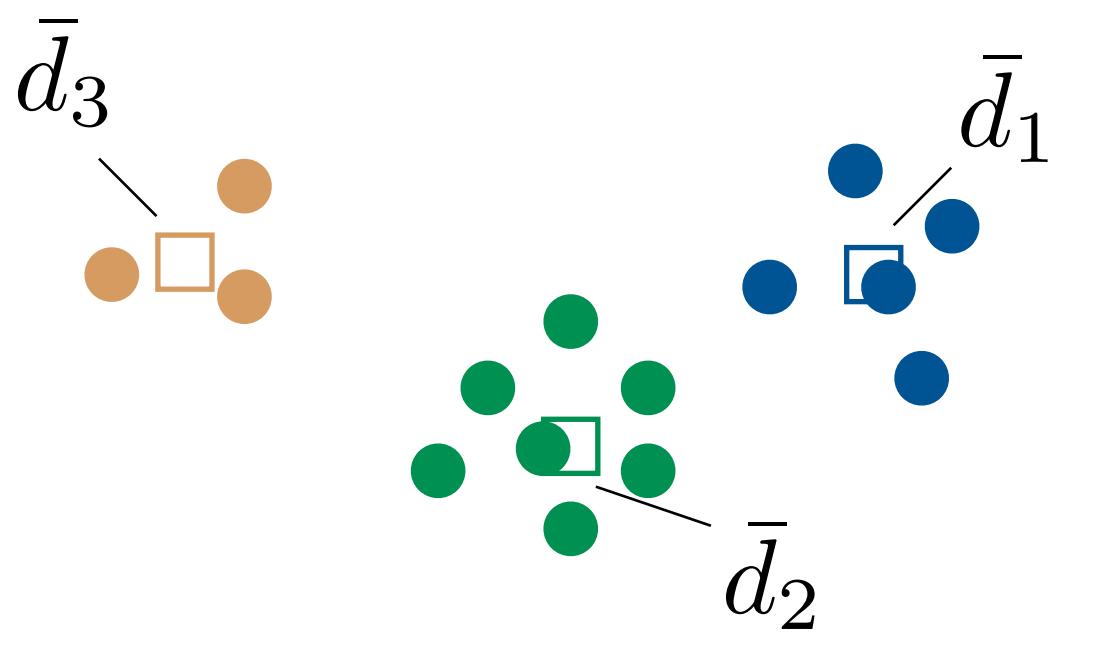
cluster  
weights      cluster  
centers



# Uncertainty set

$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

cluster weights      order      cluster centers



# Uncertainty set

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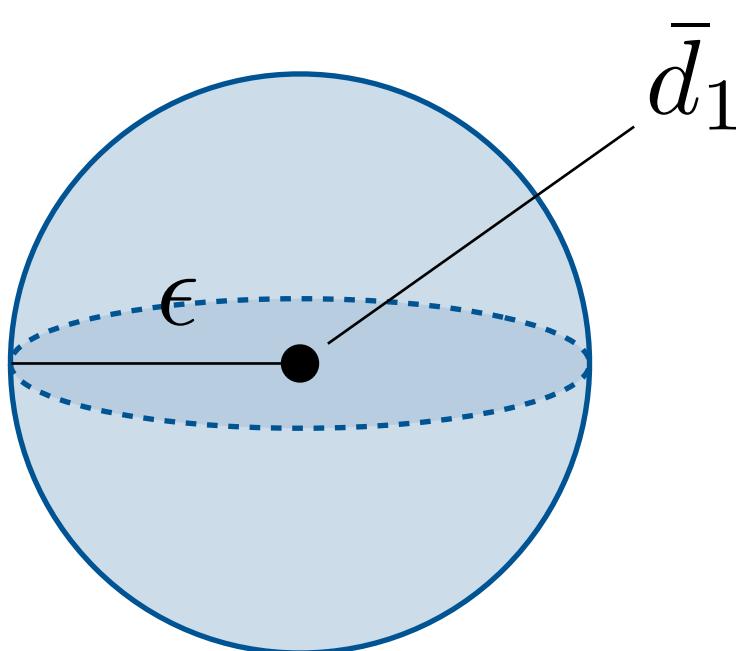
# Examples

# cluster centers

The diagram illustrates three distinct cluster types, each represented by a central square marker surrounded by circular points:

- $d_3$ : A cluster of orange points. The central square marker is orange.
- $d_1$ : A cluster of blue points. The central square marker is blue.
- $d_2$ : A cluster of green points. The central square marker is green.

$$K = 1$$



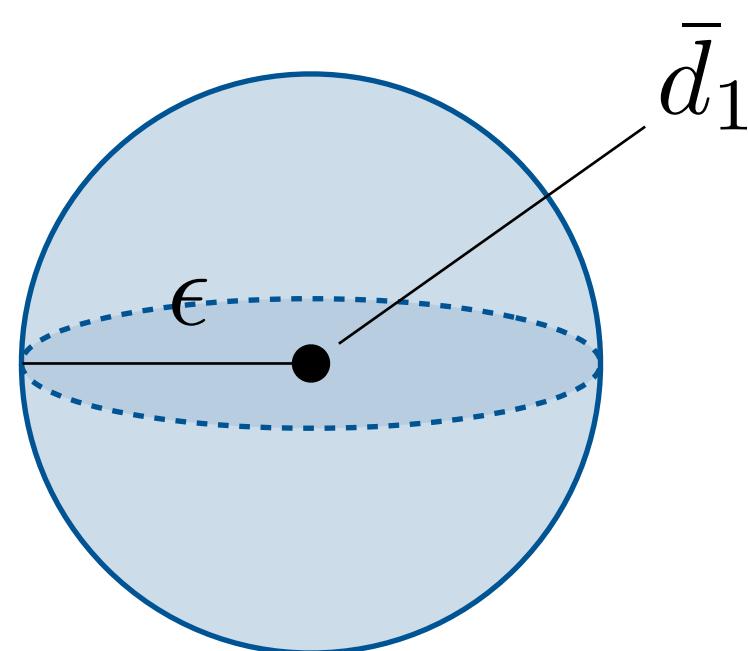
# Uncertainty set

$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

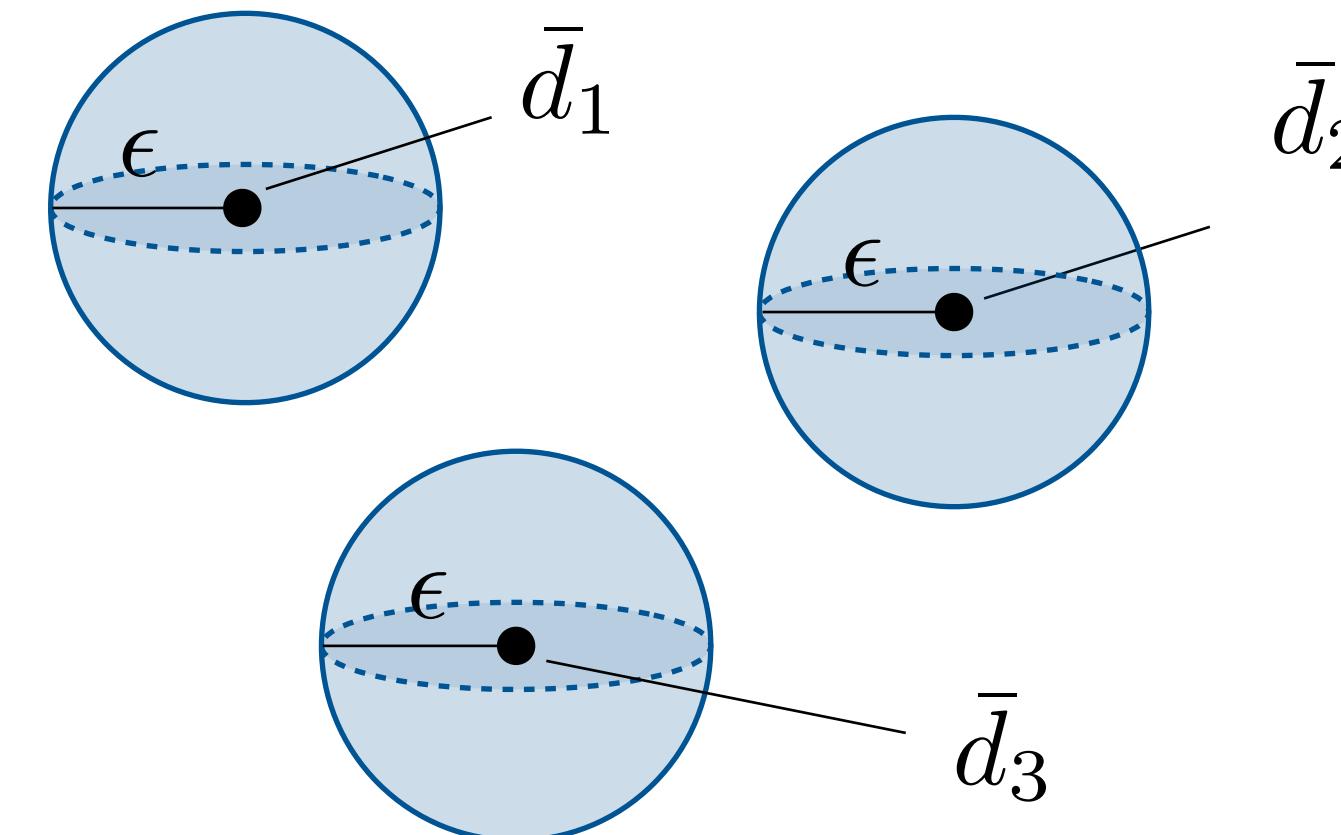
Examples

$K$

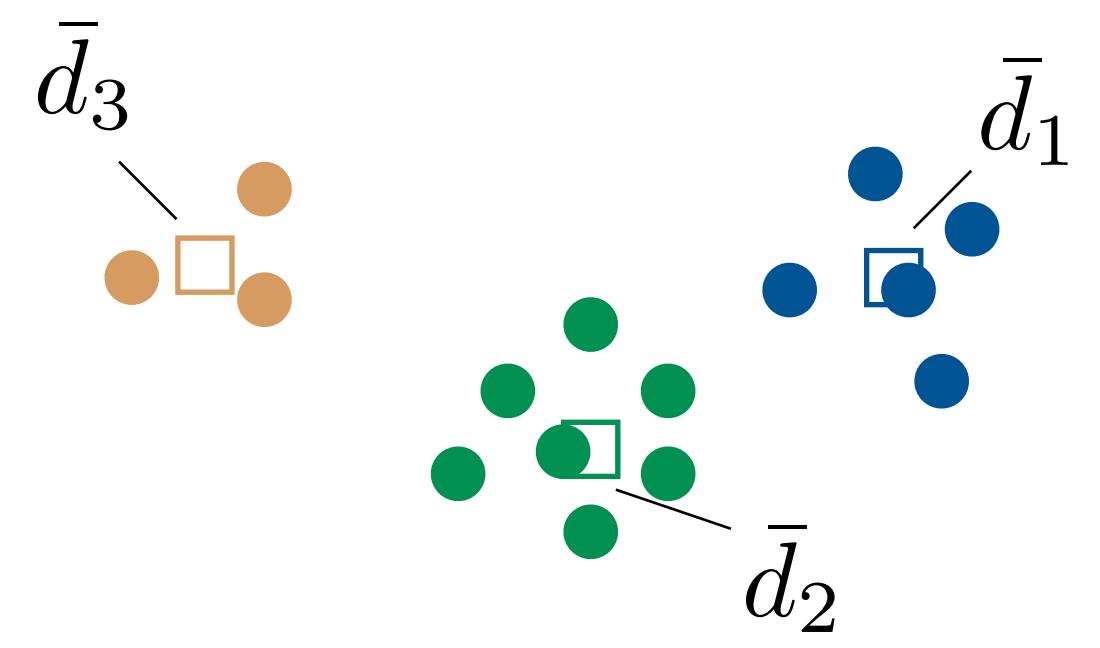
$$K = 1$$



$$K = 3, p = \infty$$



cluster weights  
order  
cluster centers



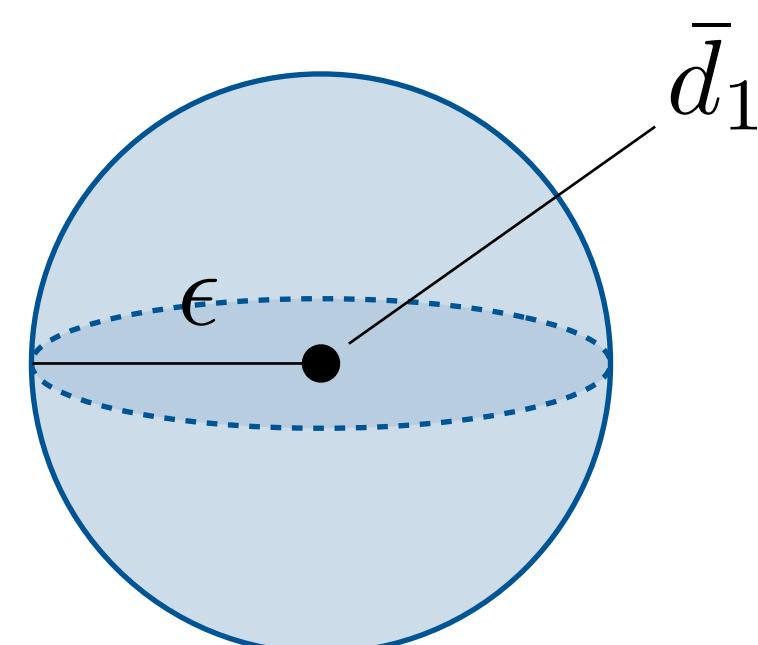
# Uncertainty set

$$\mathcal{U}(K, \epsilon) = \left\{ u = (v_1, \dots, v_K) \mid \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

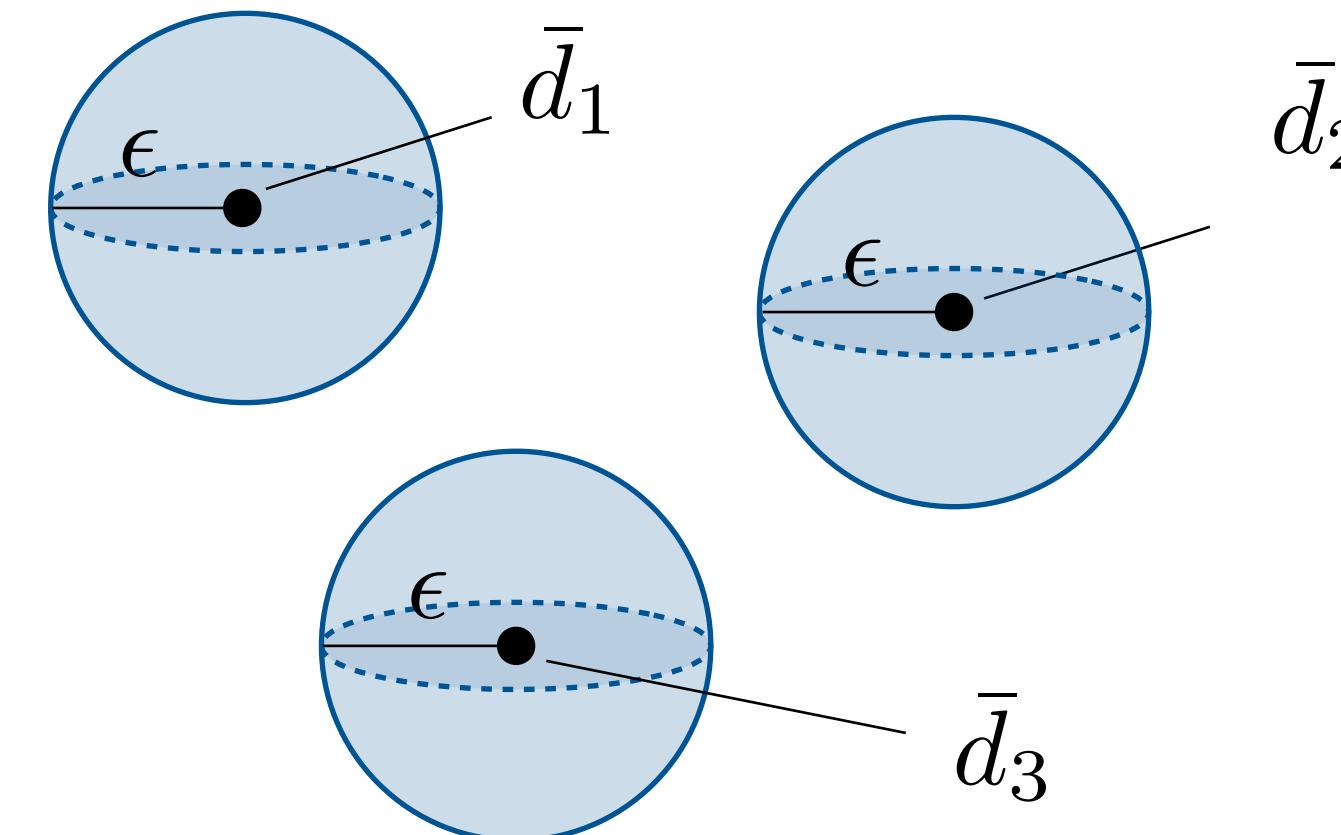
Examples

$K$

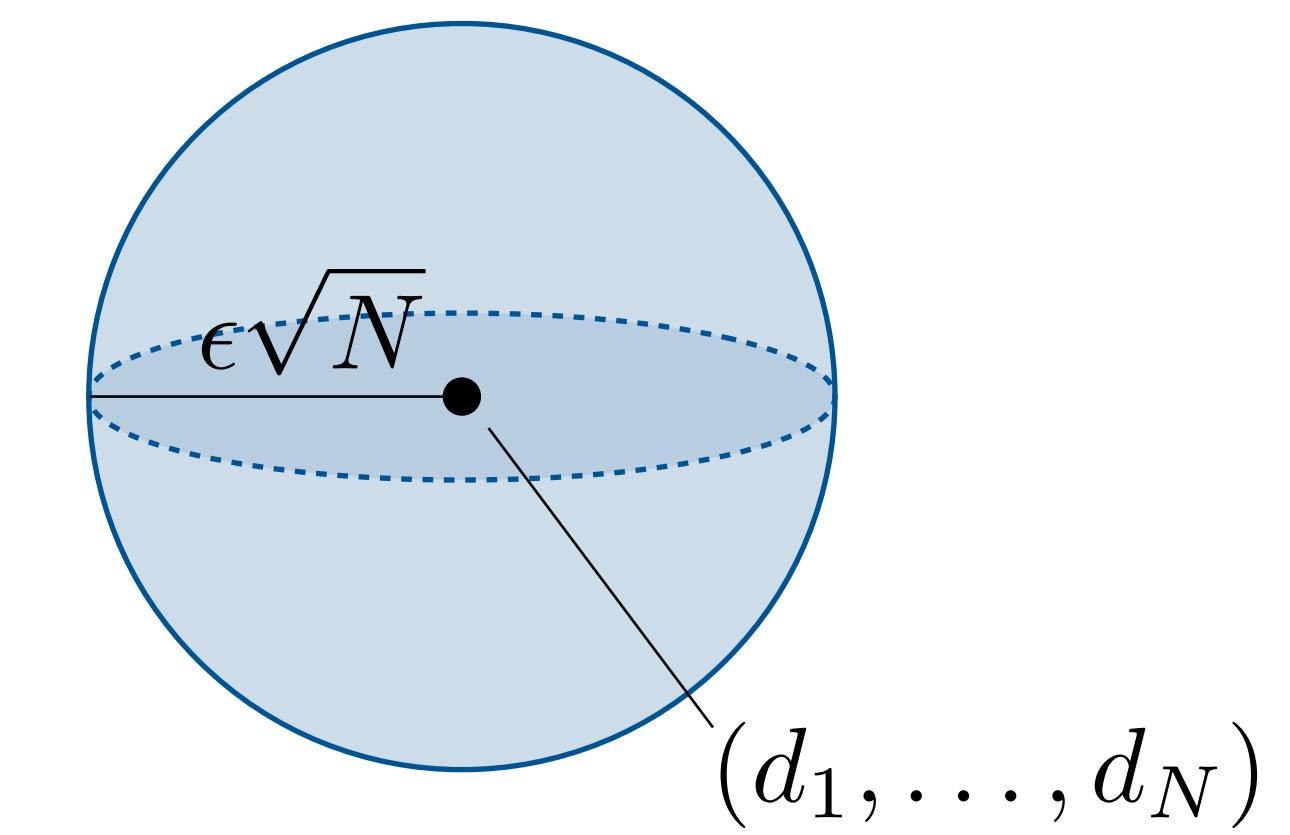
$$K = 1$$



$$K = 3, p = \infty$$



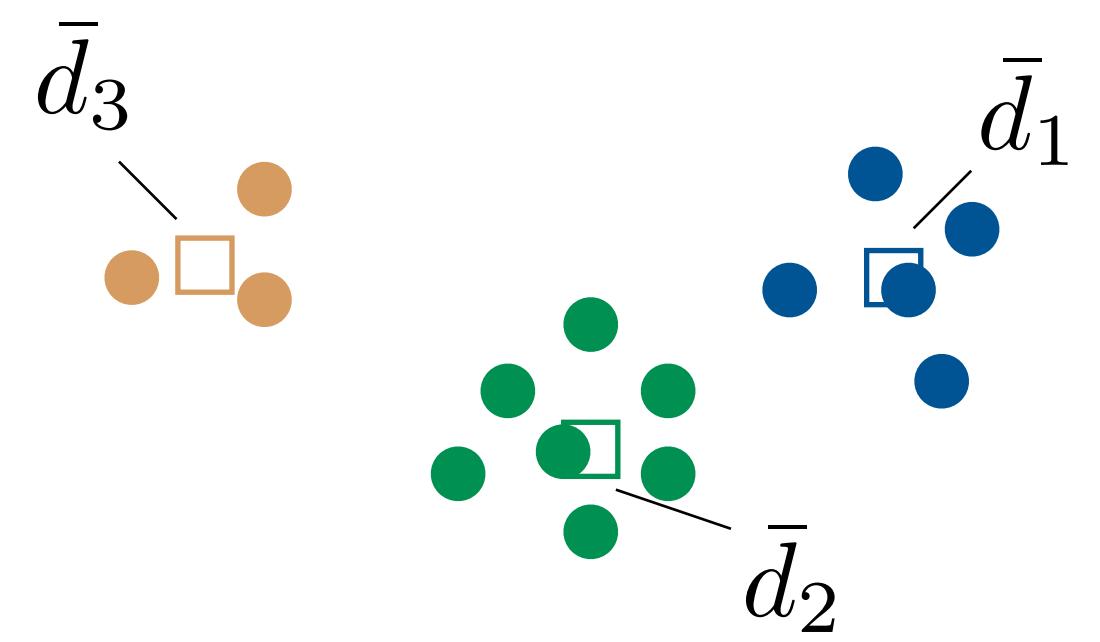
$$K = N, p = 2$$



cluster  
weights

order

cluster  
centers



# Mean Robust Optimization Problem

Uncertain variable lifting

$$u = (v_1, \dots, v_K)$$



$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && \bar{g}(u, x) \leq 0 \quad \forall u \in \mathcal{U}(K, \epsilon) \end{aligned}$$

# Mean Robust Optimization Problem

Uncertain variable lifting  
 $u = (v_1, \dots, v_K)$



minimize  $f(x)$   
subject to  $\bar{g}(u, x) \leq 0 \quad \forall u \in \mathcal{U}(K, \epsilon)$

uncertainty set

$$\left\{ \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$



# Mean Robust Optimization Problem

Uncertain variable lifting  
 $u = (v_1, \dots, v_K)$



minimize       $f(x)$   
subject to     $\bar{g}(u, x) \leq 0 \quad \forall u \in \mathcal{U}(K, \epsilon)$

constraint  
function

$$\sum_{k=1}^K w_k g(v_k, x)$$

uncertainty set

$$\left\{ \sum_{k=1}^K w_k \|v_k - \bar{d}_k\|^p \leq \epsilon^p \right\}$$

# Solving the MRO problem

Dualize constraint  $\bar{g}(u, x) \leq 0, \forall u \in \mathcal{U}(K, \epsilon)$

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && \sum_{k=1}^K w_k s_k \leq 0 \\ & && [-g]^*(z_k, x) - z_k^T \bar{d}_k + \phi(p) \lambda \|z_k/\lambda\|_*^{p/(p-1)} + \lambda \epsilon^p \leq s_k, \quad k = 1, \dots, K \\ & && \lambda \geq 0 \end{aligned}$$

# Solving the MRO problem

Dualize constraint  $\bar{g}(u, x) \leq 0, \forall u \in \mathcal{U}(K, \epsilon)$

minimize  $f(x)$

subject to  $\sum_{k=1}^K w_k s_k \leq 0$

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$$\lambda \geq 0$$

conjugate  
function

# Solving the MRO problem

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minimize  $f(x)$

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conjugate  
function



cluster  
centers

# Solving the MRO problem

Dualize constraint  $\bar{g}(u, x) \leq 0, \forall u \in \mathcal{U}(K, \epsilon)$

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$$\lambda \geq 0$$

conjugate  
function

cluster  
centers

function of  $p \geq 1$   
 $\phi(p) \rightarrow 1$  as  $p \rightarrow \infty$   
 $\phi(1) = 0$

# Solving the MRO problem

Dualize constraint  $\bar{g}(u, x) \leq 0, \forall u \in \mathcal{U}(K, \epsilon)$

minimize  $f(x)$

subject to  $\sum_{k=1}^K w_k s_k \leq 0$

$$[-g]^*(z_k, x) - z_k^T \bar{d}_k + \phi(p) \lambda \|z_k/\lambda\|_*^{p/(p-1)} + \lambda \epsilon^p \leq s_k, \quad k = 1, \dots, K$$

$\lambda \geq 0$

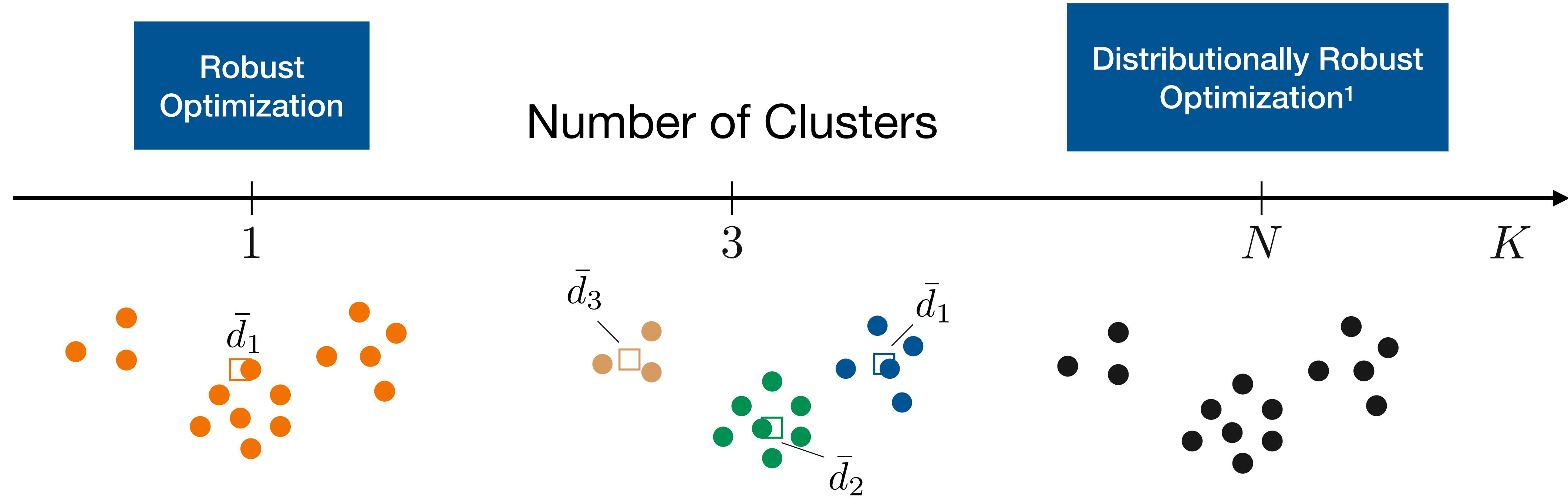
conjugate  
function

cluster  
centers

function of  $p \geq 1$   
 $\phi(p) \rightarrow 1$  as  $p \rightarrow \infty$   
 $\phi(1) = 0$

It can be very expensive when  $K$  is large (e.g.,  $K = N$ )

# MRO bridges RO and DRO



1. D Kuhn, P M Esfahani, V A Nguyen, and S Shafieezadeh-Abadeh, "Wasserstein Distributionally Robust Optimization: Theory and Applications in Machine Learning"

# **Guarantees**

# Satisfying the probabilistic guarantees

$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

# Satisfying the probabilistic guarantees

probability of  
constraint  
satisfaction



$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

# Satisfying the probabilistic guarantees

probability of  
constraint  
satisfaction

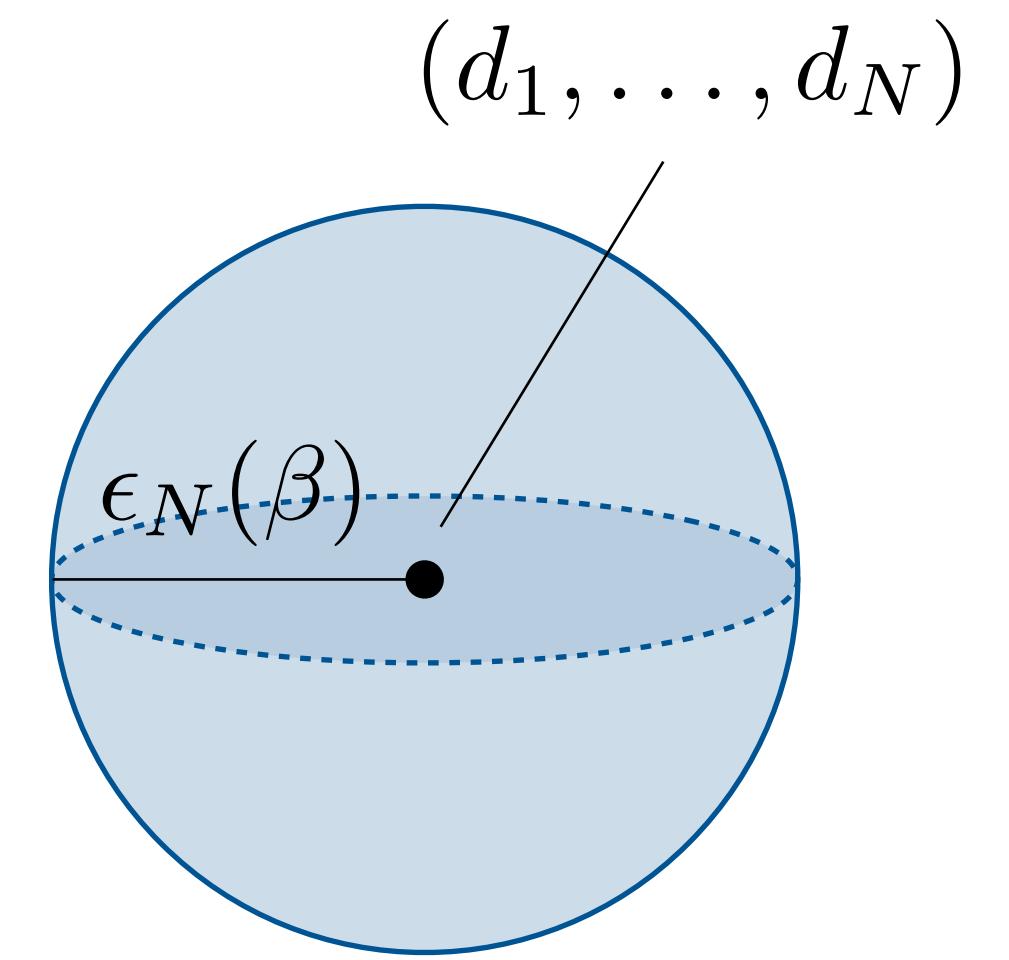
↓

$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

light-tailed

uncertainty set  
radius

↓

$$\mathcal{U}(N, \epsilon_N(\beta))$$


# Satisfying the probabilistic guarantees

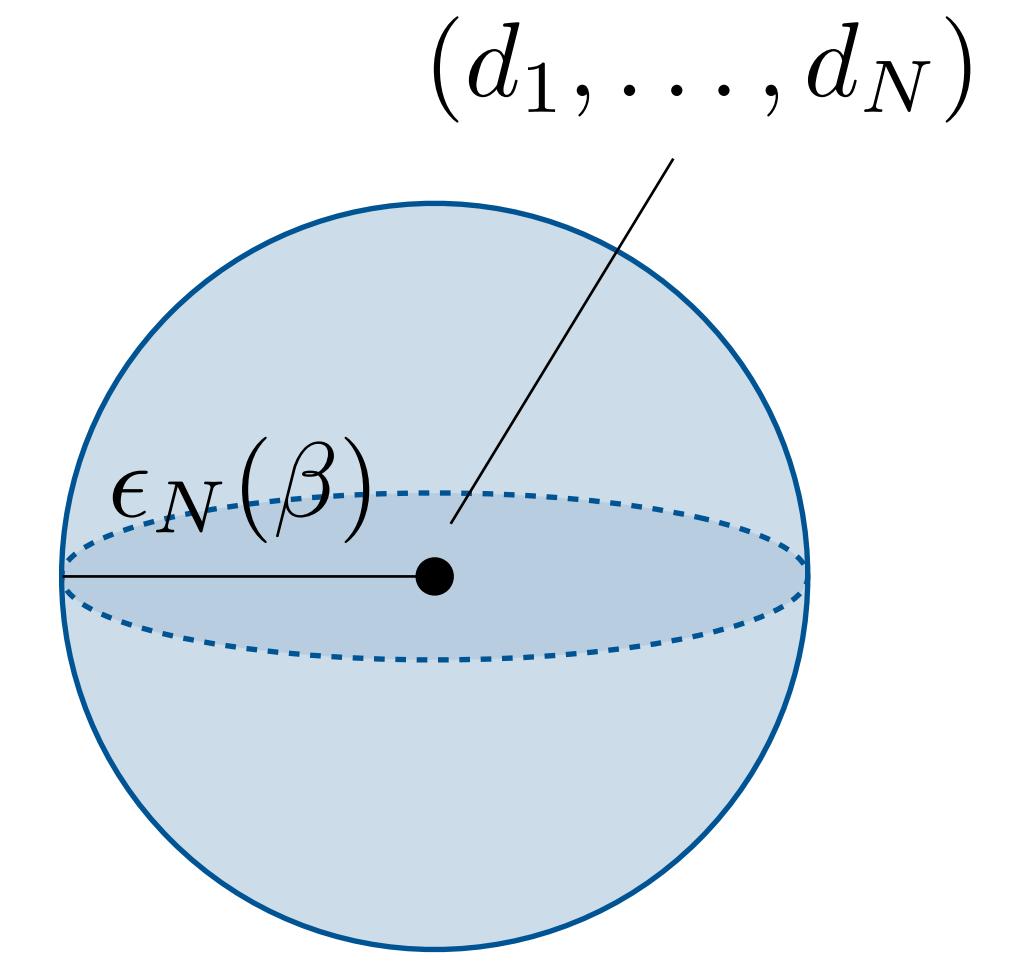
probability of  
constraint  
satisfaction

$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

light-tailed

uncertainty set  
radius

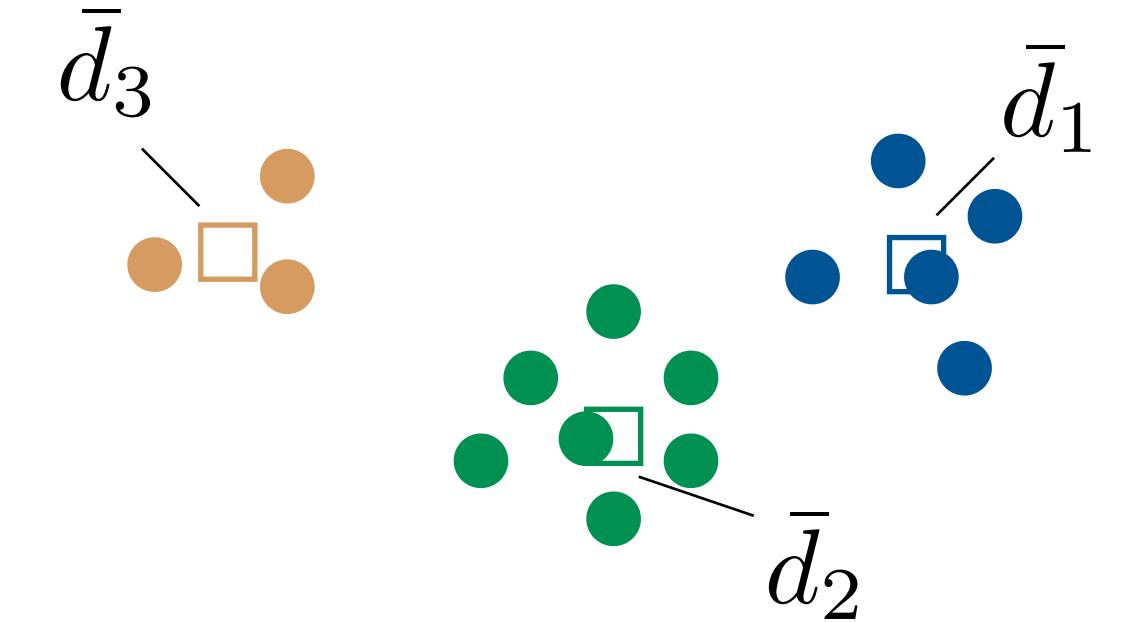
$$\mathcal{U}(N, \epsilon_N(\beta))$$



MRO clustering

$$\mathcal{U}(K, \epsilon_N(\beta) + \eta_N(K))$$

$$\frac{1}{N} \sum_{k=1}^K \sum_{d_i \in C_k} \|d_i - \bar{d}_k\|^p$$



# Satisfying the probabilistic guarantees

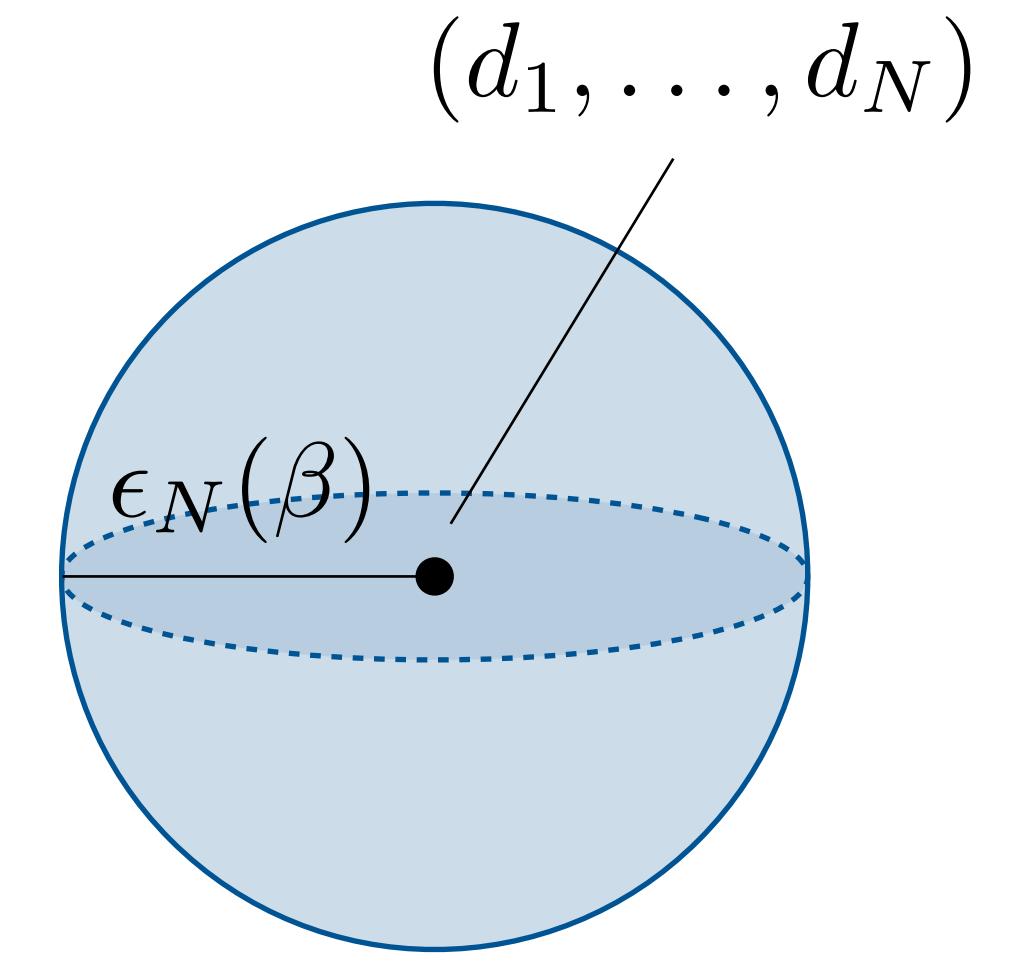
probability of  
constraint  
satisfaction

$$\mathbf{P}^N (\mathbf{E}(g(u, \hat{x}_N)) \leq 0) \geq 1 - \beta$$

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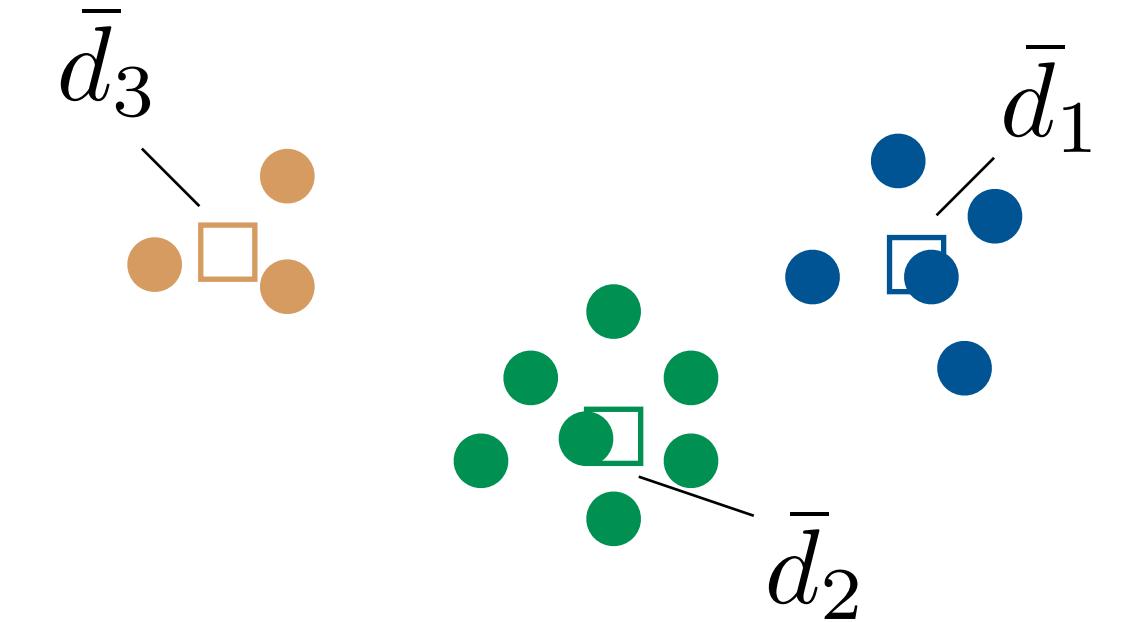
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$$\frac{1}{N} \sum_{k=1}^K \sum_{d_i \in C_k} \|d_i - \bar{d}_k\|^p$$



Quite conservative bounds... can we do better?

# Bounding the conservatism

MRO constraint

$$\bar{g}(u, x) \leq 0 \quad \forall u \in \mathcal{U}(K, \epsilon)$$

Worst-case values

$$\bar{g}^N(x) = \underset{u \in \mathcal{U}(N, \epsilon)}{\text{maximize}} \quad \bar{g}(u, x)$$

$$\bar{g}^K(x) = \underset{u \in \mathcal{U}(K, \epsilon)}{\text{maximize}} \quad \bar{g}(u, x)$$

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## Theorem

If  $-g$  is  $L$ -smooth in  $u$ , we have

$$\bar{g}^N(x) \leq \bar{g}^K(x) \leq \bar{g}^N(x) + \frac{L}{2} D(K)$$

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**MRO constraint**

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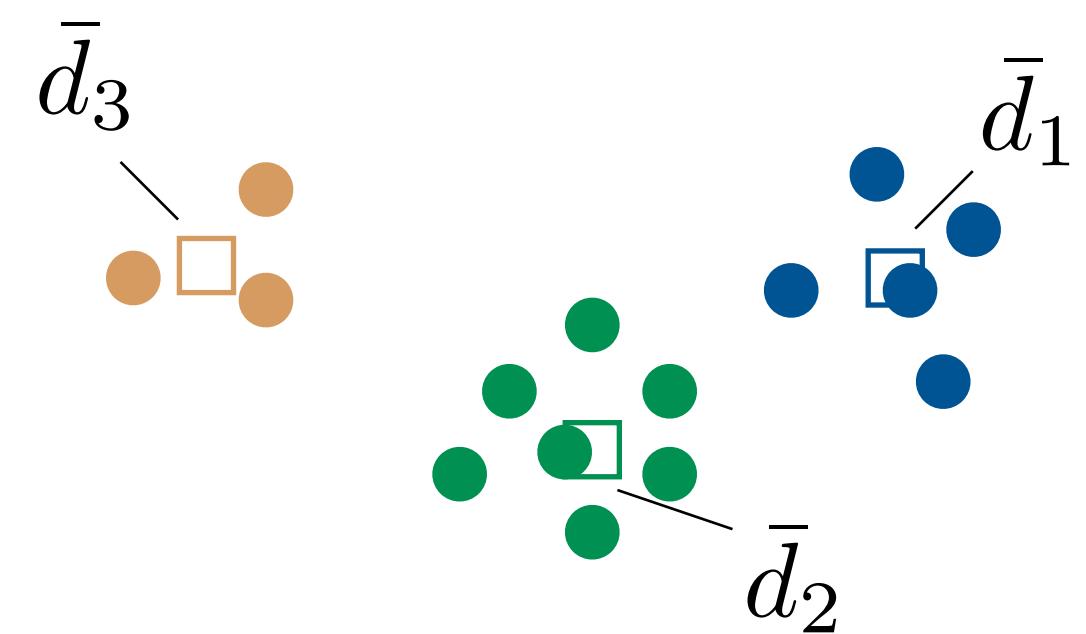
$$\bar{g}^N(x) \leq \bar{g}^K(x) \leq \bar{g}^N(x) + \frac{L}{2} D(K) \leftarrow \min \quad \frac{1}{N} \sum_{k=1}^K \sum_{d_i \in C_k} \|d_i - \bar{d}_k\|^2$$

clustering  
objective

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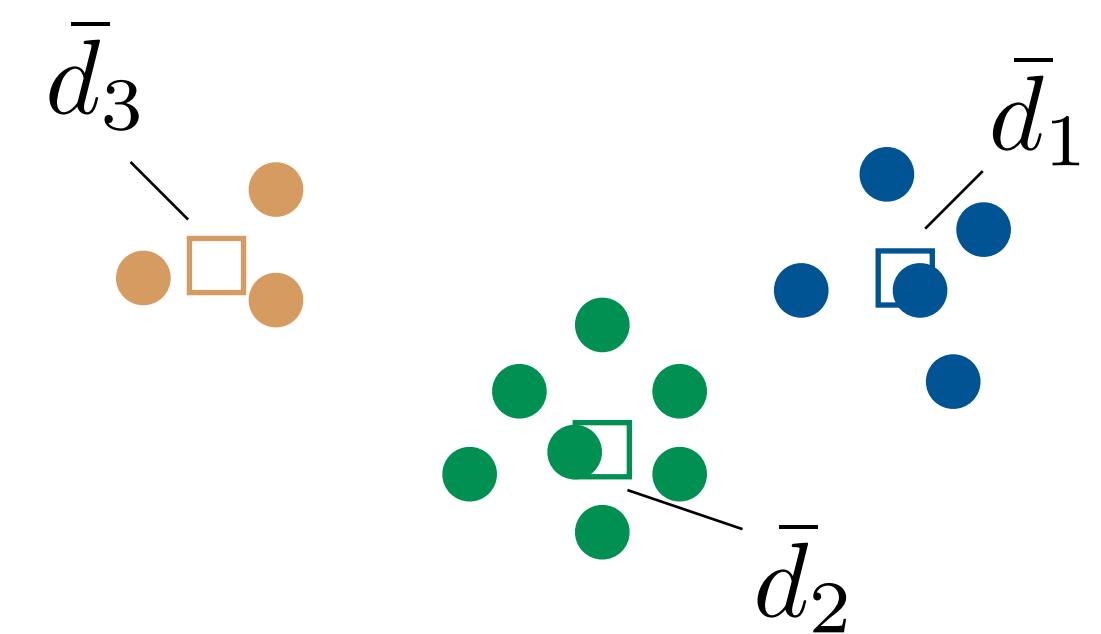
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When  $g$  is affine in  $u$  ( $L = 0$ ), clustering makes no difference to the optimal value or optimal solution

# Example MRO with linear constraints

$$p = \infty \quad (a + Pu)^T x \leq b \quad \longrightarrow \quad g(u, x) = (a + Pu)^T x - b$$

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$\uparrow$

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## Convex reformulation

$$\text{minimize} \quad f(x)$$

$$\text{subject to} \quad a^T x - b + (P^T x)^T \sum_{k=1}^K w_k \bar{d}_k + \epsilon \|P^T x\|_* \leq 0$$

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(clustering makes no difference)  $\bar{d}$  average

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(clustering makes  
no difference)

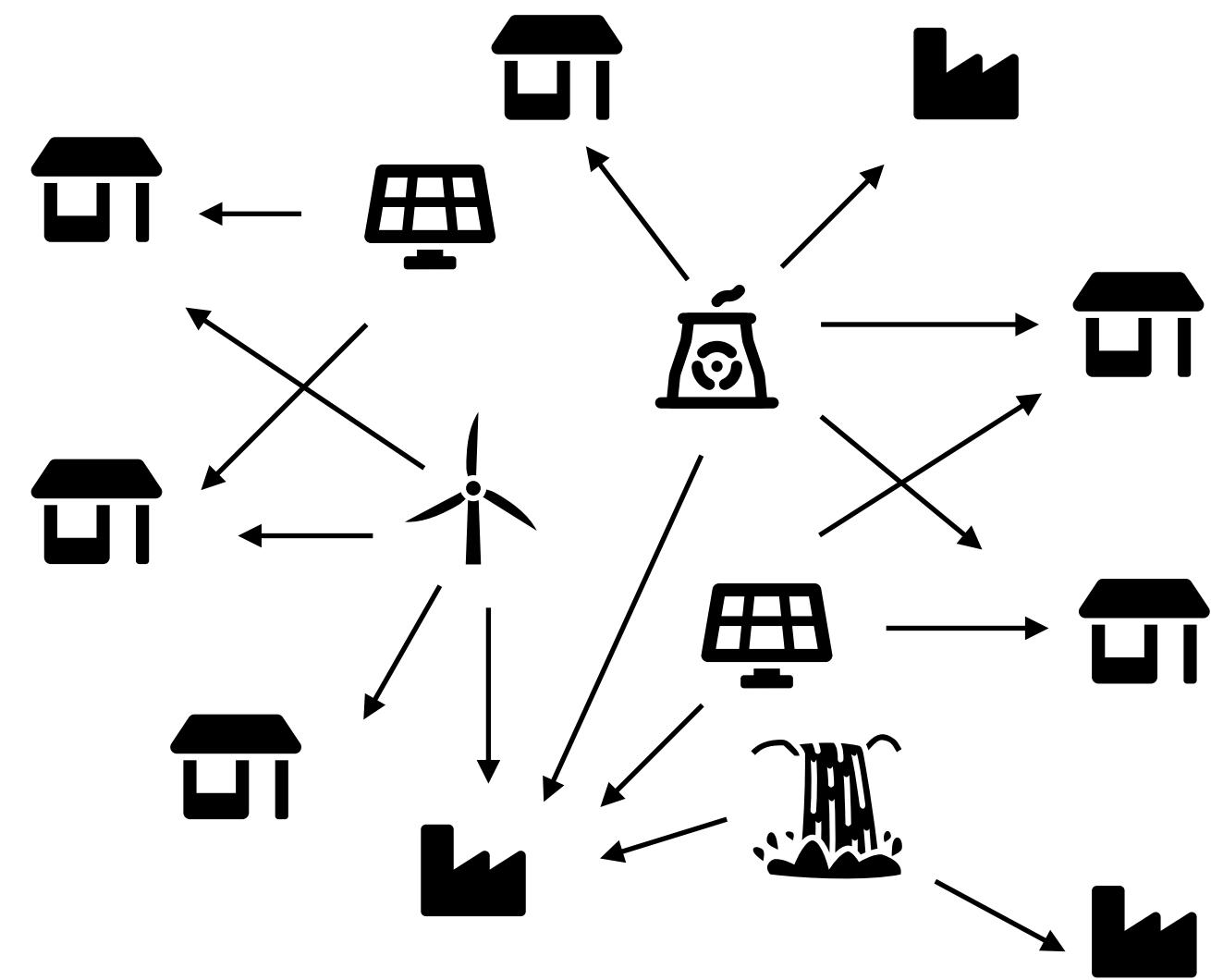
average  
 $\bar{d}$

**Classical  
Robust Optimization  
reformulation**

# Numerical examples

# Facility location example

minimize  $c^T x + \text{tr}(C^T X)$   
subject to  $\mathbf{1}^T X_j = 1, \quad j = 1, \dots, m$   
 $(X^T)_i u \leq r_i x_i, \quad i = 1, \dots, n$   
 $x \in \{0, 1\}^n, \quad X \in \mathbf{R}^{n \times m}$



# Facility location example

cost of  
opening facilities

minimize

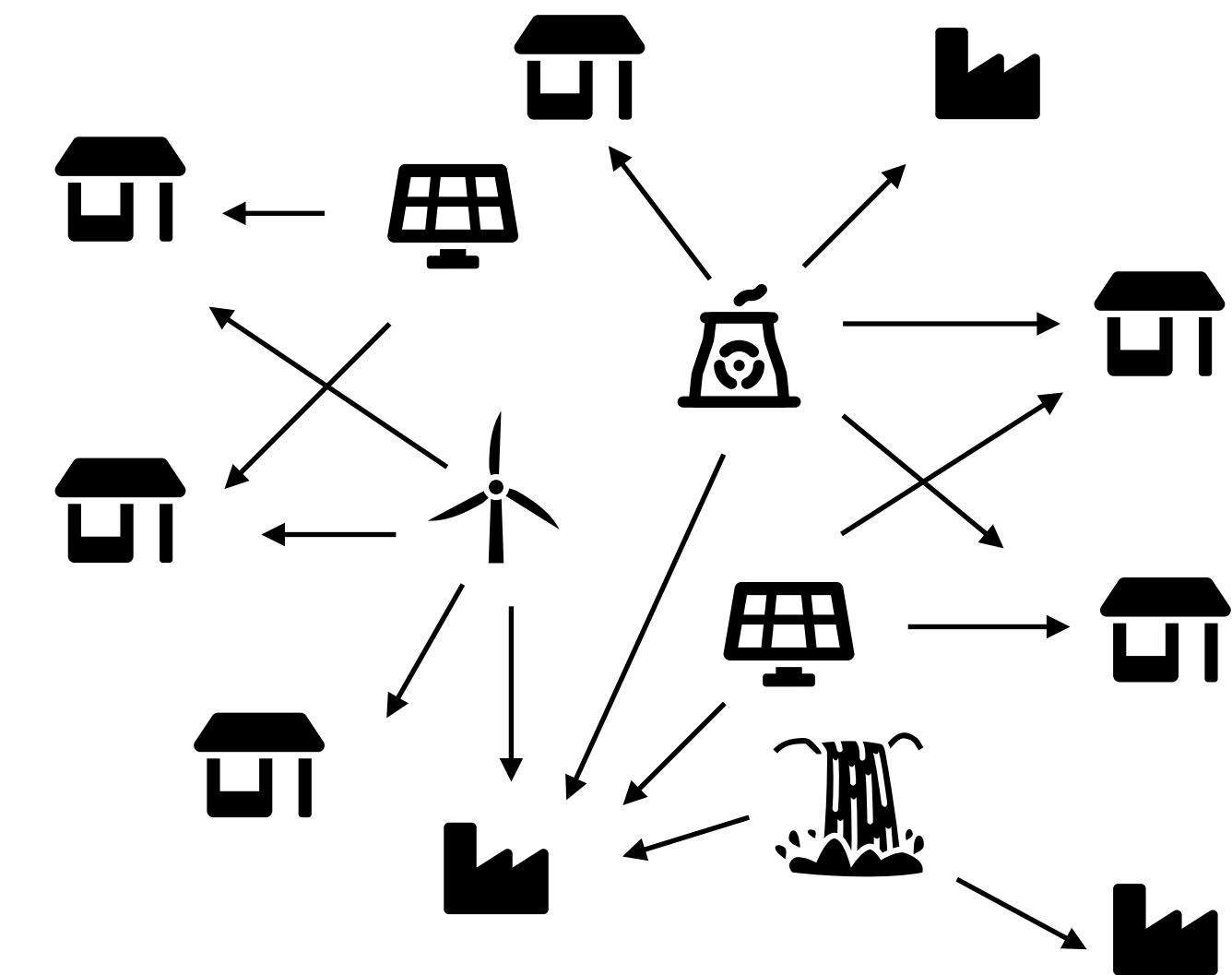
$$c^T x + \text{tr}(C^T X)$$

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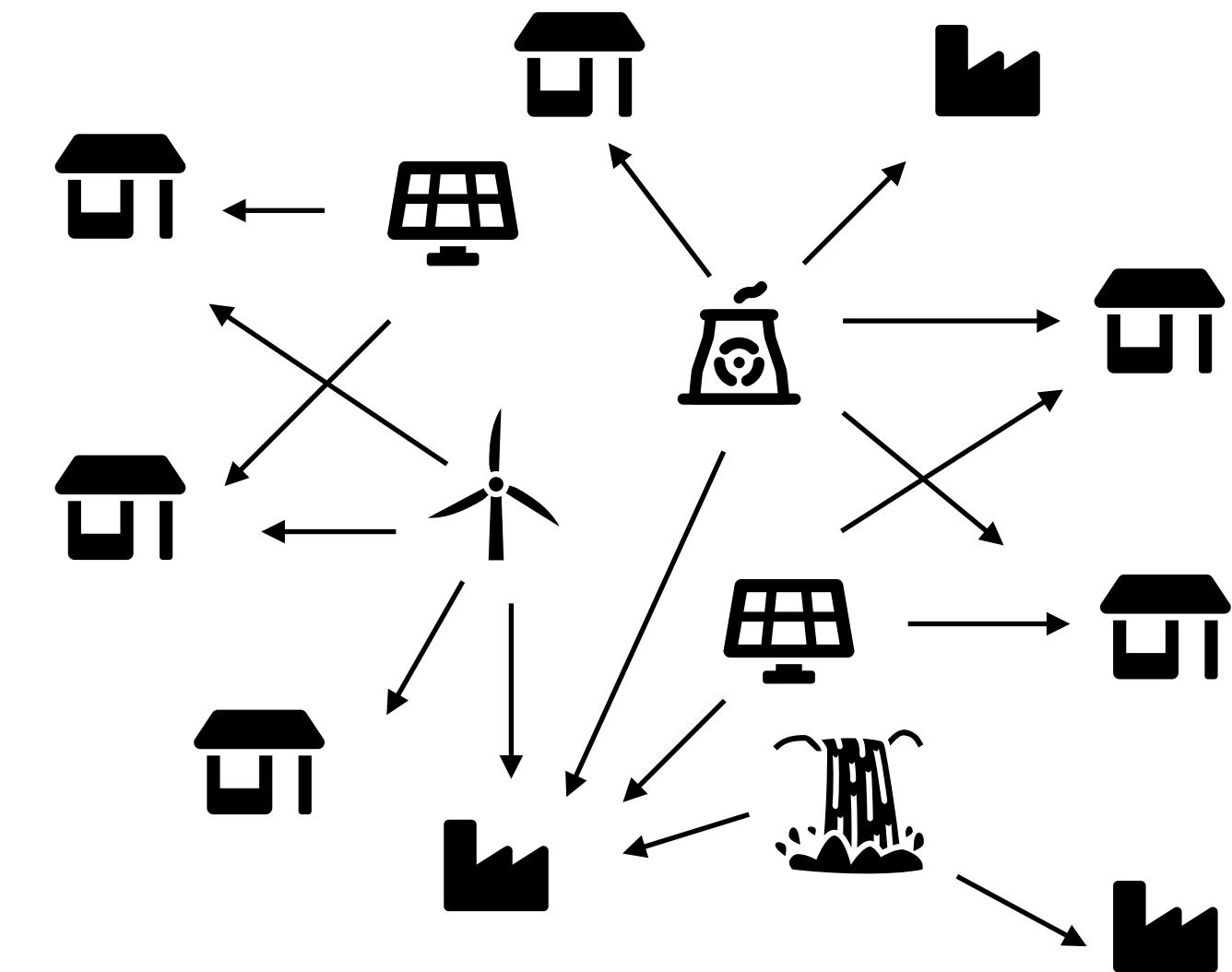
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cost of  
energy distribution



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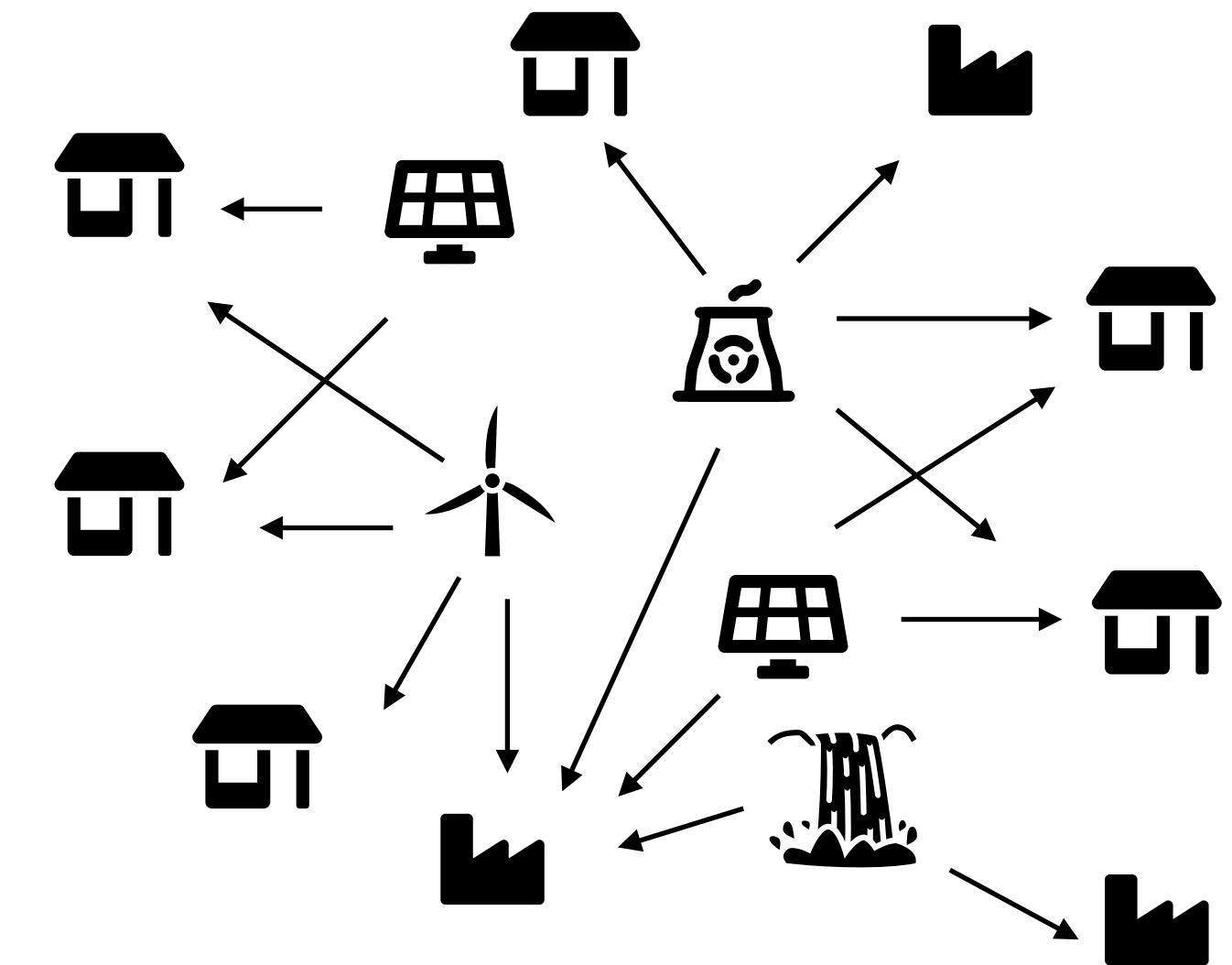
$$\mathbf{1}^T X_j = 1, \quad j = 1, \dots, m$$

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cost of  
energy distribution

capacity  
constraints  
 $g(u, x, X) \leq 0$



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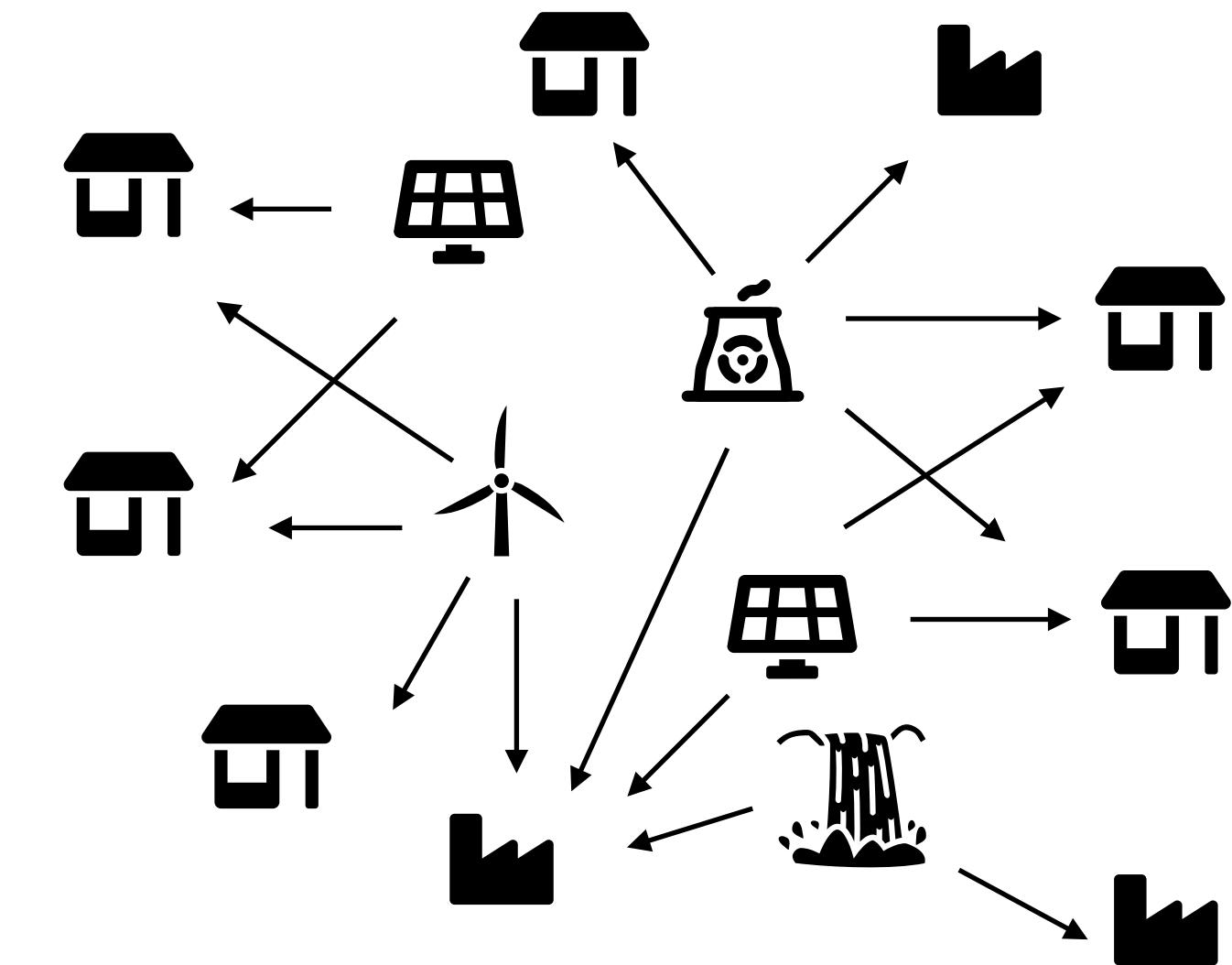
vector of uncertain  
energy demands

$$(X^T)_i u \leq r_i x_i, \quad i = 1, \dots, n$$

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cost of  
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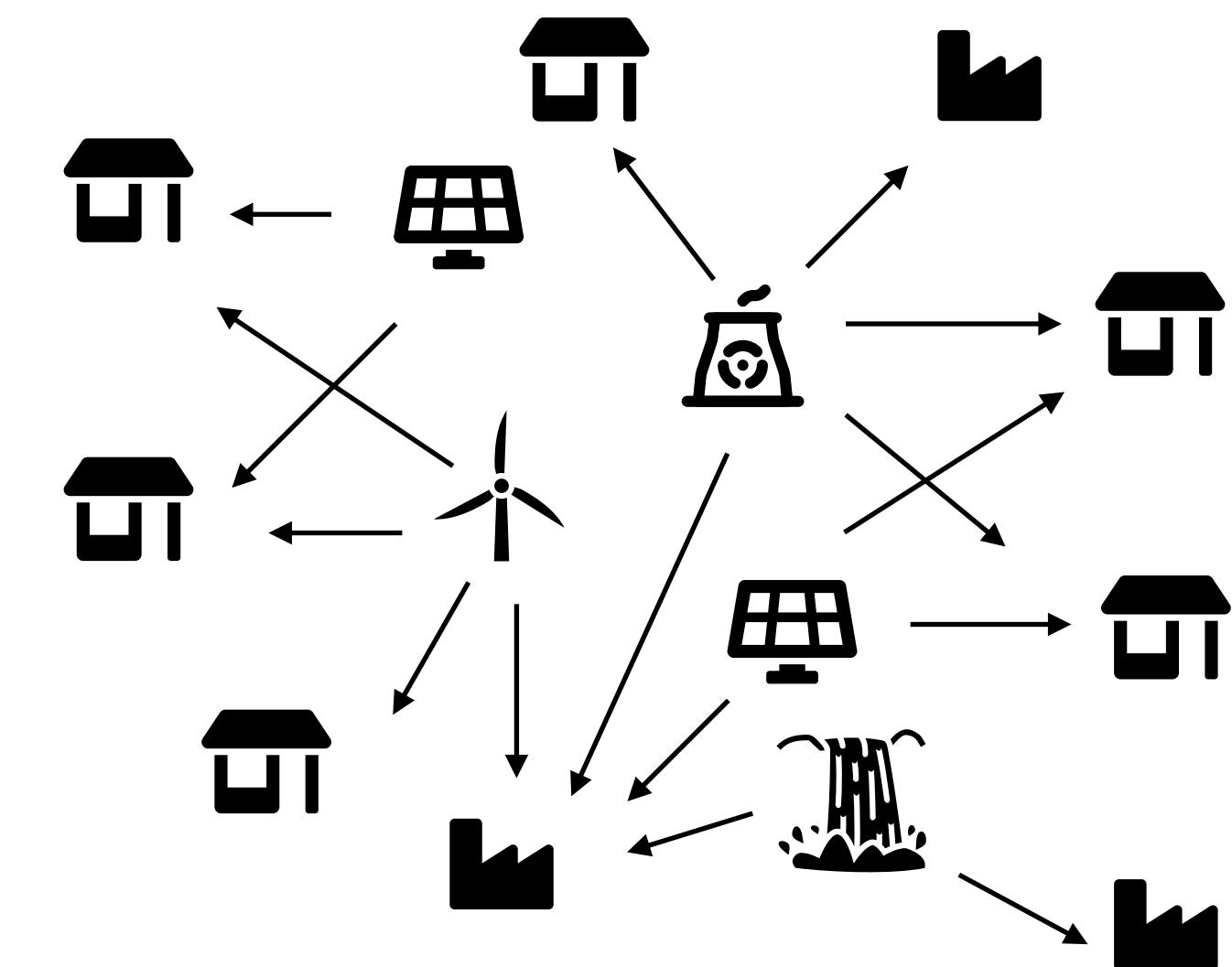
vector of uncertain  
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cost of  
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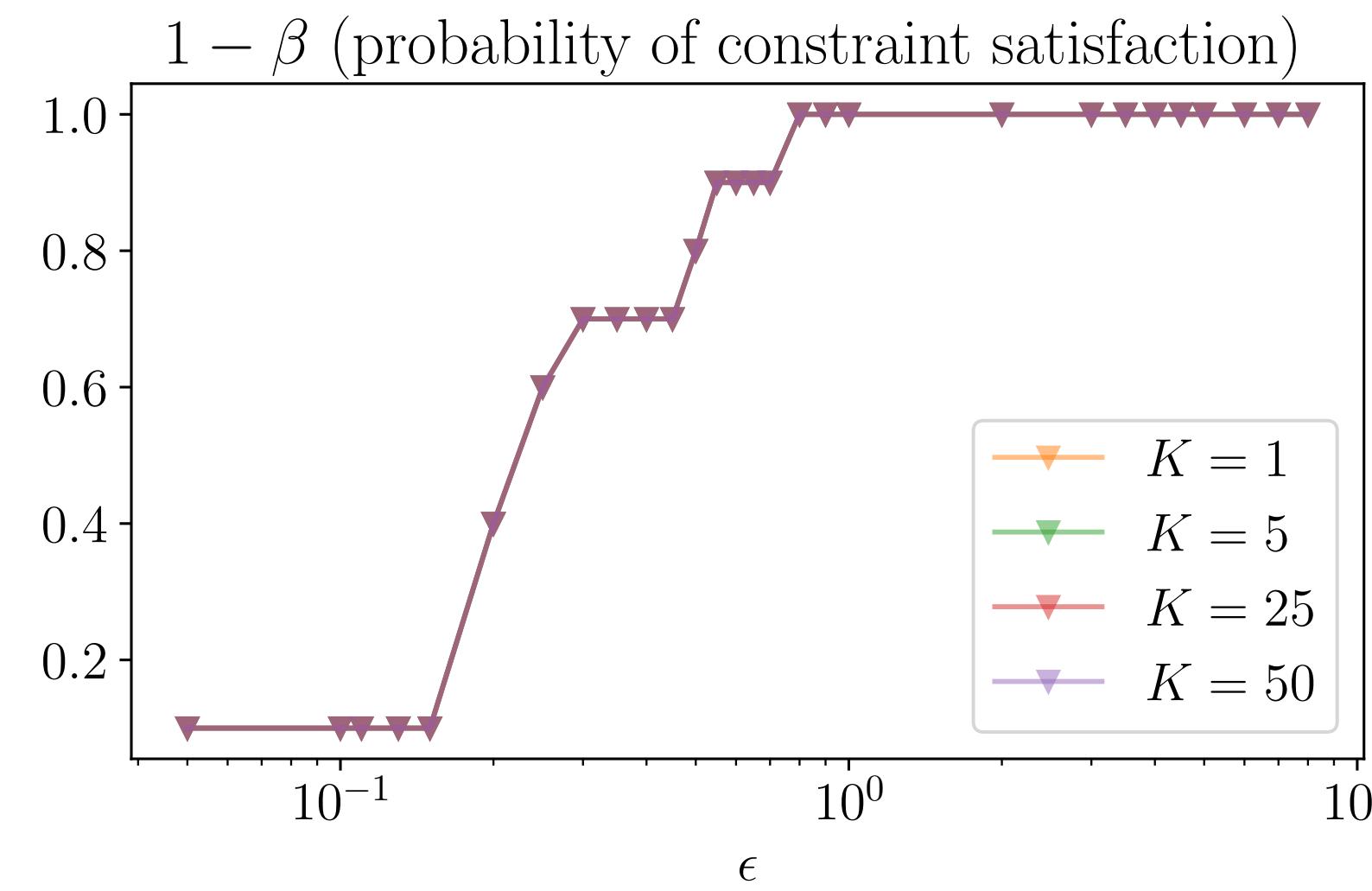
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clustering  
does not  
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# Facility location example

cost of opening facilities

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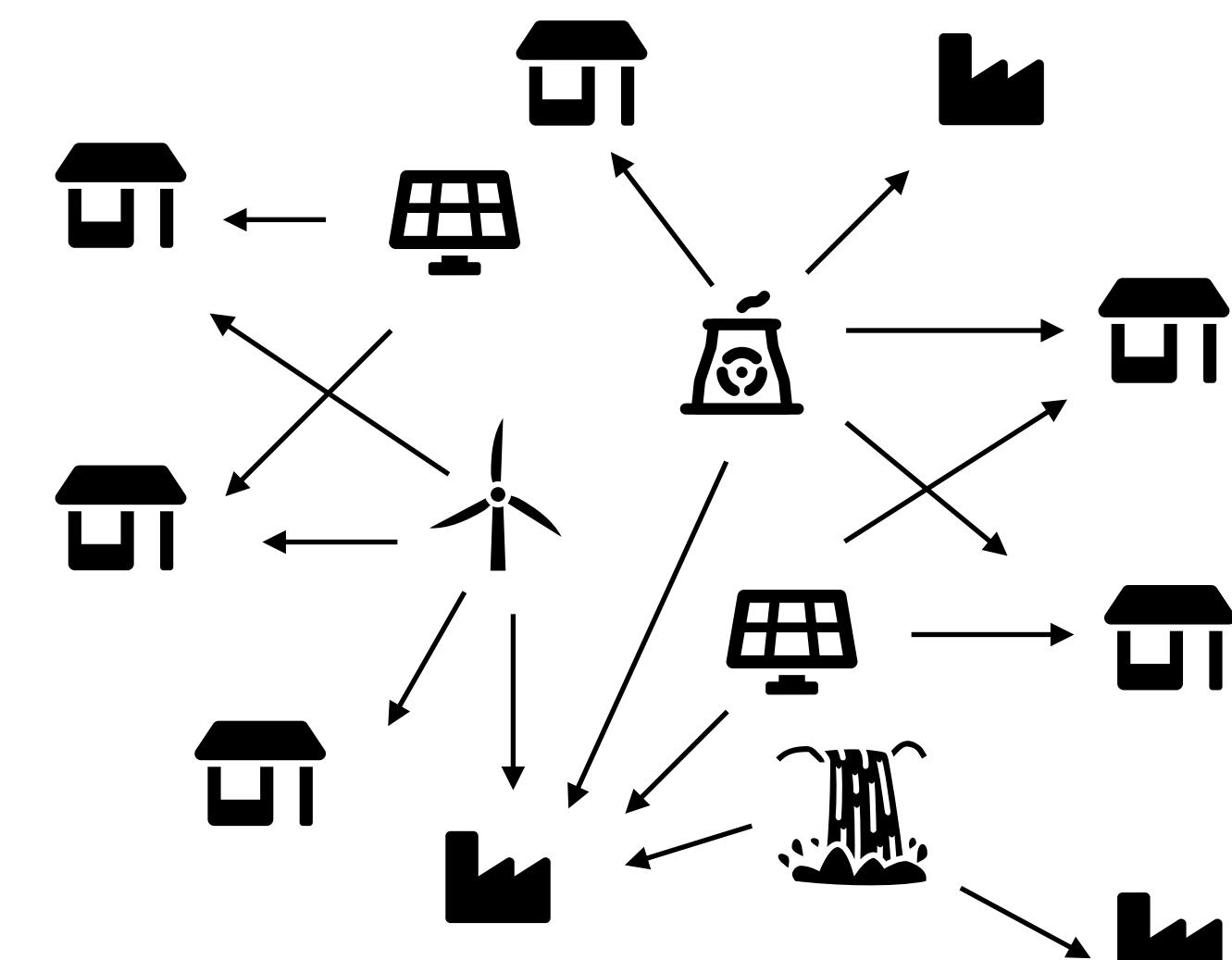
subject to

$$\begin{aligned} & \mathbf{1}^T X_j = 1, \quad j = 1, \dots, m \\ & (X^T)_i u \leq r_i x_i, \quad i = 1, \dots, n \\ & x \in \{0, 1\}^n, \quad X \in \mathbf{R}^{n \times m} \end{aligned}$$

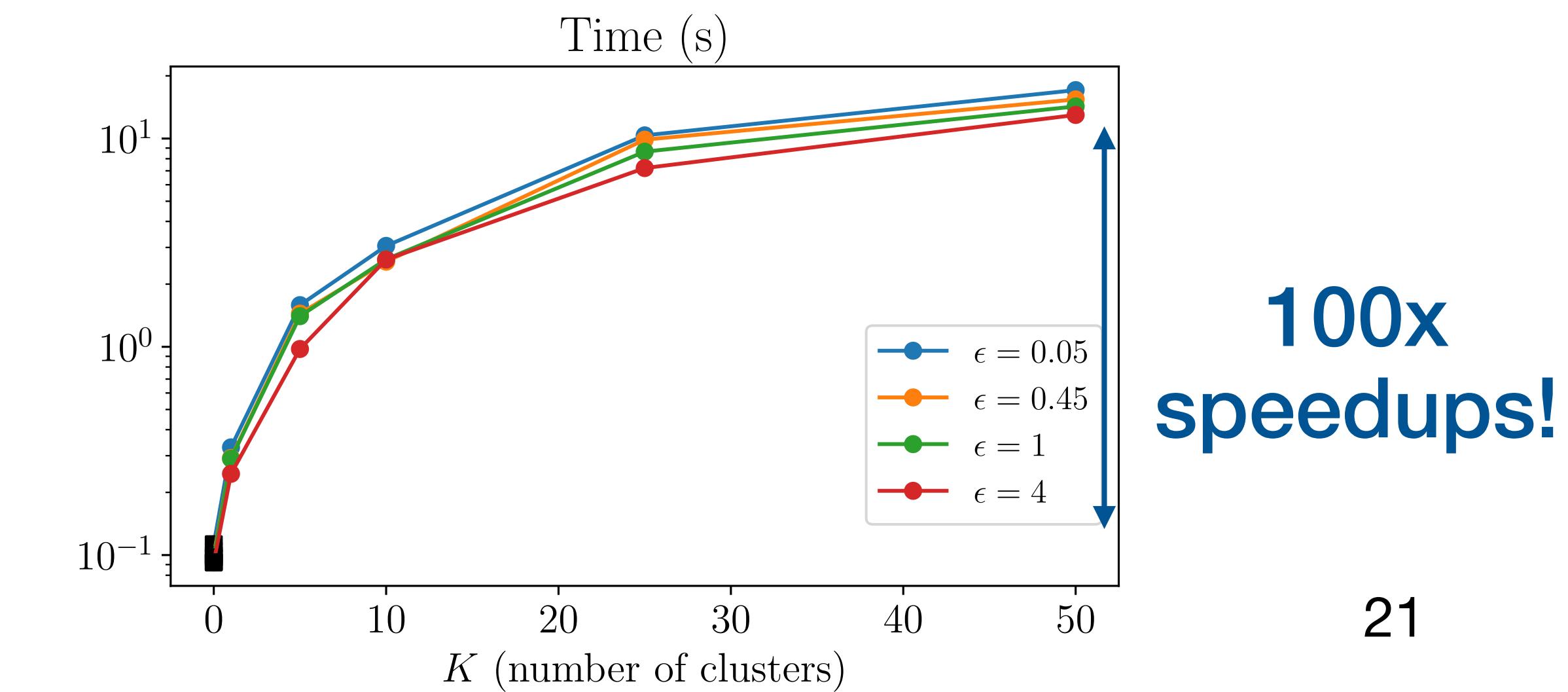
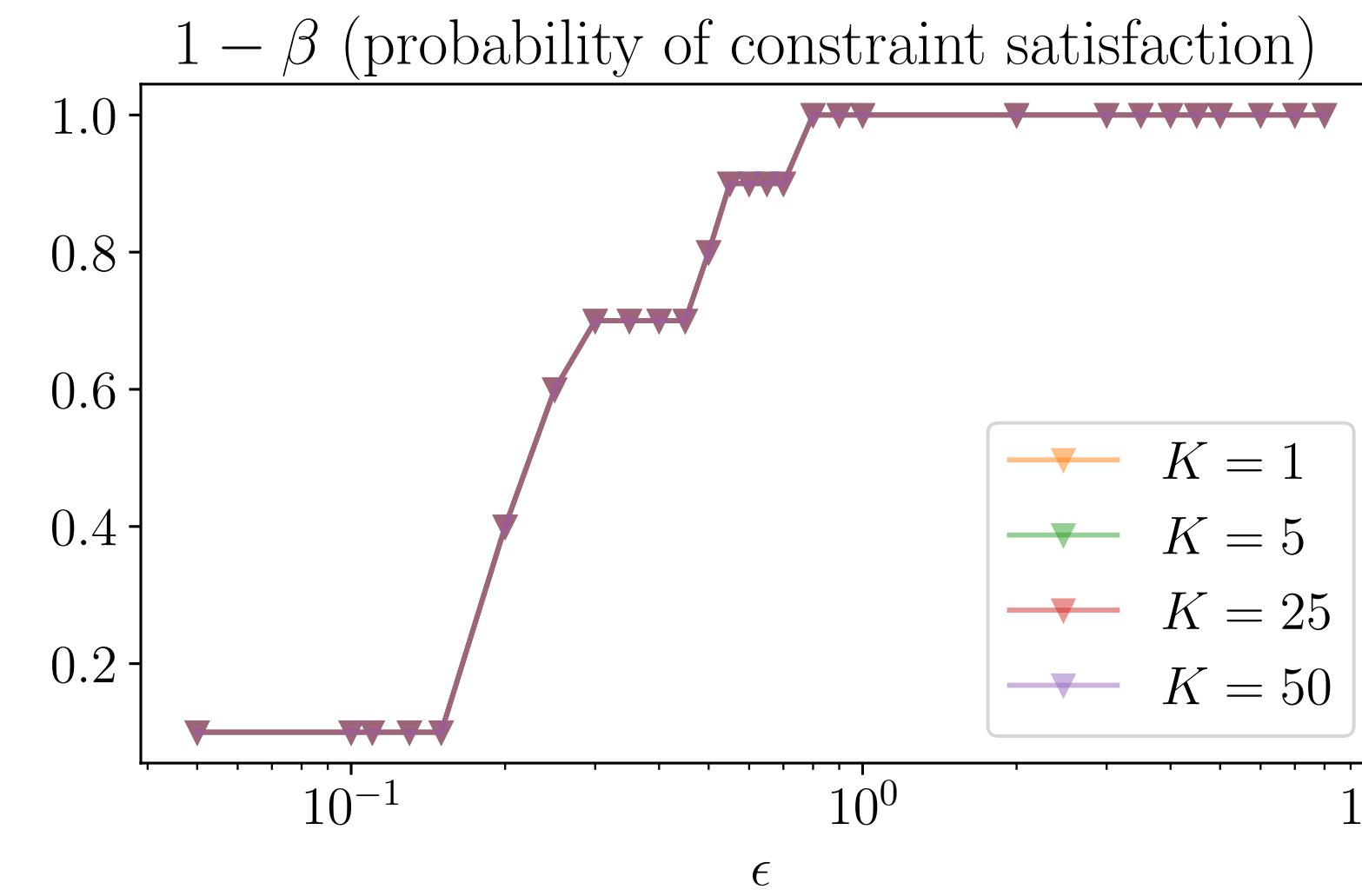
vector of uncertain energy demands

cost of energy distribution

capacity constraints

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clustering does not affect constraint satisfaction



# Capital budgeting example

## Problem

$$\text{maximize} \quad \eta(u)^T x$$

$$\text{subject to} \quad a^T x \leq b$$

$$x \in \{0, 1\}^n$$

# Capital budgeting example

Problem	total net present value (NPV)
maximize	$\eta(u)^T x$
subject to	$a^T x \leq b$
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Problem	total net present value (NPV)
maximize	$\eta(u)^T x$
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budget  
constraint

# Capital budgeting example

Problem                          total  
maximize                          net present value (NPV)  
subject to                         $\eta(u)^T x$  ←  
                                       $a^T x \leq b$  ←  
                                      budget  
                                      constraint  
 $x \in \{0, 1\}^n$

NPV of project  $j$

$$\eta_j(u) = \sum_{t=1}^T \frac{F_{jt}}{(1 + u_j)^t}$$

cash flow ←  
discount rate ←

# Capital budgeting example

**Problem**

maximize       $\eta(u)^T x$       total net present value (NPV)

subject to       $a^T x \leq b$       budget constraint

$x \in \{0, 1\}^n$

The diagram illustrates a binary knapsack problem. It features three main components: an objective function  $\eta(u)^T x$  (highlighted in a light blue box), a budget constraint  $a^T x \leq b$  (highlighted in a light brown box), and a set of variables  $x \in \{0, 1\}^n$ . Labels on the right side identify these components: "total net present value (NPV)" is associated with the objective function, and "budget constraint" is associated with the inequality  $a^T x \leq b$ .

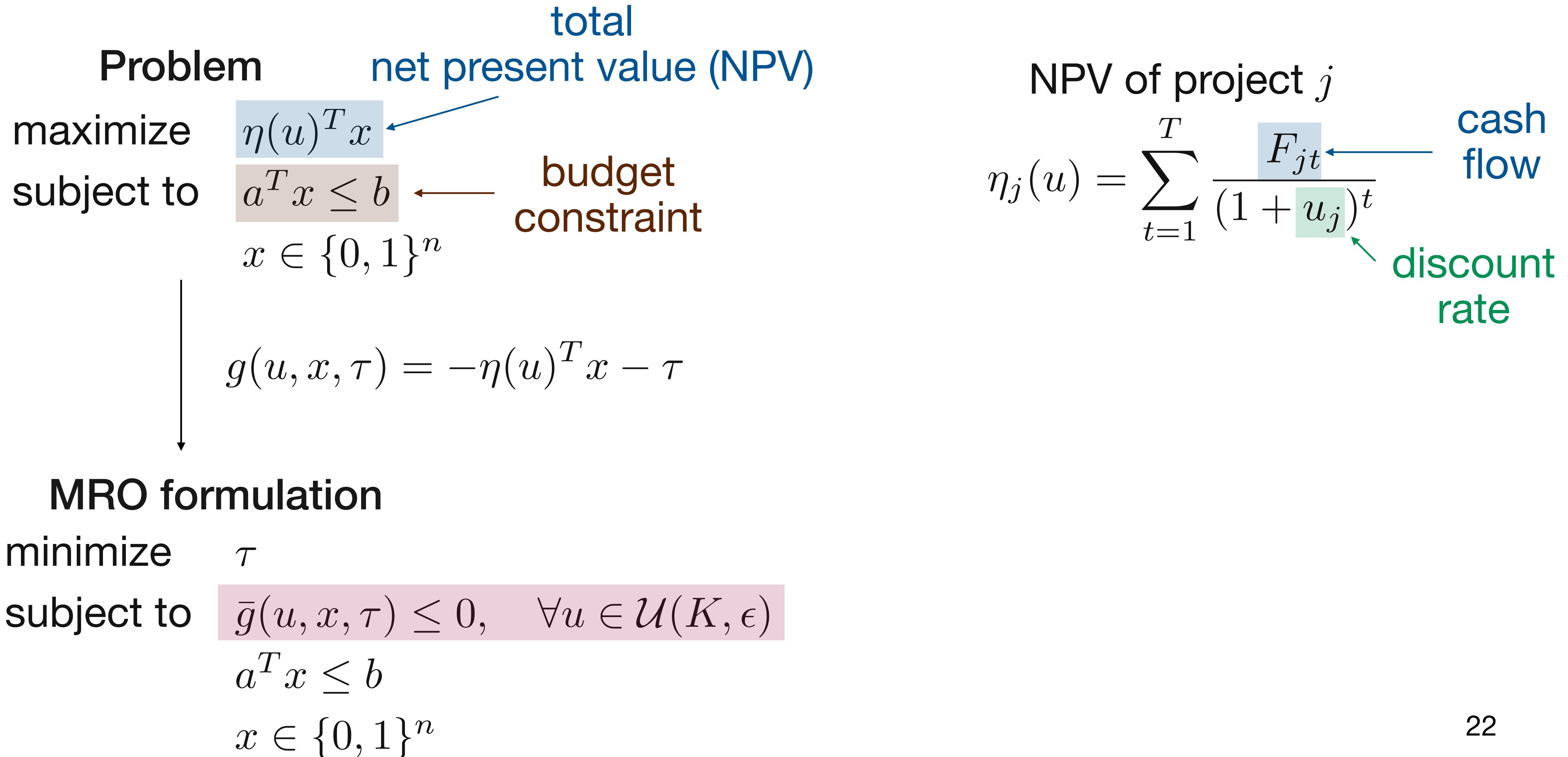
$$g(u, x, \tau) = -\eta(u)^T x - \tau$$

$$\text{NPV of project } j$$
$$\mathcal{C}_j(u) = \sum_{t=1}^T \frac{F_{jt}}{(1 + u_j)^t}$$

cash flow

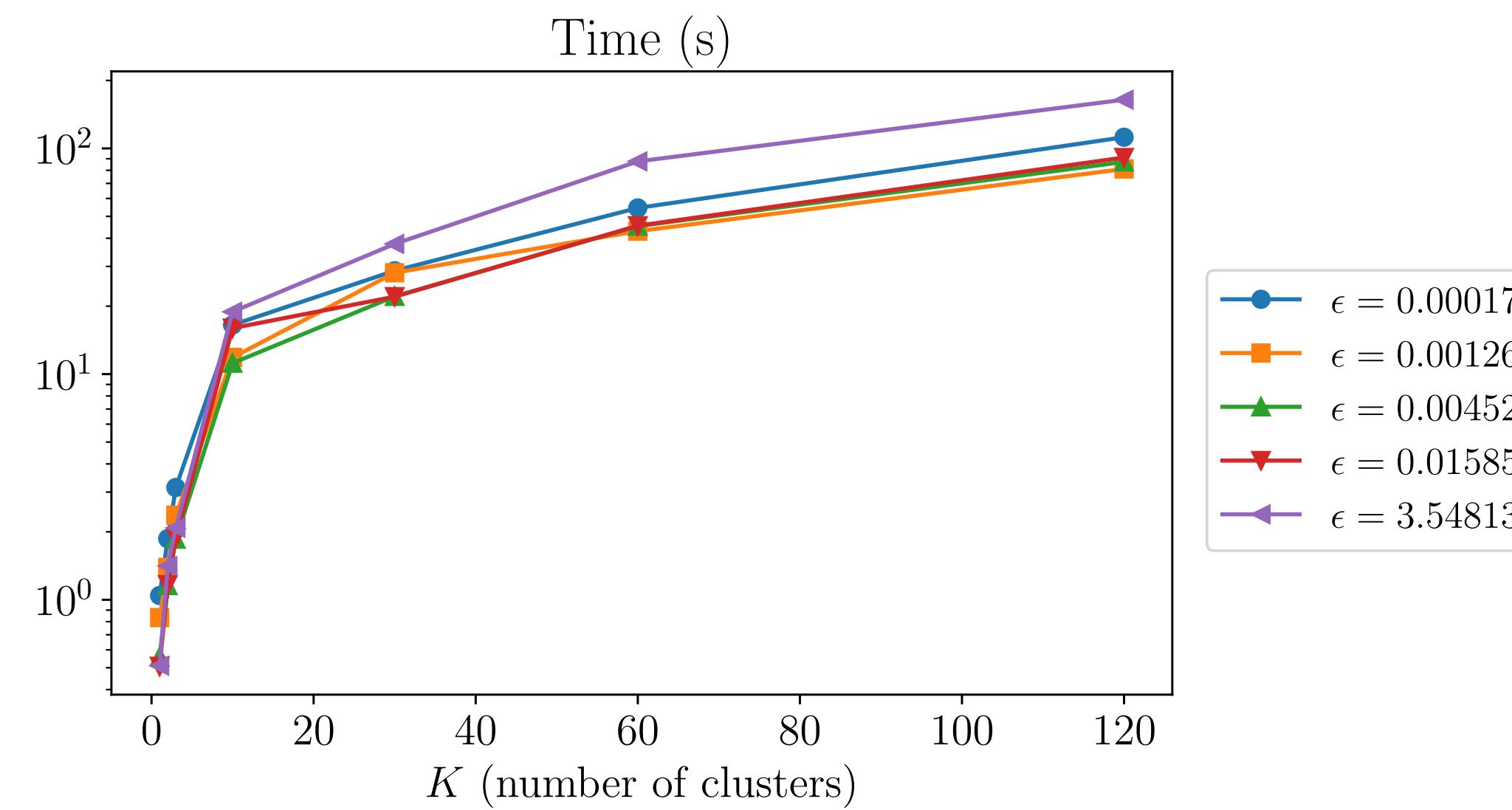
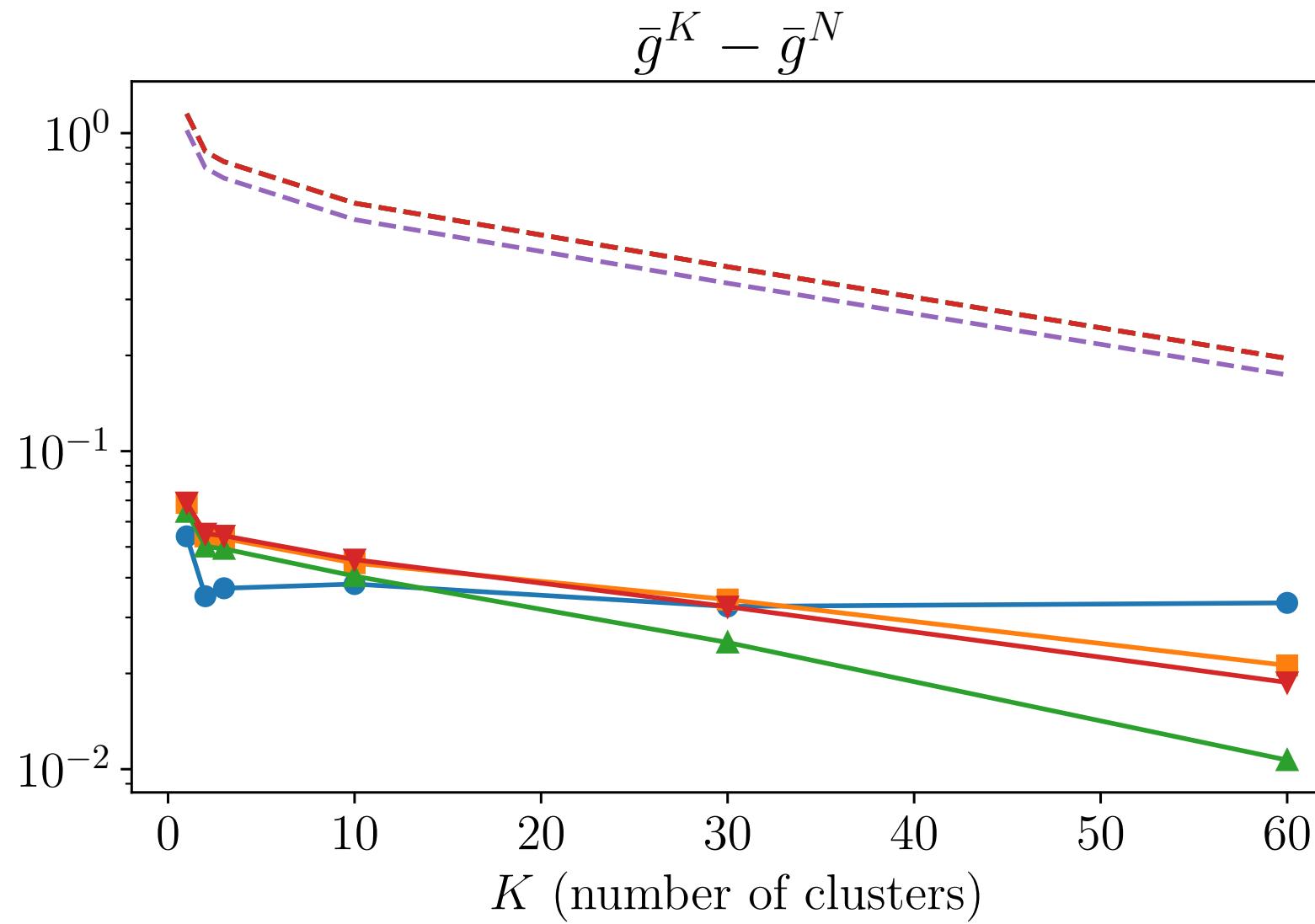
discount rate

# Capital budgeting example



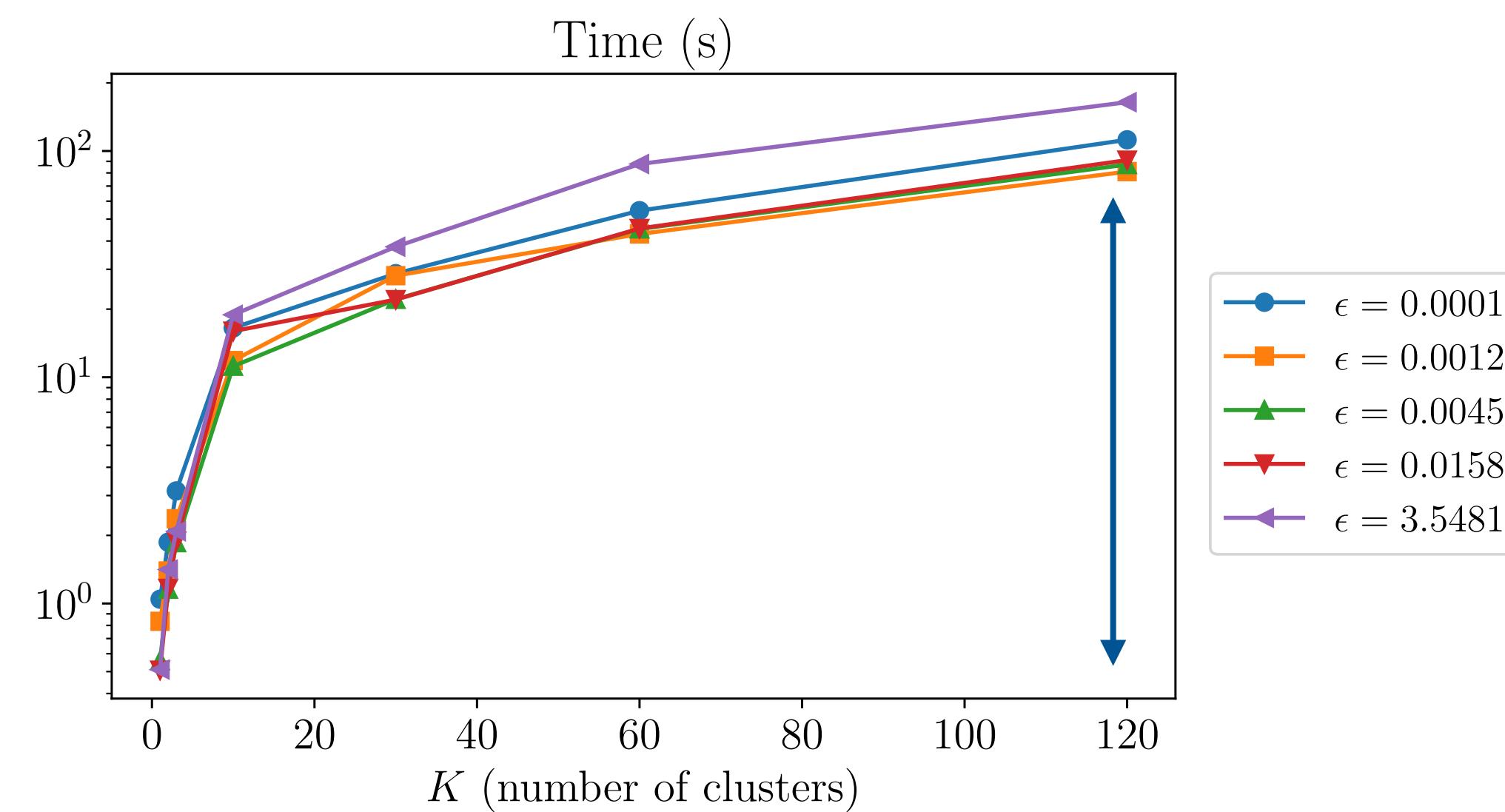
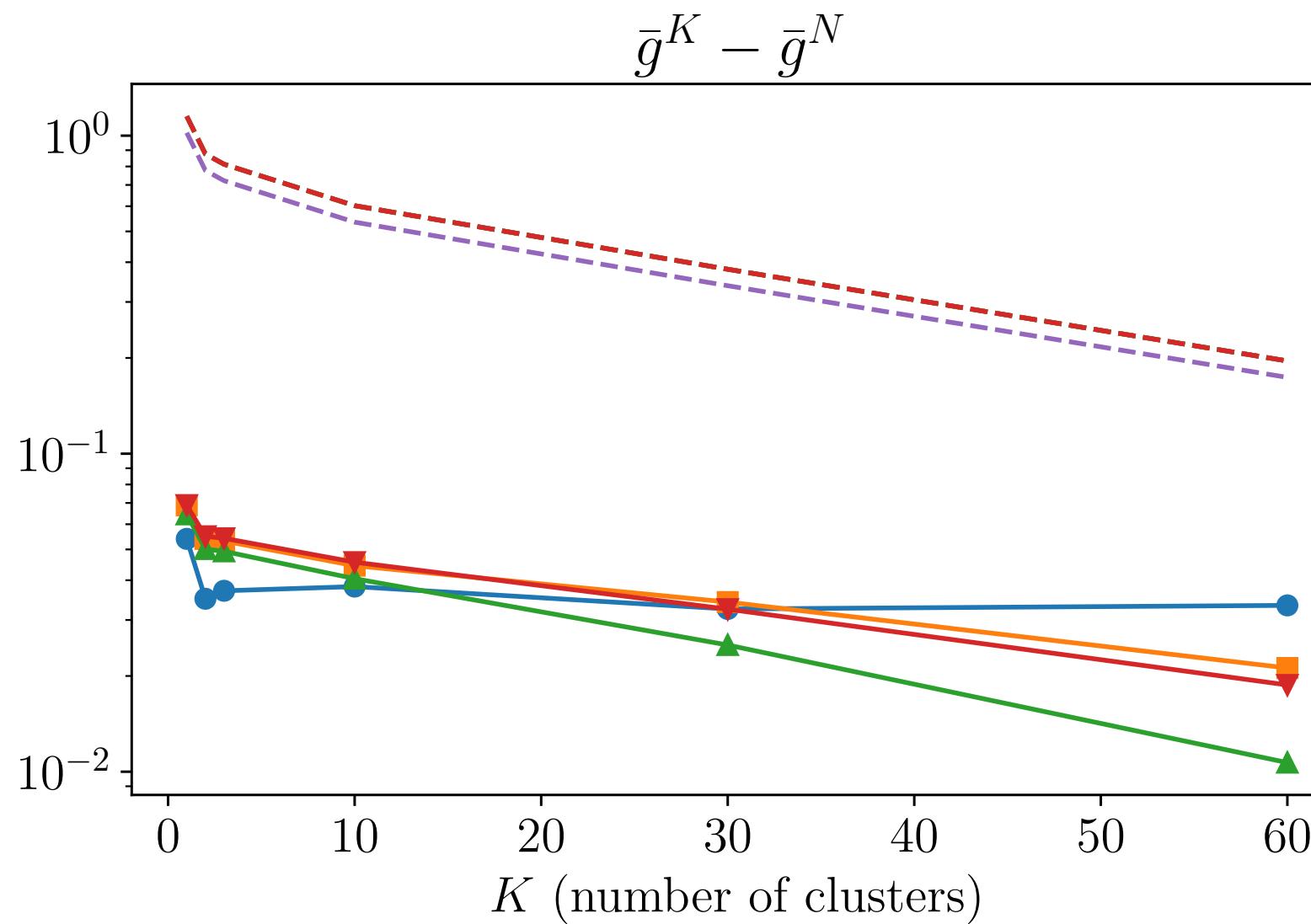
# Capital budgeting results

$$n = 20, N = 120, T = 5$$



# Capital budgeting results

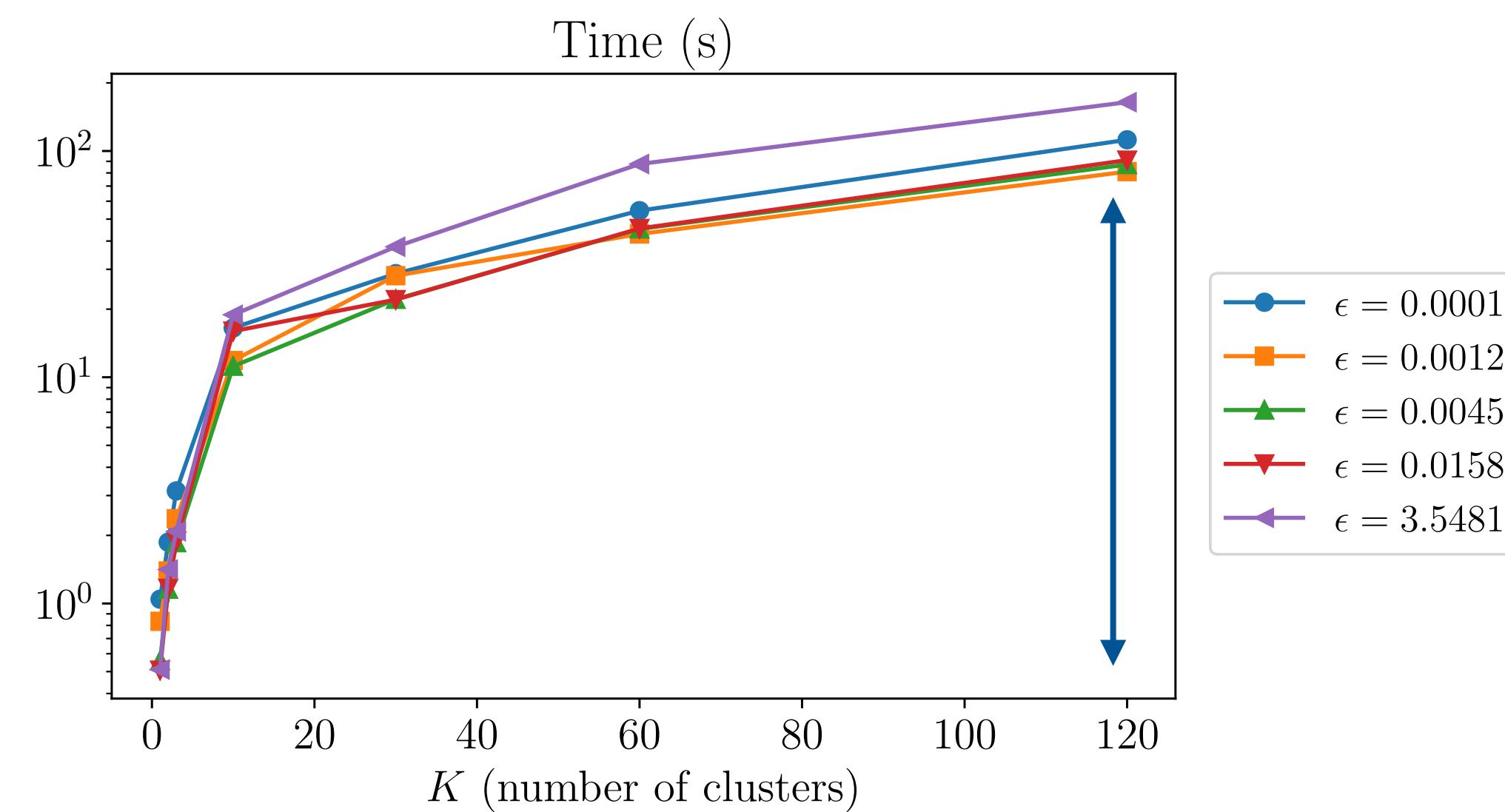
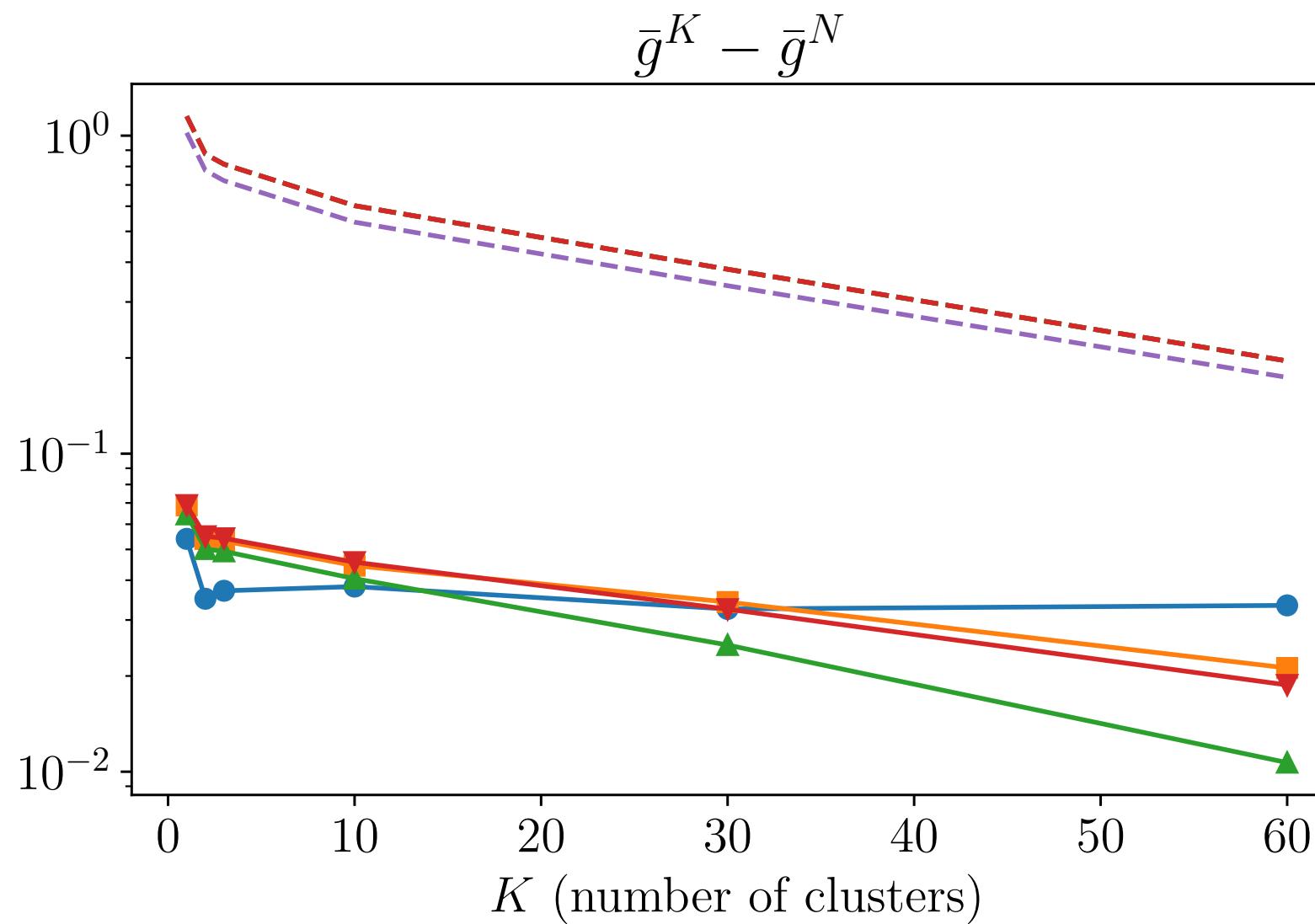
$$n = 20, N = 120, T = 5$$



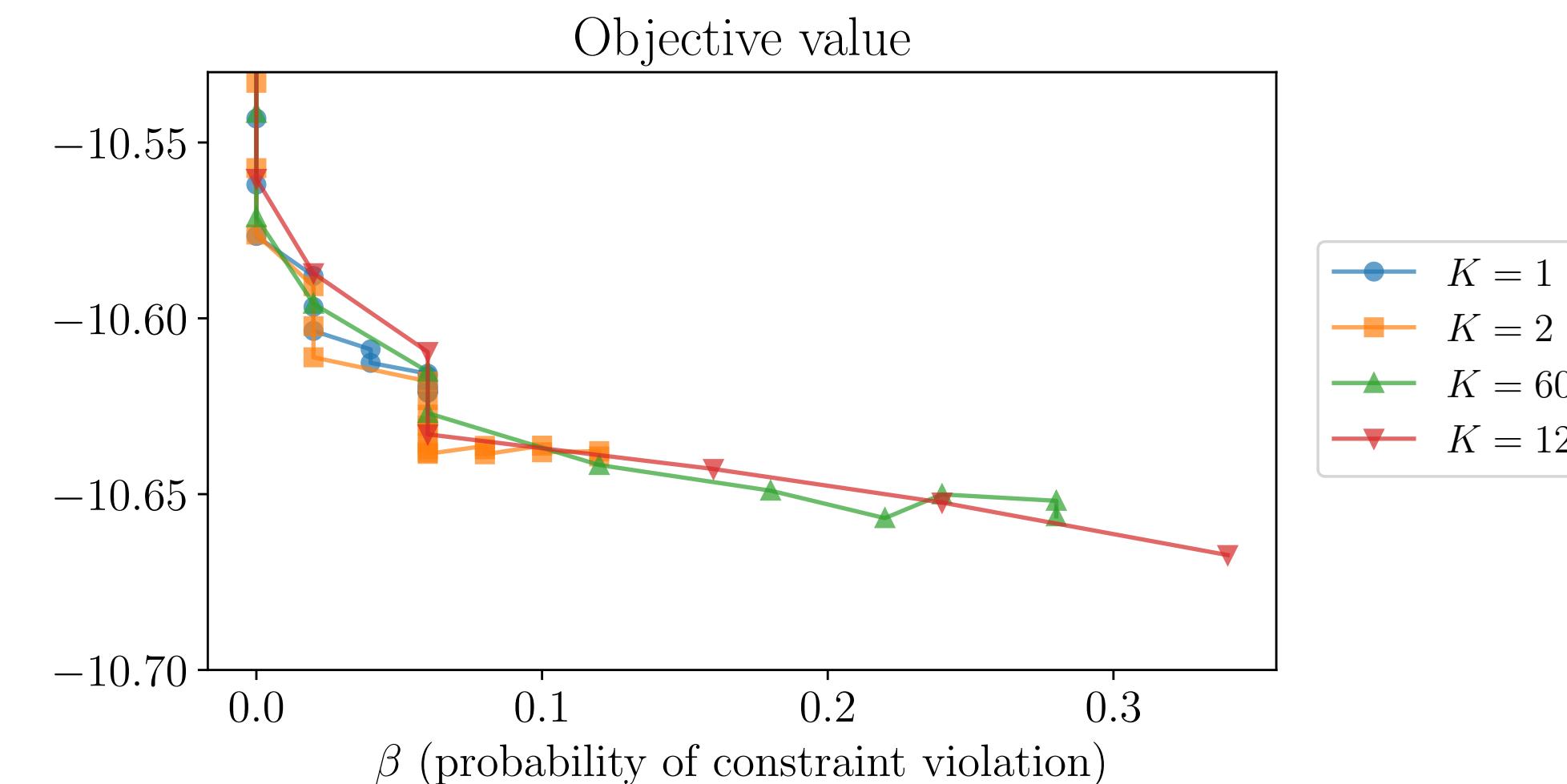
100x speedups!

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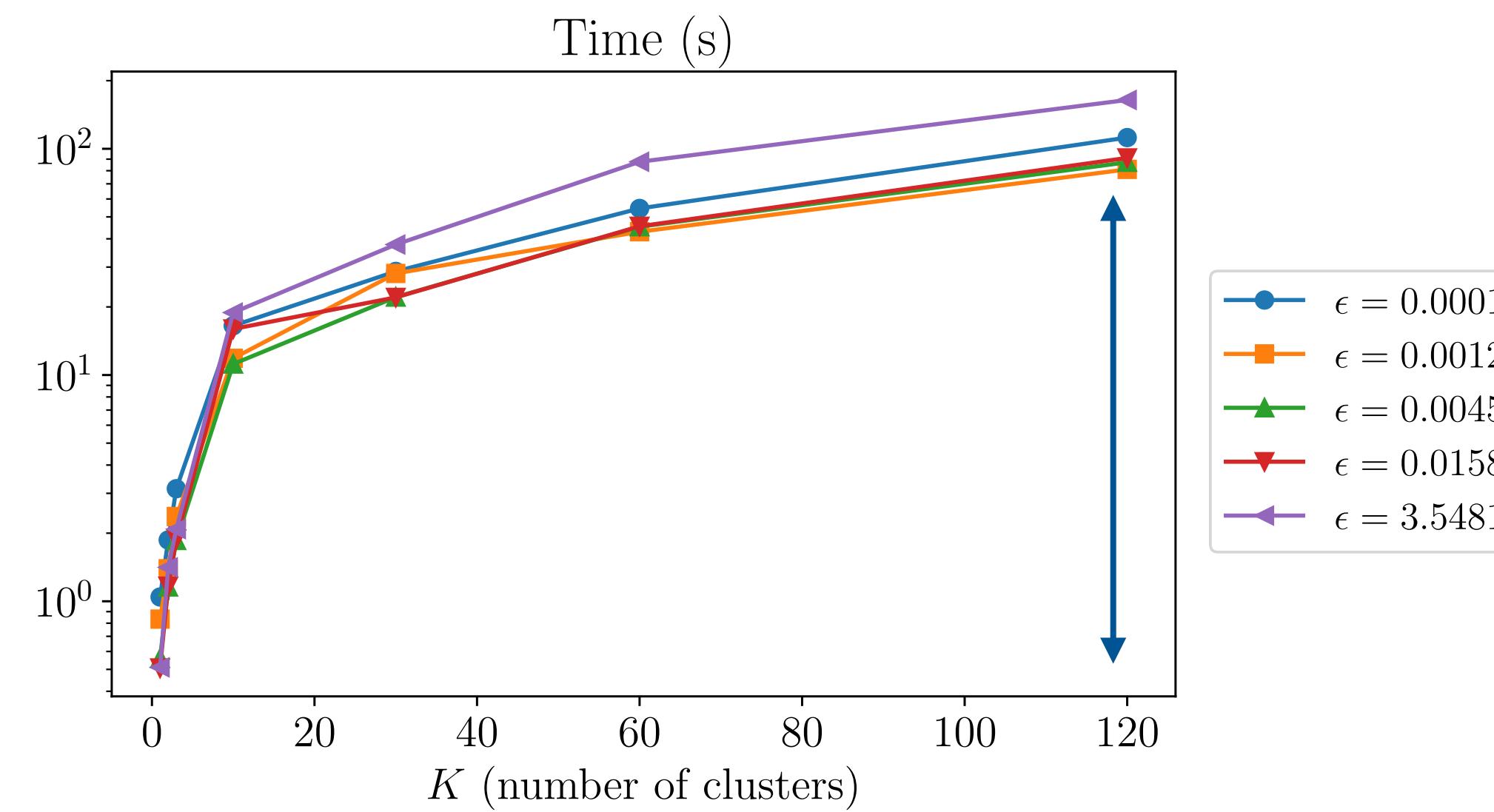
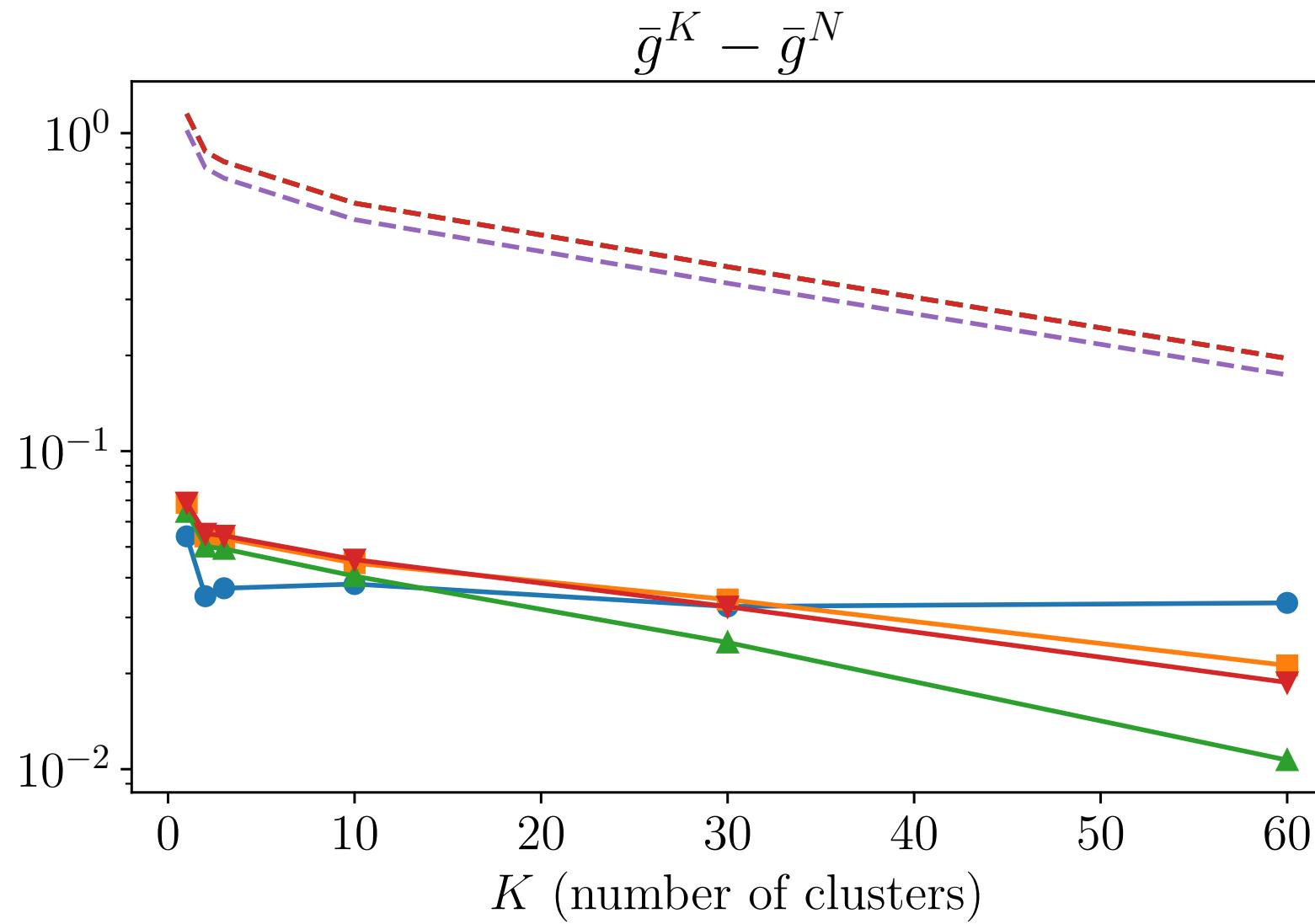


100x speedups!

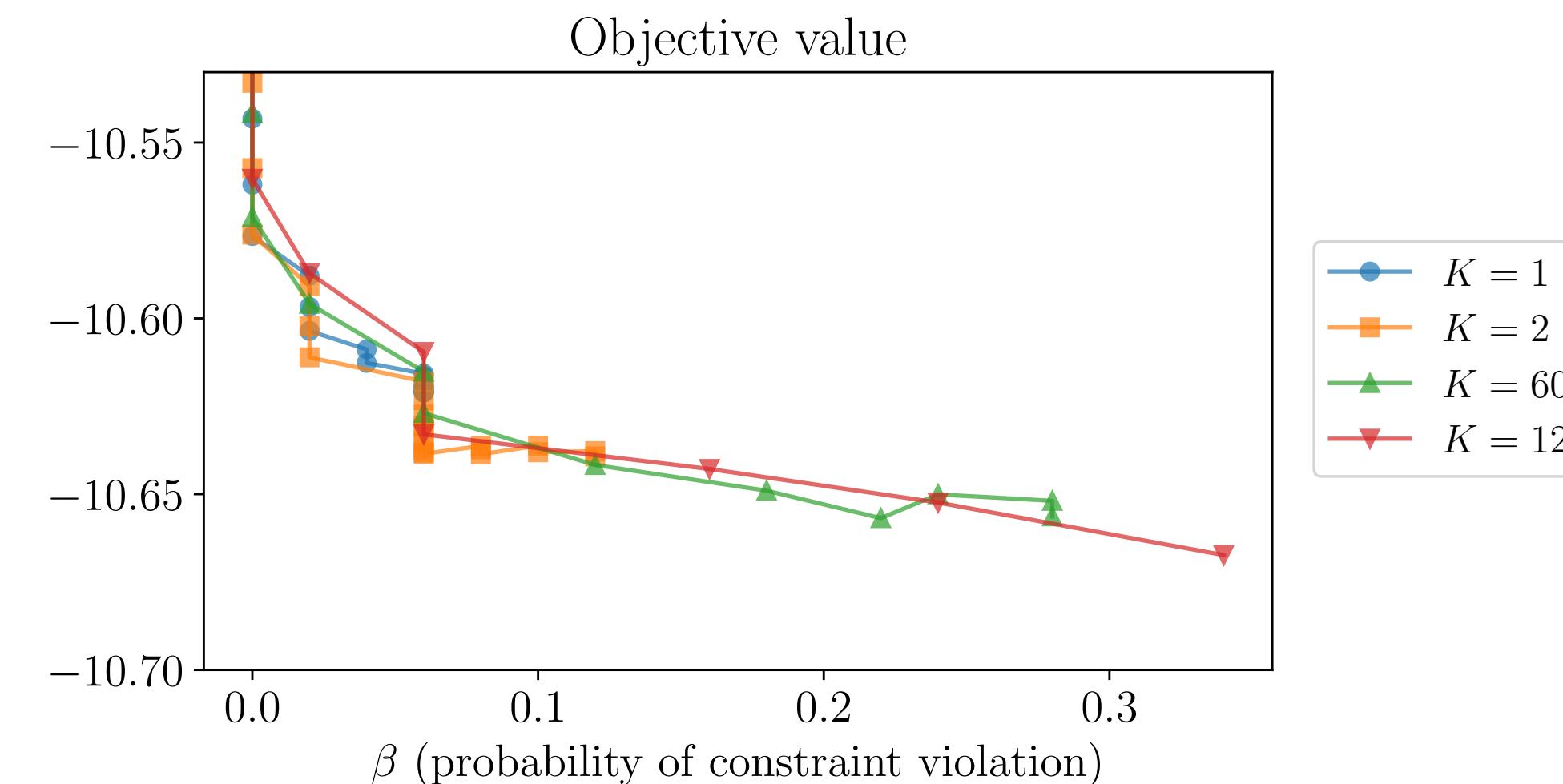


# Capital budgeting results

$$n = 20, N = 120, T = 5$$



100x speedups!



2 clusters give near-optimal performance

# **Conclusions**

# Acknowledgements

Irina Wang



Cole Becker



Bart Van Parys



Princeton

Princeton

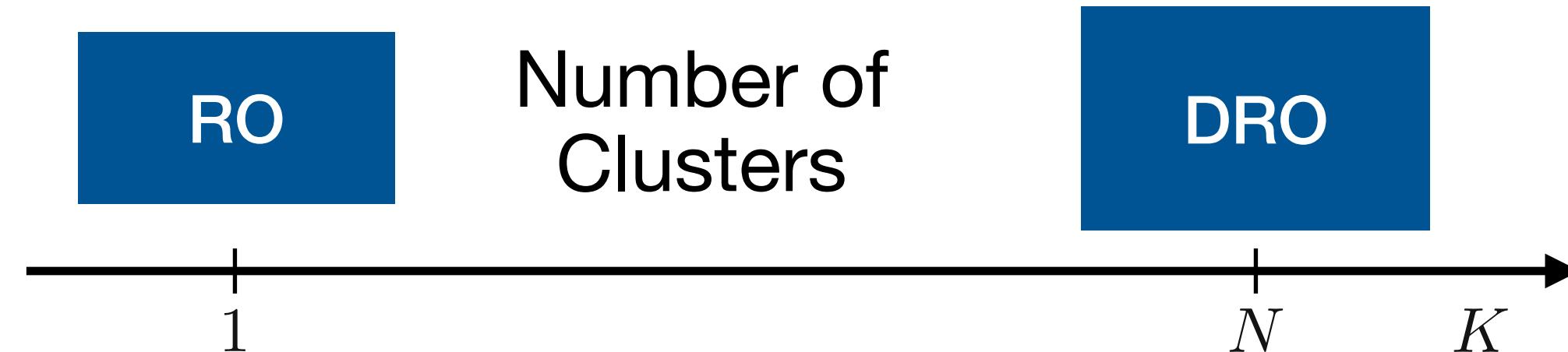
MIT

# Mean Robust Optimization

- Bridge RO and DRO
- Clustering effect
- Multiple **orders of magnitude** speedups

# Mean Robust Optimization

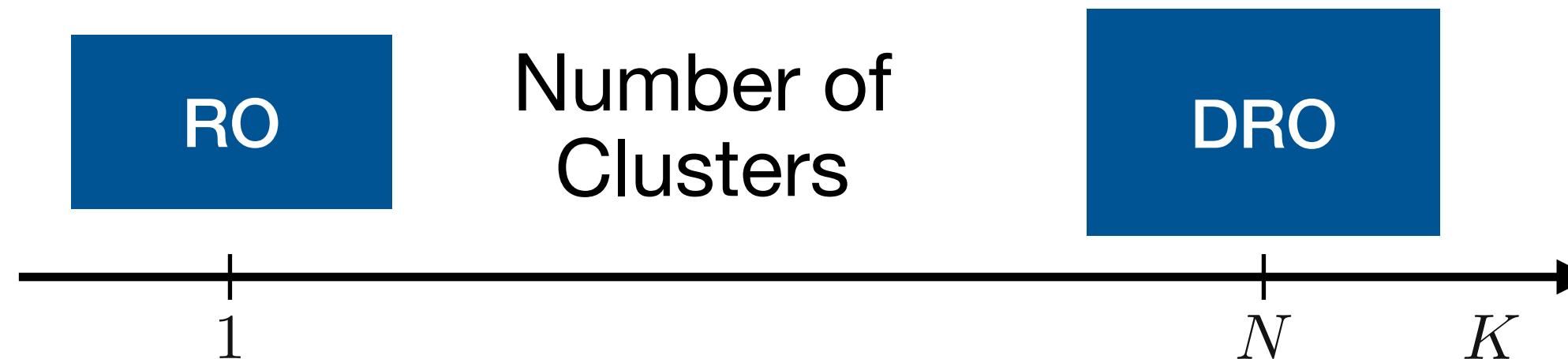
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# Mean Robust Optimization

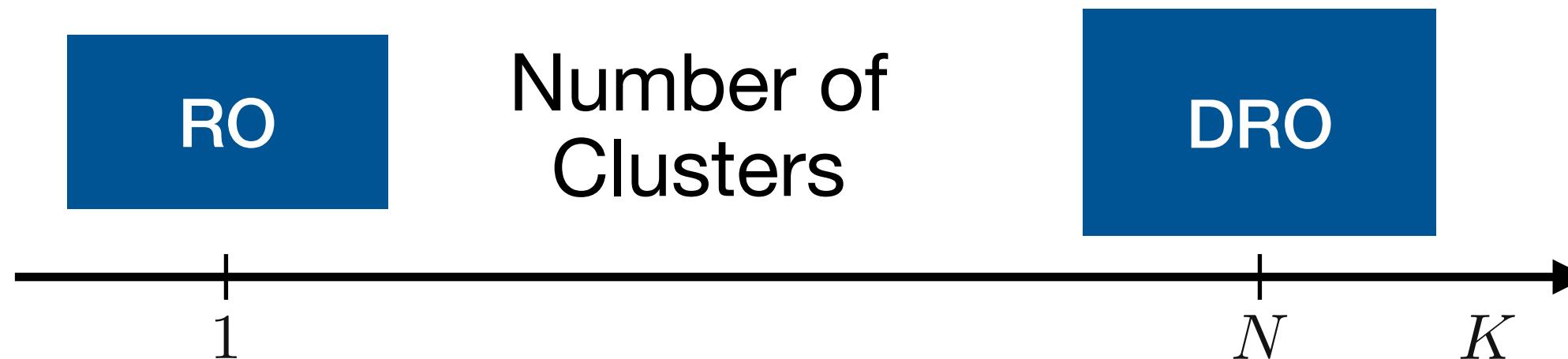
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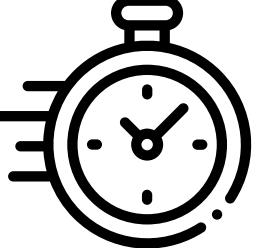


- Clustering effect
  - $g$  affine in  $u$   $\longrightarrow$  zero clustering effect!
  - $g$  concave in  $u$   $\longrightarrow$  performance bound
- Multiple orders of magnitude speedups

# Mean Robust Optimization

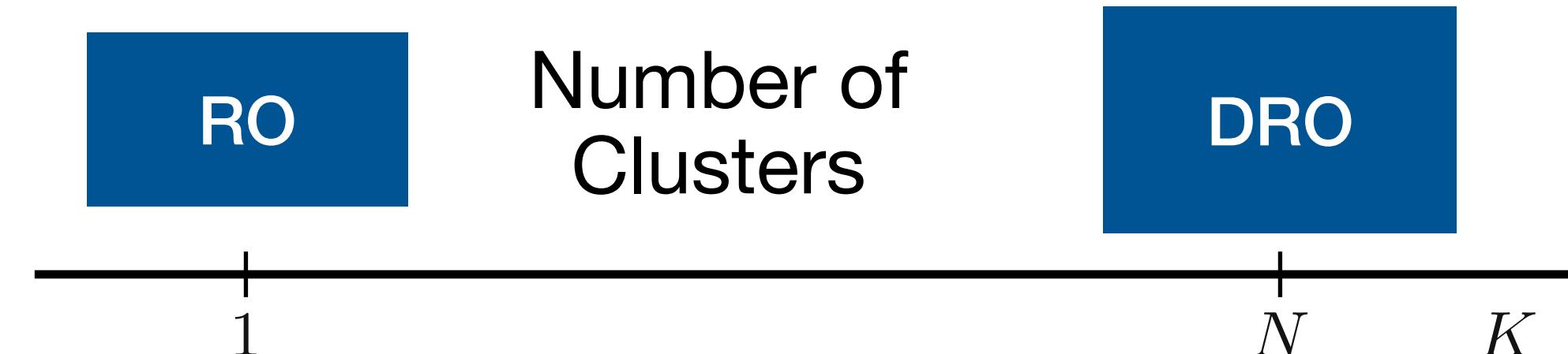
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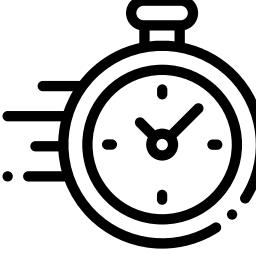


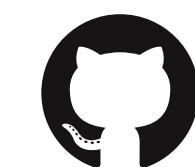
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# Mean Robust Optimization

- Bridge RO and DRO



- Clustering effect
  - $g$  affine in  $u$  → zero clustering effect!
  - $g$  concave in  $u$  → performance bound
- Multiple orders of magnitude speedups 



[https://github.com/stellatogrp/mro\\_experiments](https://github.com/stellatogrp/mro_experiments)



Mean Robust Optimization  
I. Wang, C. Becker, B. Van Parys, and B. Stellato  
[arXiv e-prints:2207.10820](https://arxiv.org/abs/2207.10820), 2022



INFORMS Computing Society  
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# Takeaway message

**Machine Learning**  
can help us  
**formulate optimization problems**



stellato.io



bstellato@princeton.edu



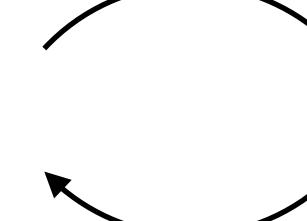
@b\_stellato

# Takeaway message

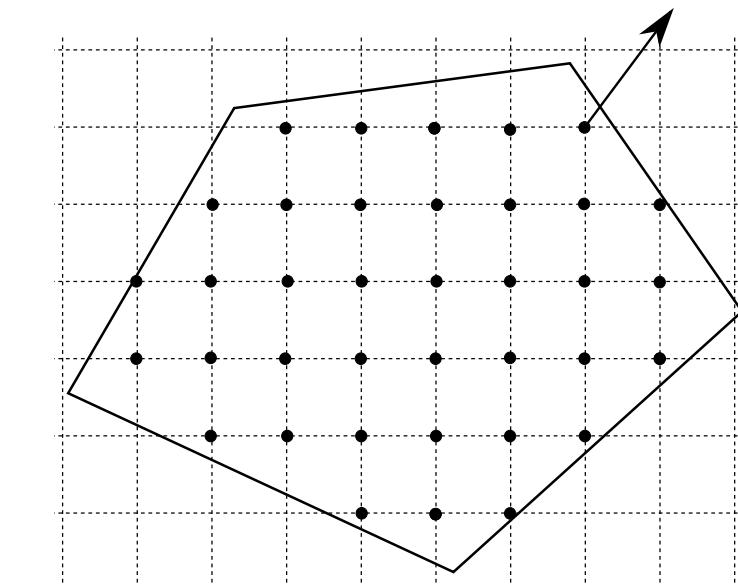
Machine Learning  
can help us  
**formulate optimization problems**

Many opportunities ahead!

Data



Formulations



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bstellato@princeton.edu



@b\_stellato