Optimization meets AI: trustworthy decisions via the Scenario Approach

speaker: **Simone Garatti**

(Politecnico di Milano, Italy – email: simone.garatti@polimi.it)

POLITECNICO MILANO 1863

FUTURE AI RESEARCH

Thanks to

Marco C. Campi

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Marco C. Campi

Algo Carè

Federico Ramponi

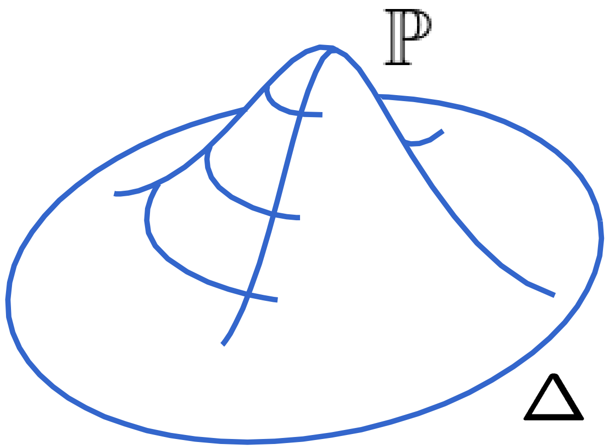
Alessandro Falsone

Kostas Margellos

Maria Prandini

Data-driven decision-making

δ = uncertain element ⇒ exercise caution



⇒

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decision x^*

Data-driven decision-making

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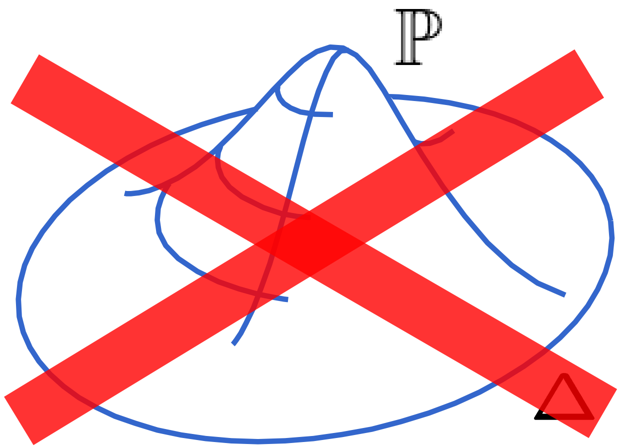

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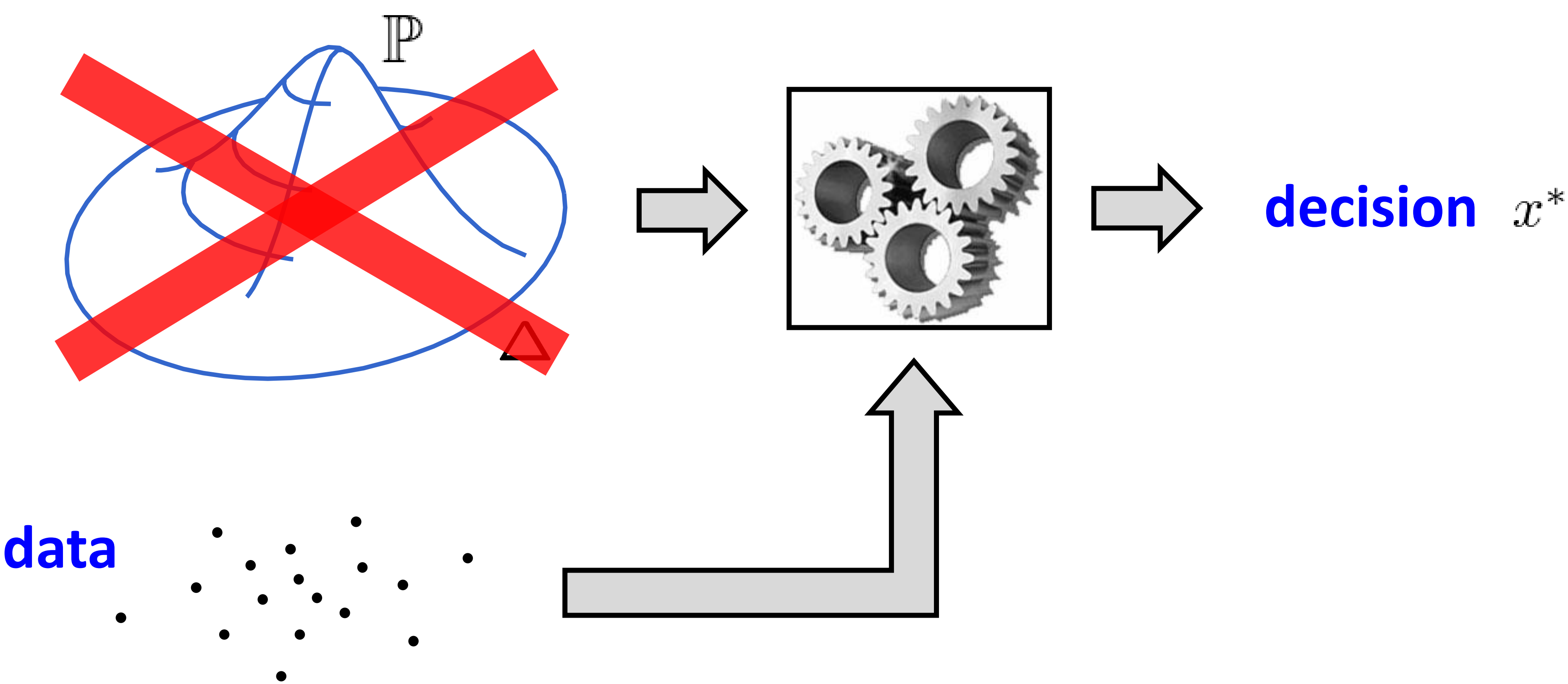


$\delta^{(1)}, \delta^{(2)}, \ldots, \delta^{(N)}$ (scenarios, i.i.d. sample)

Desiderata

Effective ⇒ no over-conservatism

Dependable ⇒ certified decisions

Agnostic ⇒ no information other than data

Desiderata

Effective → no over-conservatism

Dependable → certified decisions

Agnostic → no information other than data

The way of the scenario approach: enforce design goals heuristically, possibly in various attempts (tunable schemes); provide the user with a precise assessment of the quality of the solution(s) to decide when goals are met

Ingredients to (many) decision problems

Decision vector: $x \in \mathcal{X}$

Cost function: $c(x)$

Family of constraint sets: $\mathcal{X}_\delta$

Scenarios: $\delta^{(1)}, \delta^{(2)}, \ldots, \delta^{(N)}$

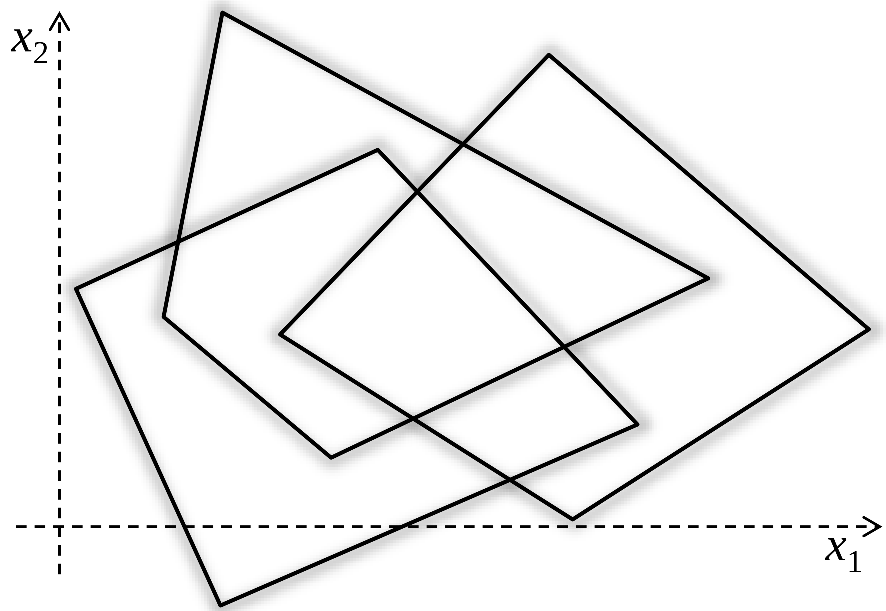
Robust scenario optimization

$$\delta^{(1)} \rightarrow \mathcal{X}_{\delta^{(1)}}$$

$$\delta^{(2)} \rightarrow \mathcal{X}_{\delta^{(2)}}$$

$$\vdots$$

$$\delta^{(N)} \rightarrow \mathcal{X}_{\delta^{(N)}}$$



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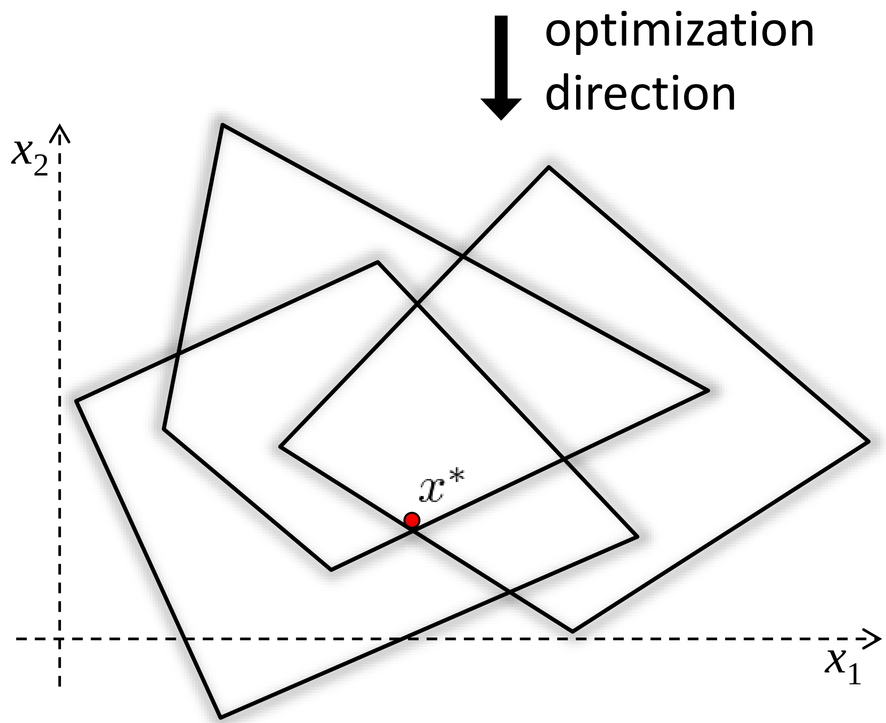
$$\begin{aligned} \min_{x \in \mathcal{X}} \quad & c(x) \\ \text{s.t.} \quad & x \in \mathcal{X}_{\delta^{(i)}} \\ & i = 1, \ldots, N \end{aligned}$$



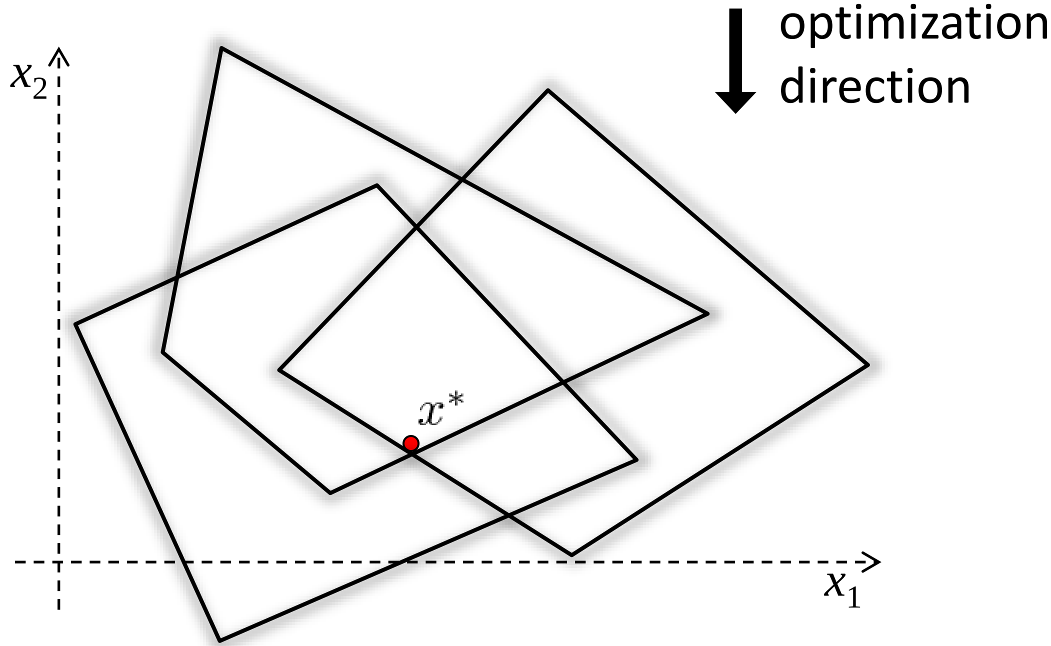
solution = x^*

Scenario optimization with constraints relaxation

$$\min_{x \in \mathcal{X}} \quad c(x)$$

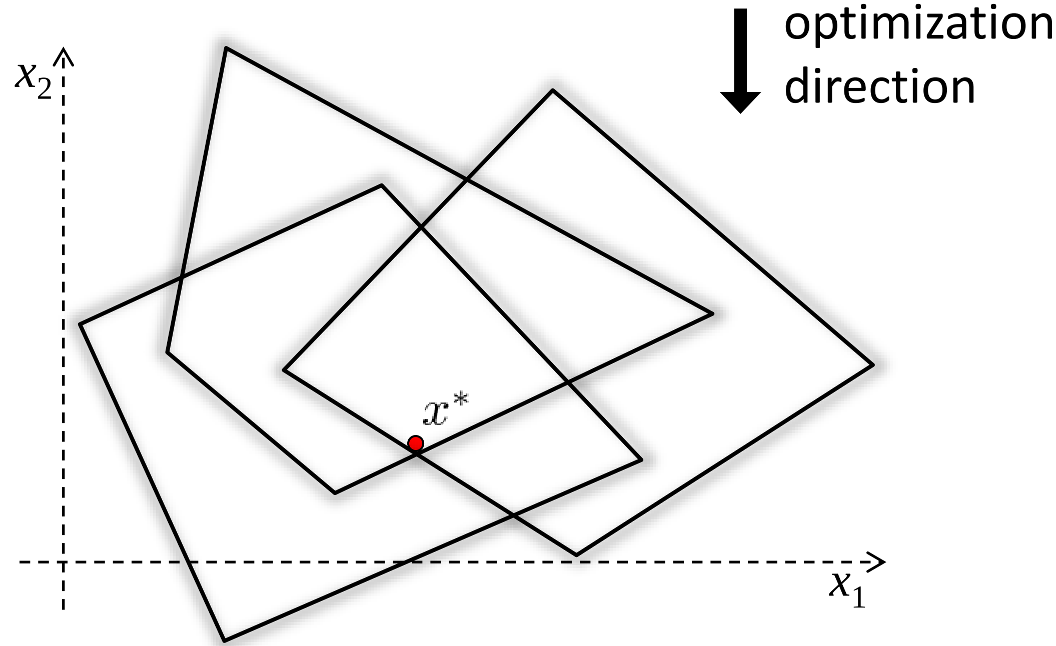
$$\text{s.t.} \quad x \in \mathcal{X}_{\delta(i)}$$

$$i = 1, \ldots, N$$



Scenario optimization with constraints relaxation

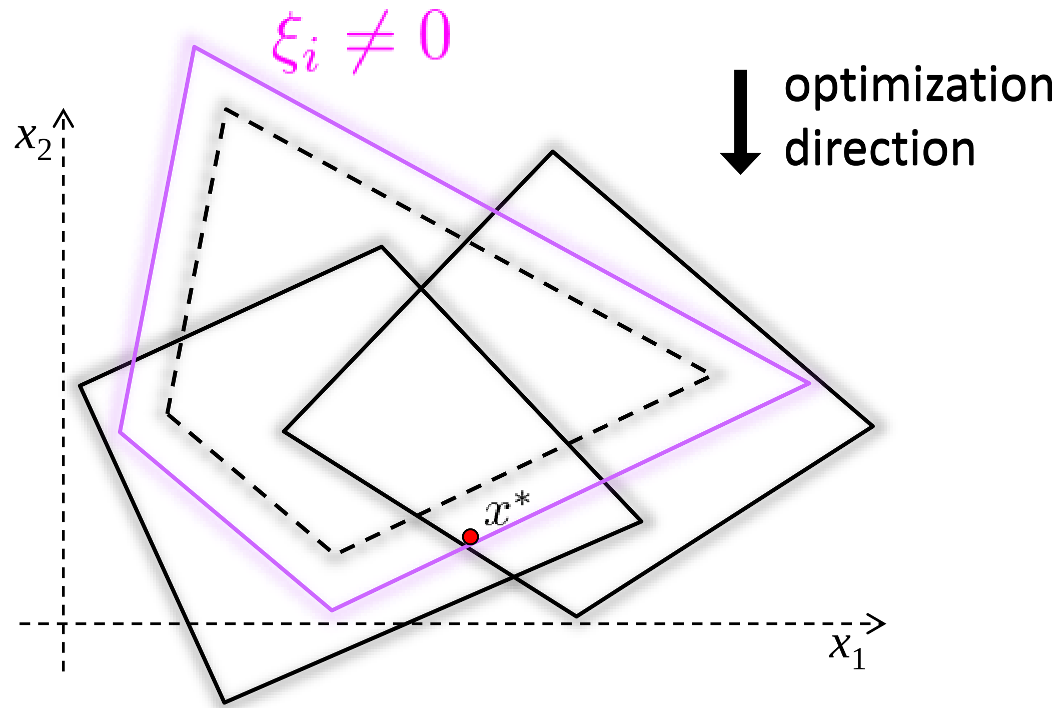
$$\min_{x \in \mathcal{X}} \quad c(x)$$
$$\text{s.t.} \quad f(x, \delta^{(i)}) \leq 0,$$
$$i = 1, \ldots, N$$



Scenario optimization with constraints relaxation

$$\min_{x \in \mathcal{X}, \xi_i \geq 0} \quad c(x) + \rho \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.} \quad f(x, \delta^{(i)}) \leq \xi_i, \quad i = 1, \ldots, N$$



solution: $x^*, \{\xi_i^* : \xi_i^* \neq 0\}$

ρ = tunable tradeoff parameter

A general scenario decision-making framework

Decision map $M: \delta^{(1)}, \ldots, \delta^{(N)} \to (x^*, w^*)$ such that when new scenarios $\delta^{(N+1)}, \ldots, \delta^{(N+H)}$ are added:

- if $\underbrace{x^* \in \mathcal{X}_{\delta^{(N+i)}}}_{x^* \text{ already feasible}}$ for all *i*, then solution does <u>not</u> change

- if $\underbrace{x^* \notin \mathcal{X}_{\delta^{(N+i)}}}_{x^* \text{ unfeasible for some cases}}$ for some *i*, then solution must change

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consistency

⇨ robust optimization, opt. with constraint relaxation, expected shortfall optimization, variational inequalities, …

Scenario approach: main features

- easy (algorithmically speaking) and widely applicable

- data used to directly target the objective

⇨ effective solutions!

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- easy (algorithmically speaking) and widely applicable

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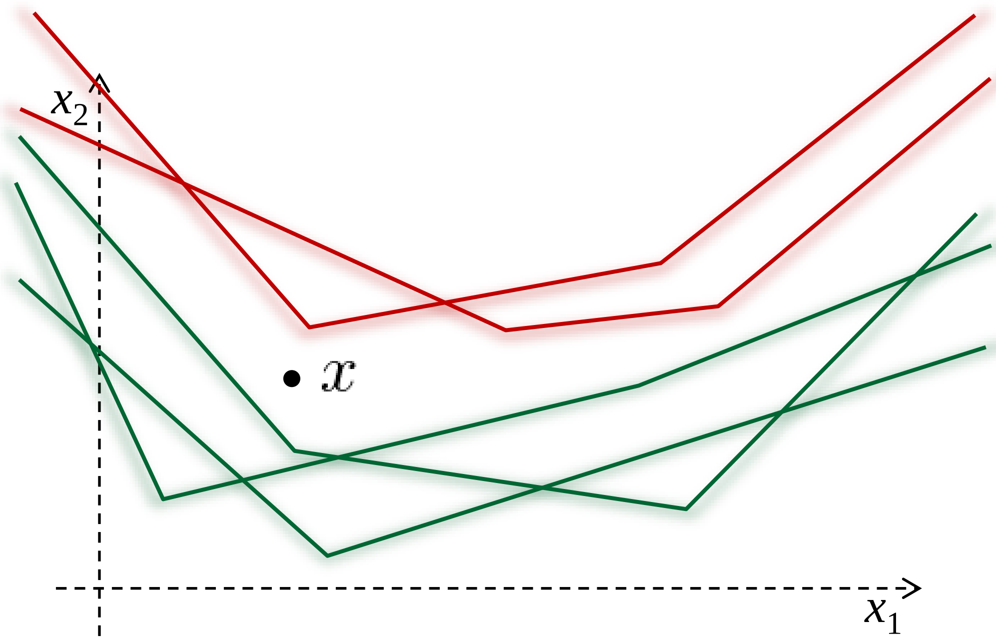
⇨ effective solutions!

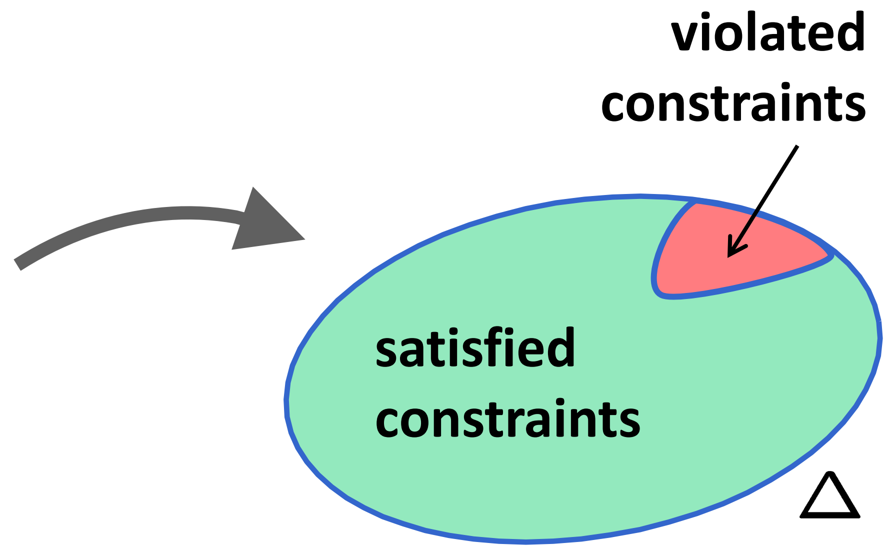
- feasibility addressed empirically

⇨ dependability of the scenario approach rests on our capability to keep control of the actual feasibility level (risk)

Risk

$V(x) = \mathbb{P}\{\delta \in \Delta : \ x \notin \mathcal{X}_\delta\}$ out-of-sample constraint violation





$V(x)$ = "size" of red region

Solution certification

$c(x)$ vs. $V(x) = \mathbb{P}\{\delta \in \Delta : \; x \notin \mathcal{X}_\delta\}$

cost   risk

$\mathbb{P}$ = mechanism by which δ is generated

scenario decision certification

- $c(x^*)$ accessible (once x^* is computed)
- $V(x^*)$

Solution certification

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- $c(x^*)$ accessible (once x^* is computed)
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⇩ cost ⇩ risk

??????????

$\mathbb{P}$ = mechanism with which the δ are generated

main goal: to evaluate $V(x^*)$

scenario solution certification

▷ $c(x^*)$ accessible (once x^* is computed)

▷ $V(x^*)$ **not accessible**

Issues

- no. of violated constraints is **not a valid** indicator of the risk

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- validation with new data is **questionable**

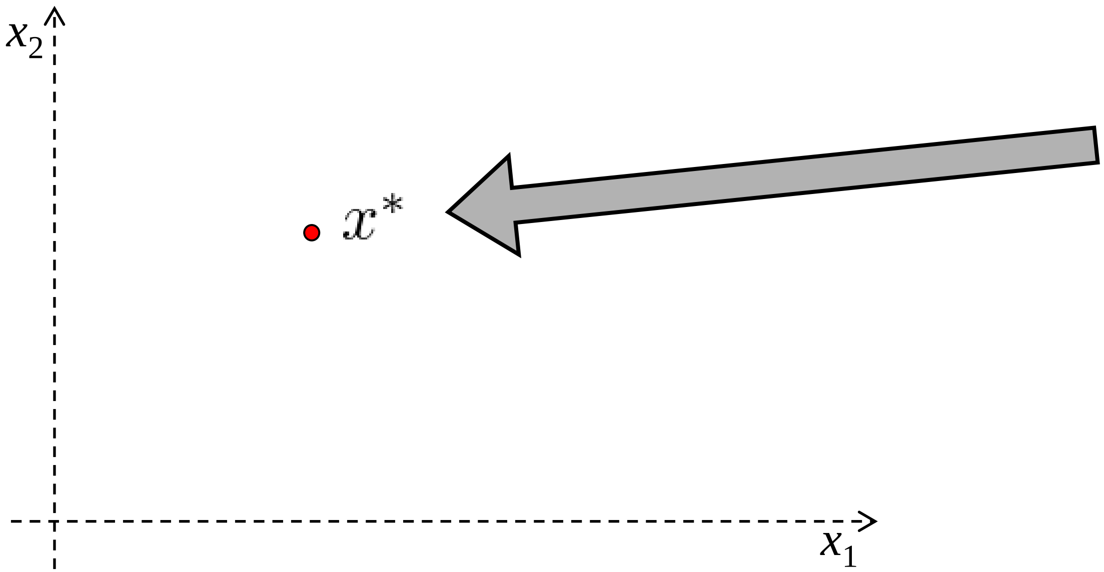
  - using some data for testing rather than designing… waste of information!

  - scenarios (data) are often limited resources (collecting data can be time-consuming or burdensome, involving a monetary cost)

  - in the present context validation is not necessary! (brand-new generalization theory)

Risk of the scenario decision

Problem: assess $V(x^*)$



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\min_{x \in \mathcal{X}, \xi_i \geq 0} \quad & c(x) + \rho \sum_{i=1}^{N} \xi_i \\
\text{s.t.} \quad & f(x, \delta^{(i)}) \leq \xi_i, \\
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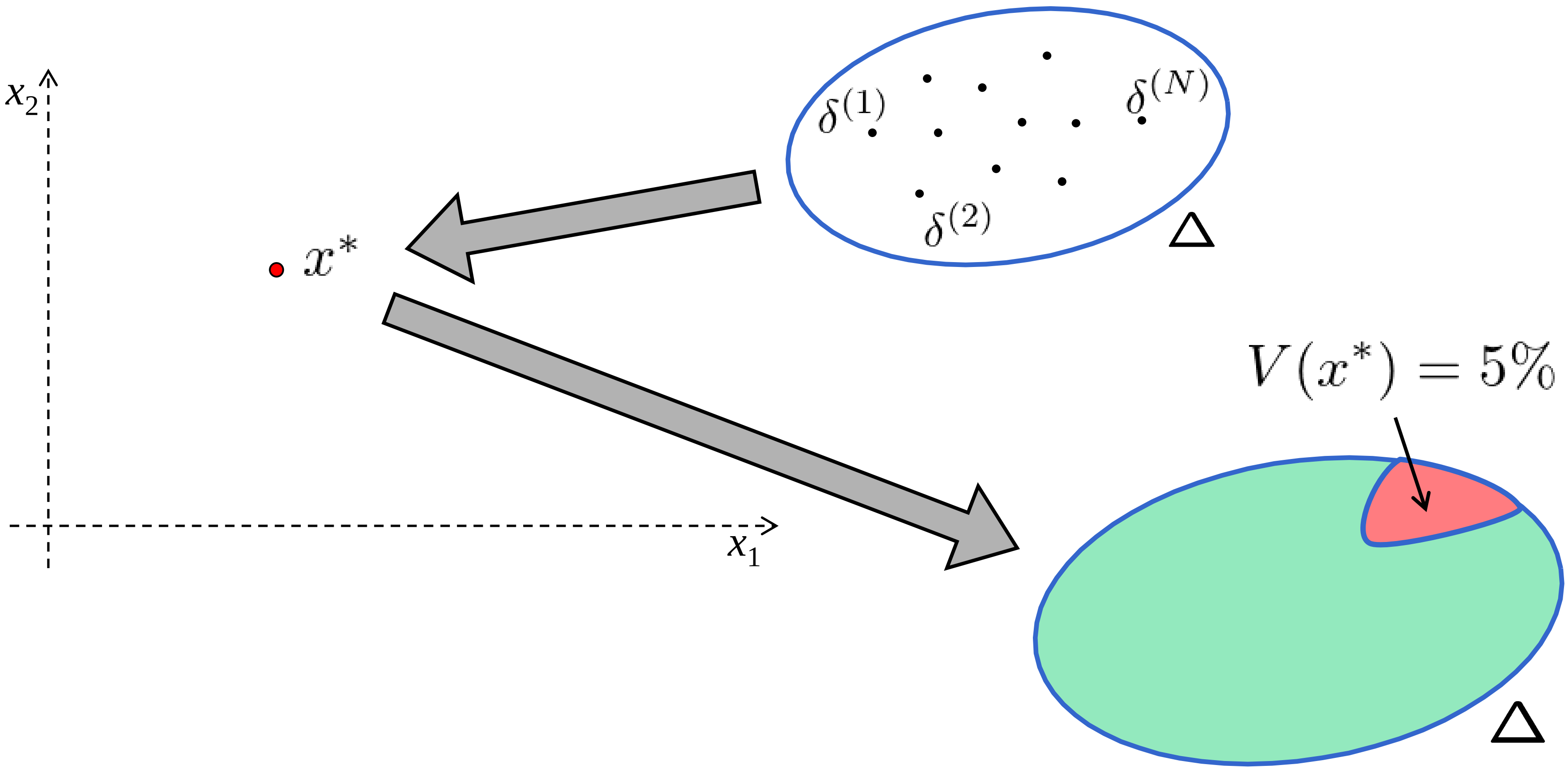
Risk of the scenario decision

Problem: assess $V(x^*) = V(x^*(\delta^{(1)}, \delta^{(2)}, \dots, \delta^{(N)}))$



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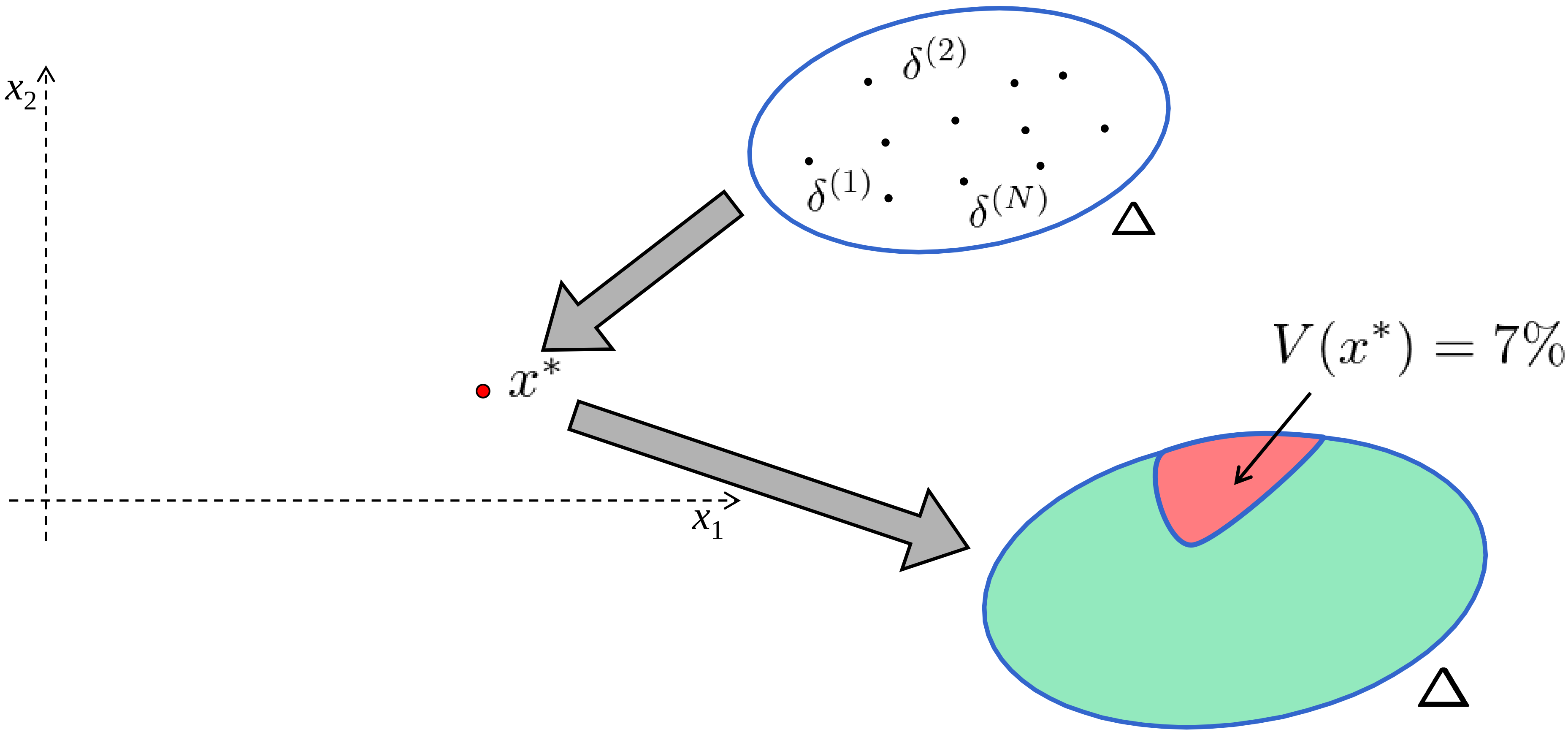


Distribution of the risk

$V(x^*)$ is a **random variable**

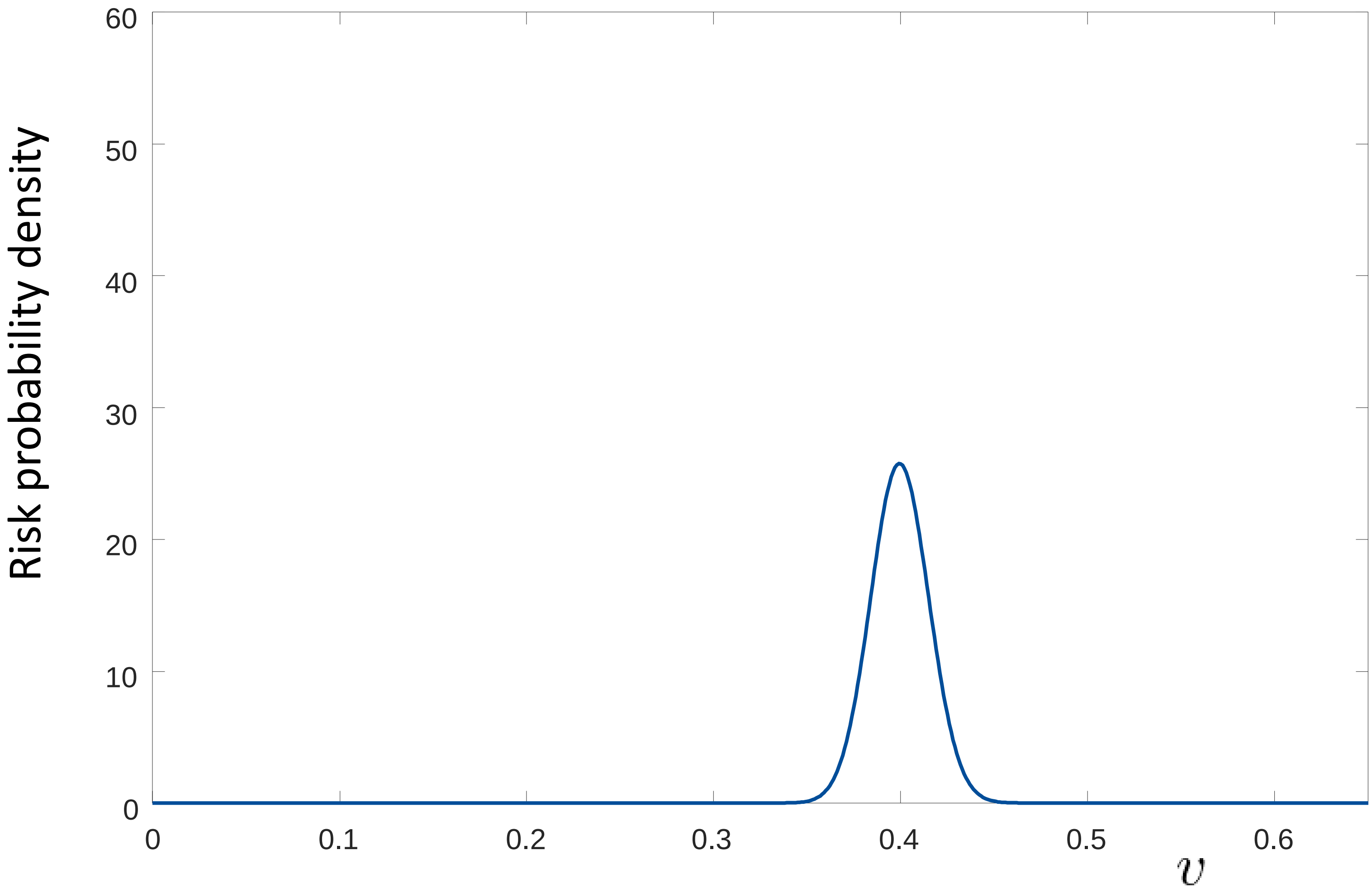
What about its probability distribution?

How does it change with $\mathbb{P}$, the mechanism generating δ ?

Is it concentrated?

Distribution of the risk: examples

Same decision problem with $N = 1000$ for various $\mathbb{P}$



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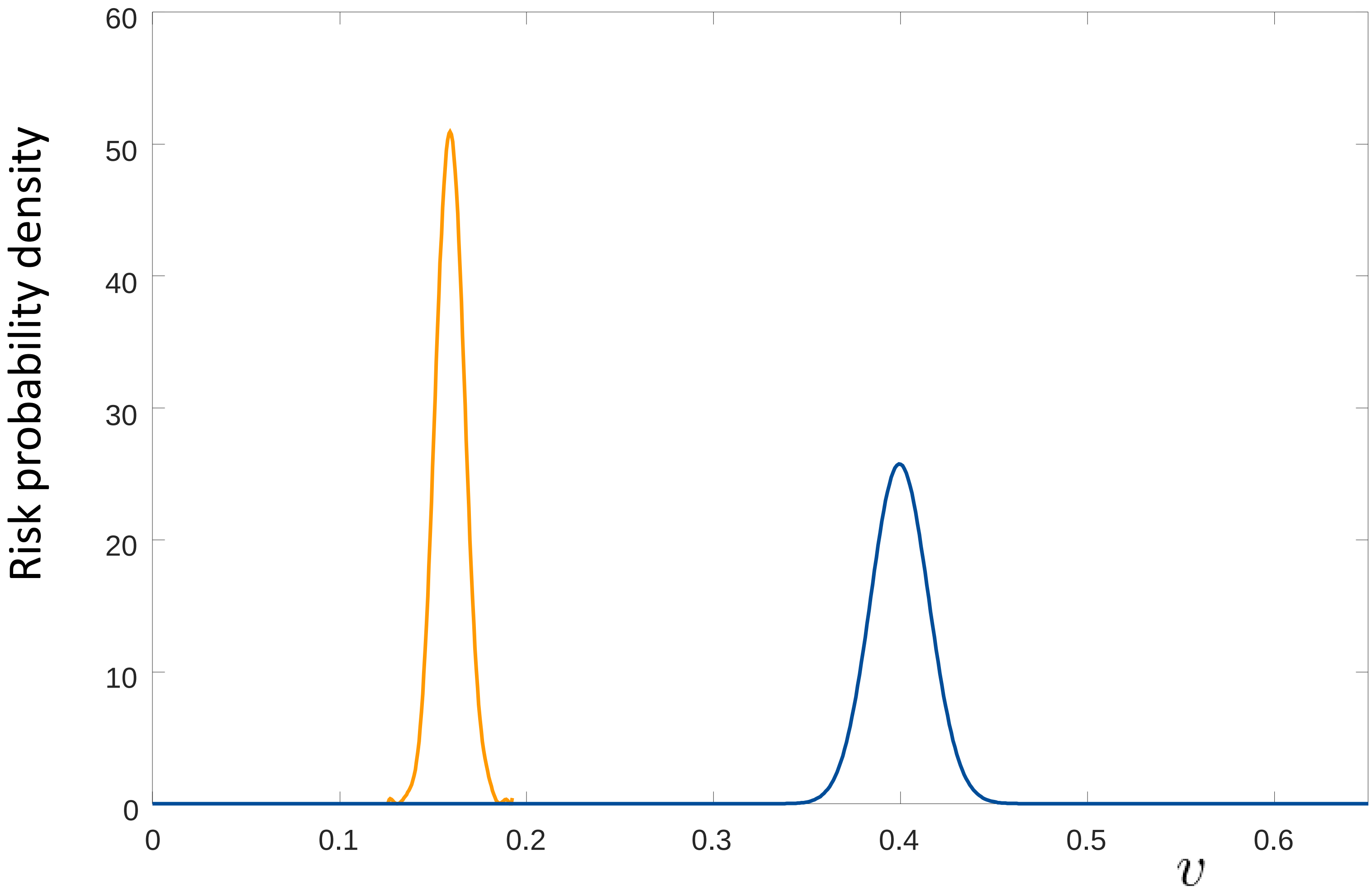

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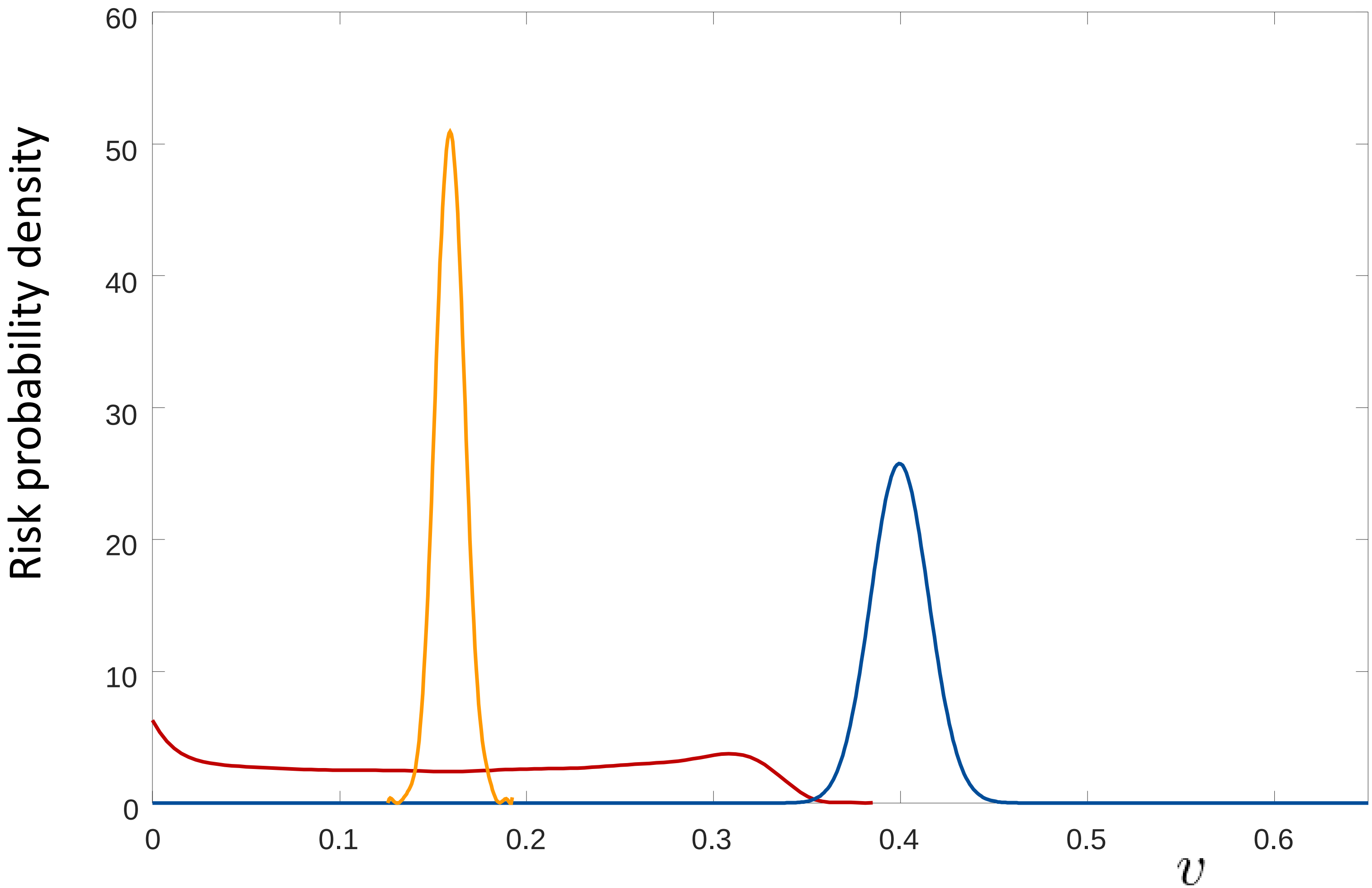

Support set and complexity

Support set: $\left\{\delta^{(i_1)}, \delta^{(i_2)}, \ldots, \delta^{(i_k)}\right\}$ such that

1. $\mathrm{sol}\left(\delta^{(i_1)}, \delta^{(i_2)}, \ldots, \delta^{(i_k)}\right) = \mathrm{sol}\left(\delta^{(1)}, \delta^{(2)}, \ldots, \delta^{(N)}\right)$
2. no $\delta^{(i_j)}$ can be further removed without changing the solution

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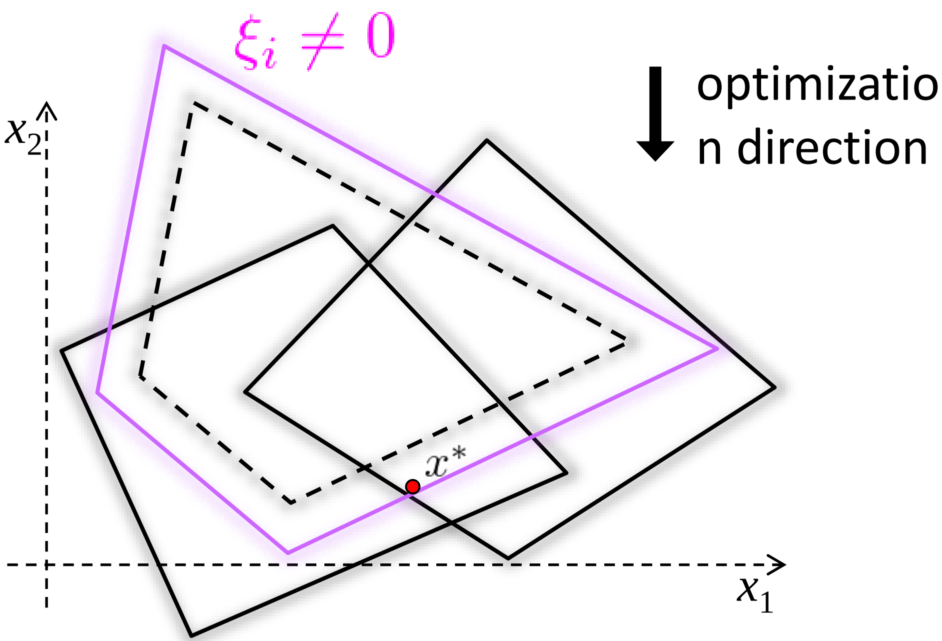

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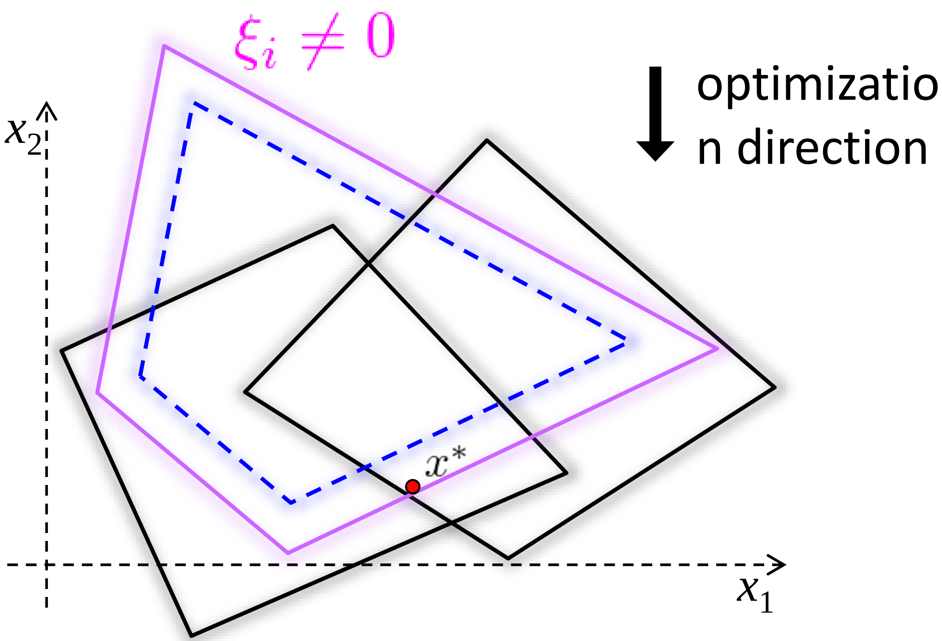

support set =

violated

solution: x^*, $\{\xi_i^* : \xi_i^* \neq 0\}$

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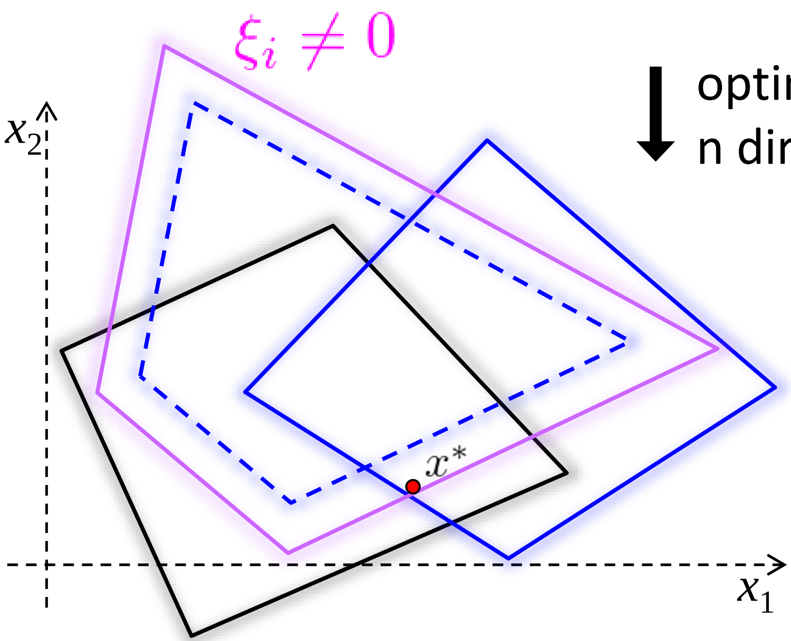

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support set =

violated + active

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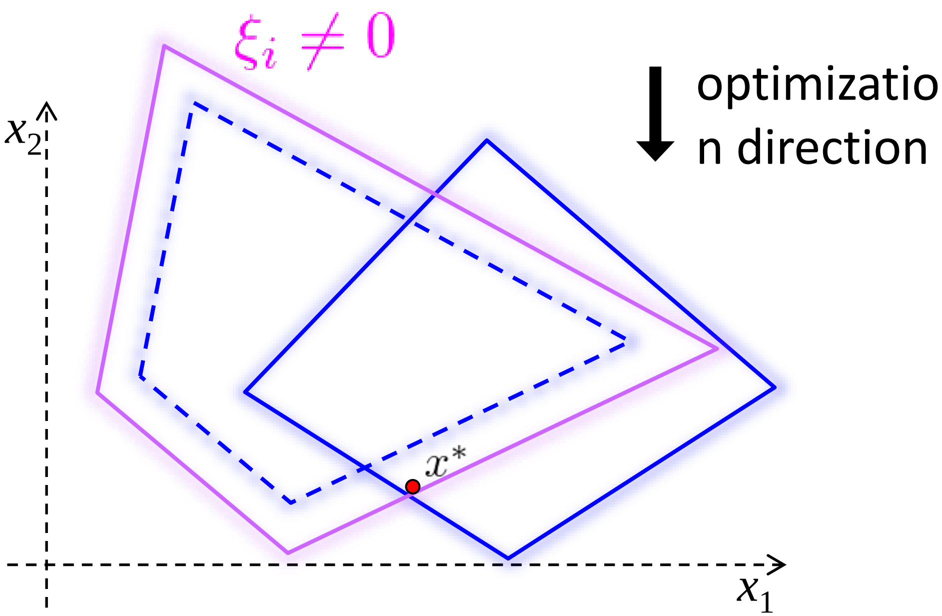

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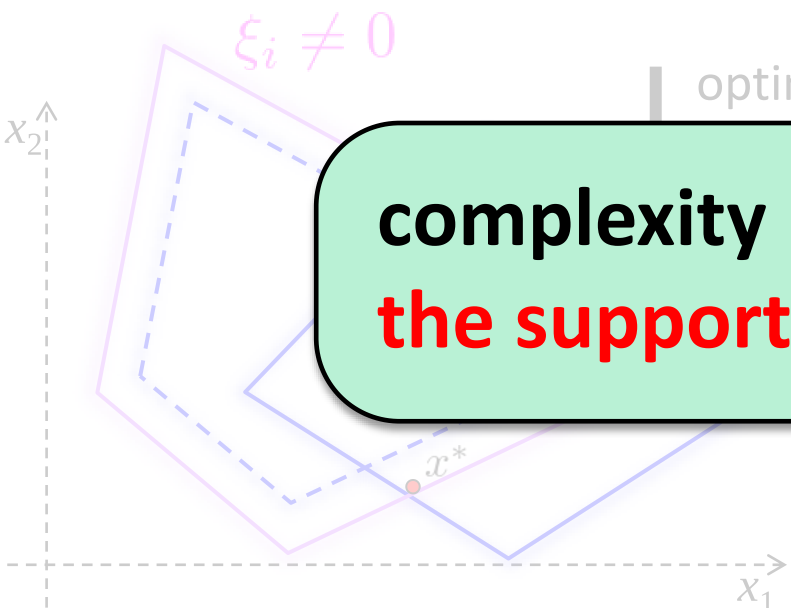

optimizatio

complexity π^* = cardinality of the support set

active

solution: $x^*, \{\xi_i^* : \xi_i^* \neq 0\}$

A new perspective

π^* is a random variable (integer, $\pi^* = k,\ k \in \{0, 1, \ldots, N\}$)

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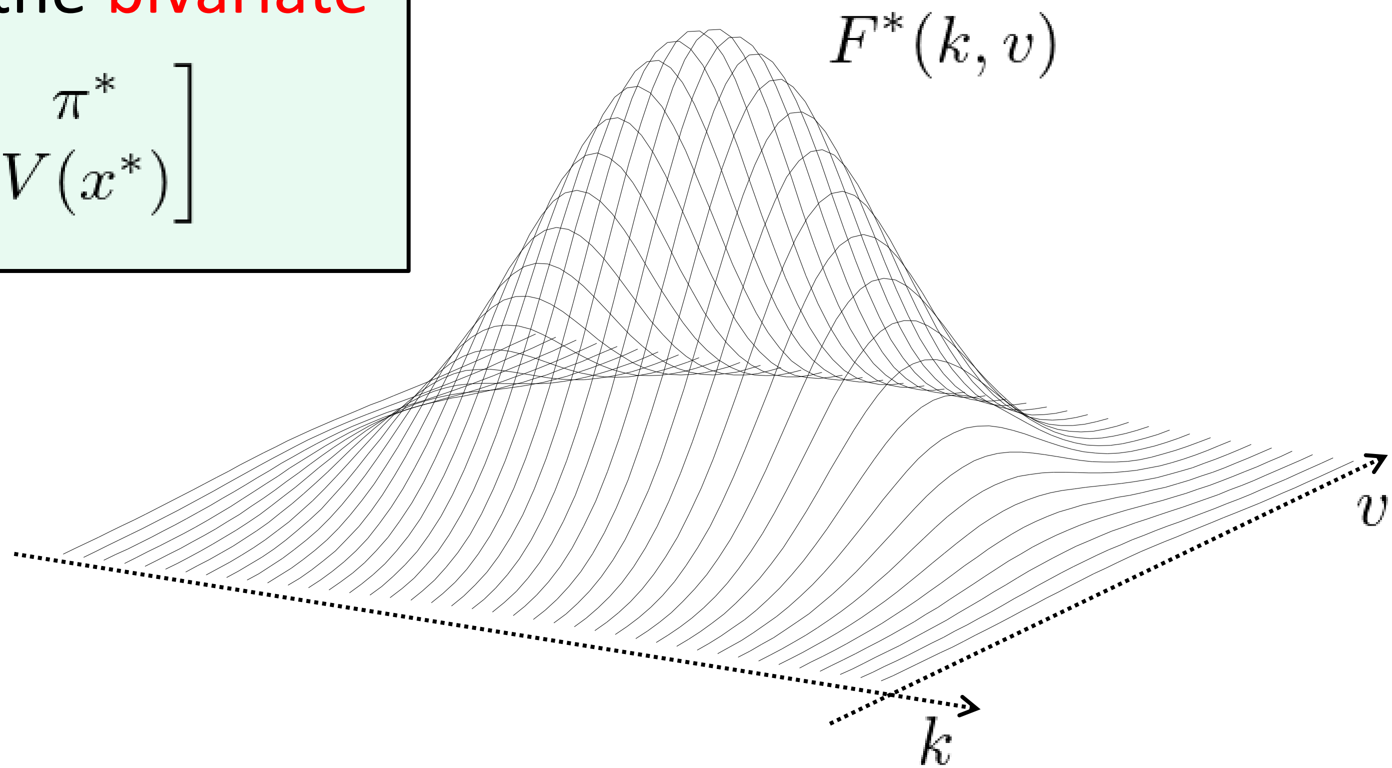
$V(x^*)$ is a random variable (real, $V(x^*) = v, \quad v \in [0, 1]$)

A new bivariate perspective

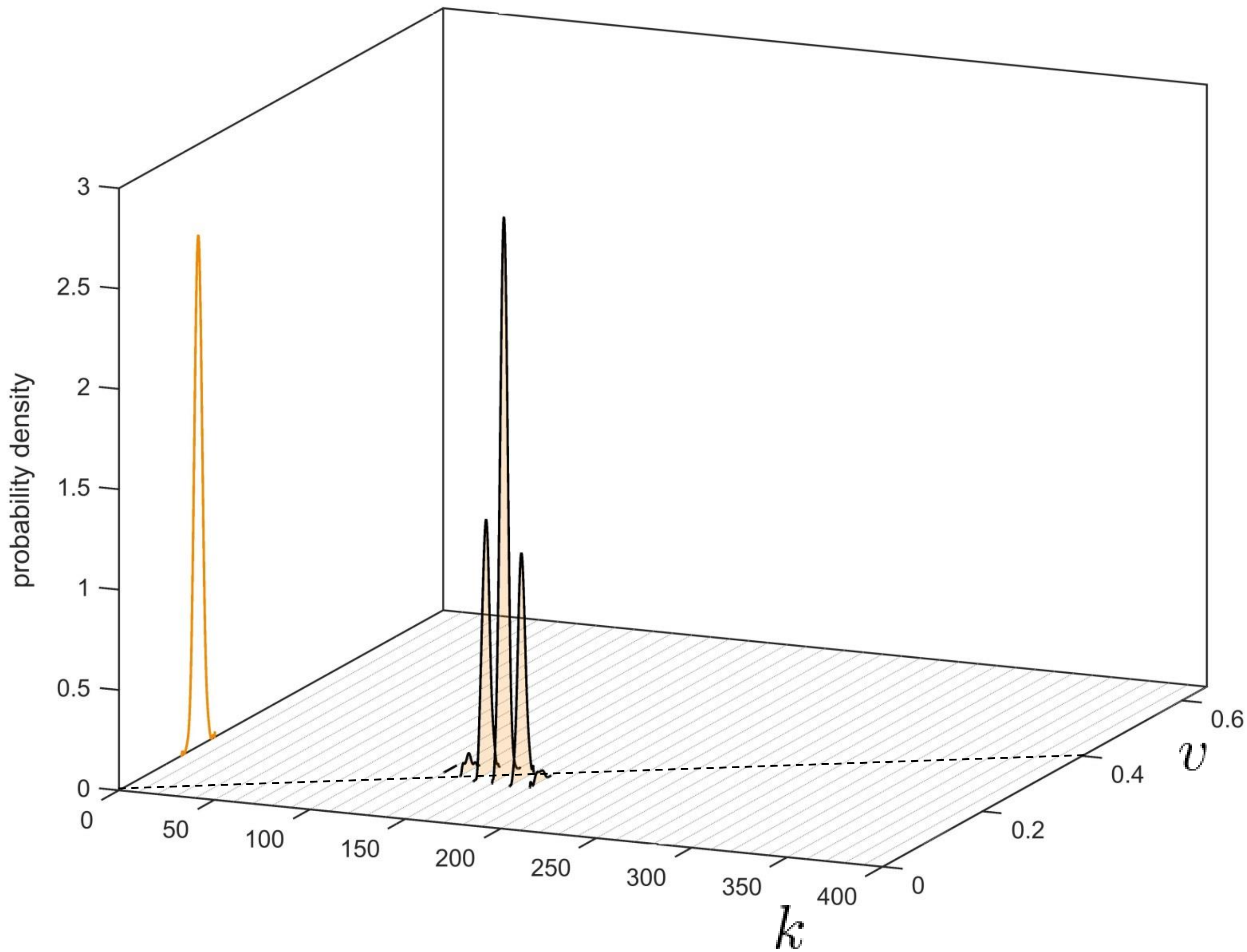
π^* is a random variable (integer, $\pi^* = k,\ k \in \{0, 1, \ldots, N\}$)

$V(x^*)$ is a random variable (real, $V(x^*) = v, \quad v \in [0, 1]$)

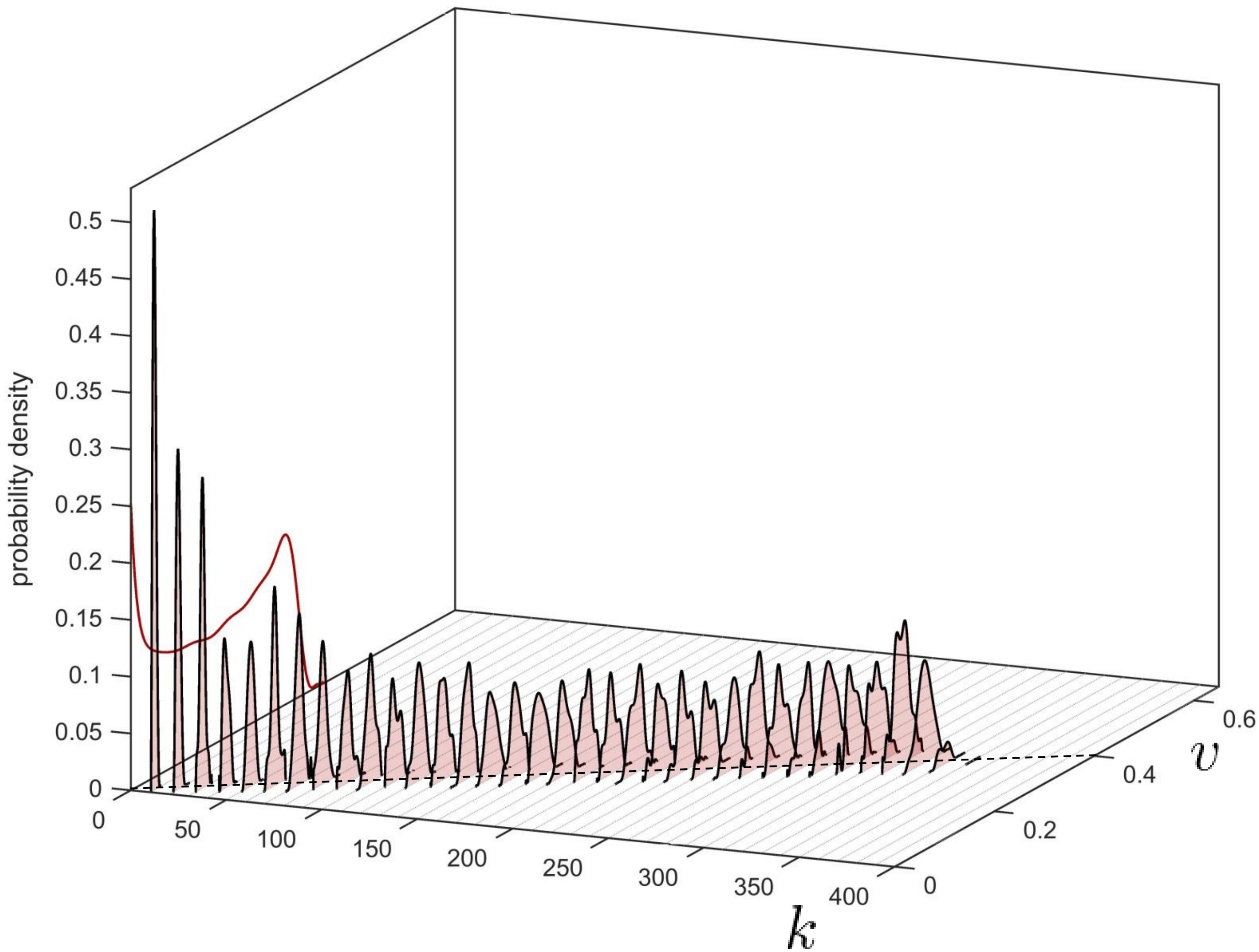
Study $F^*(k, v)$, the bivariate distribution of $\begin{bmatrix} \pi^* \\ V(x^*) \end{bmatrix}$



Bivariate risk-complexity distribution – Example 1



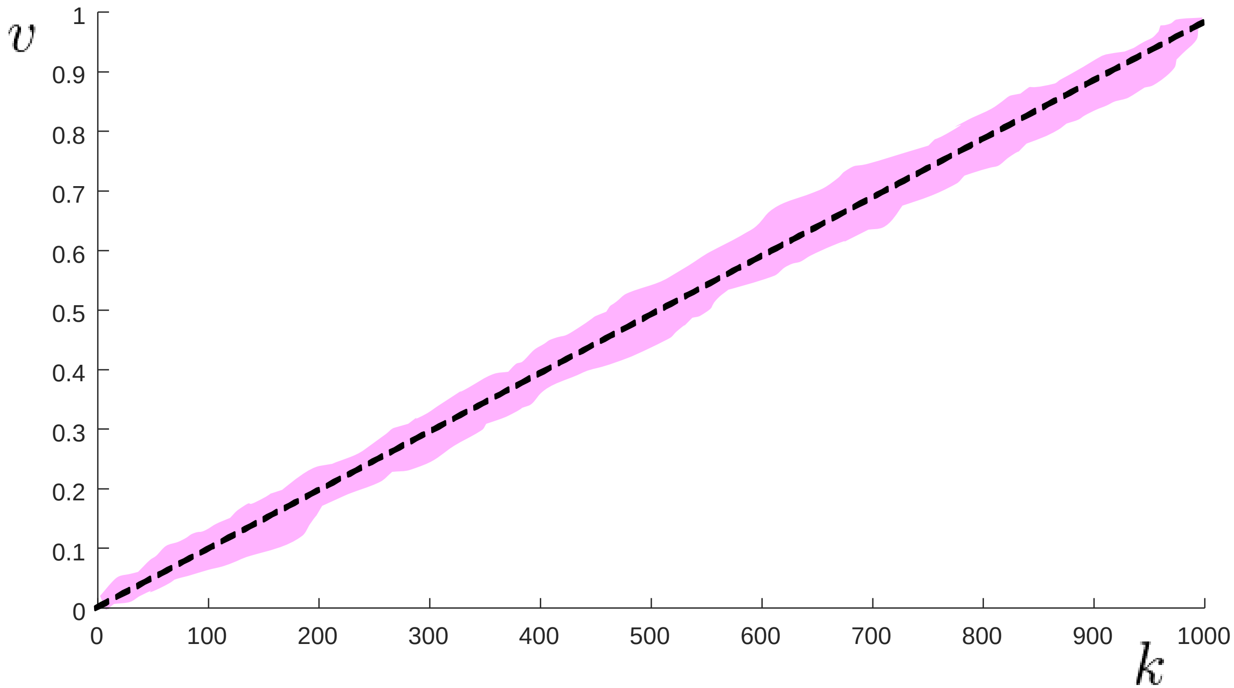
Bivariate risk-complexity distribution – Example 2



Main result (take-home message)

For all consistent decision schemes and distribution-free,

$F^*(k, v)$ concentrates around/below $v = \frac{k}{N}, \; k = 0, 1, \ldots, N$



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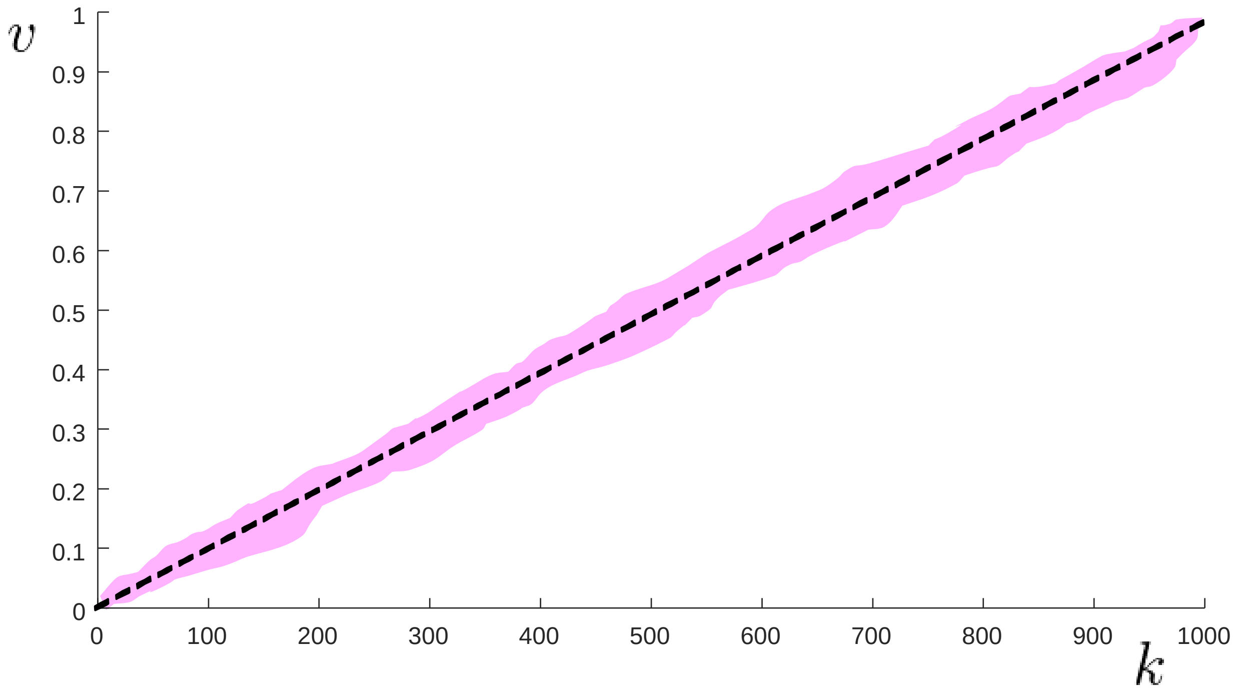

$\Rightarrow$ $V(x^*)$ **can be accurately estimated from** π^*

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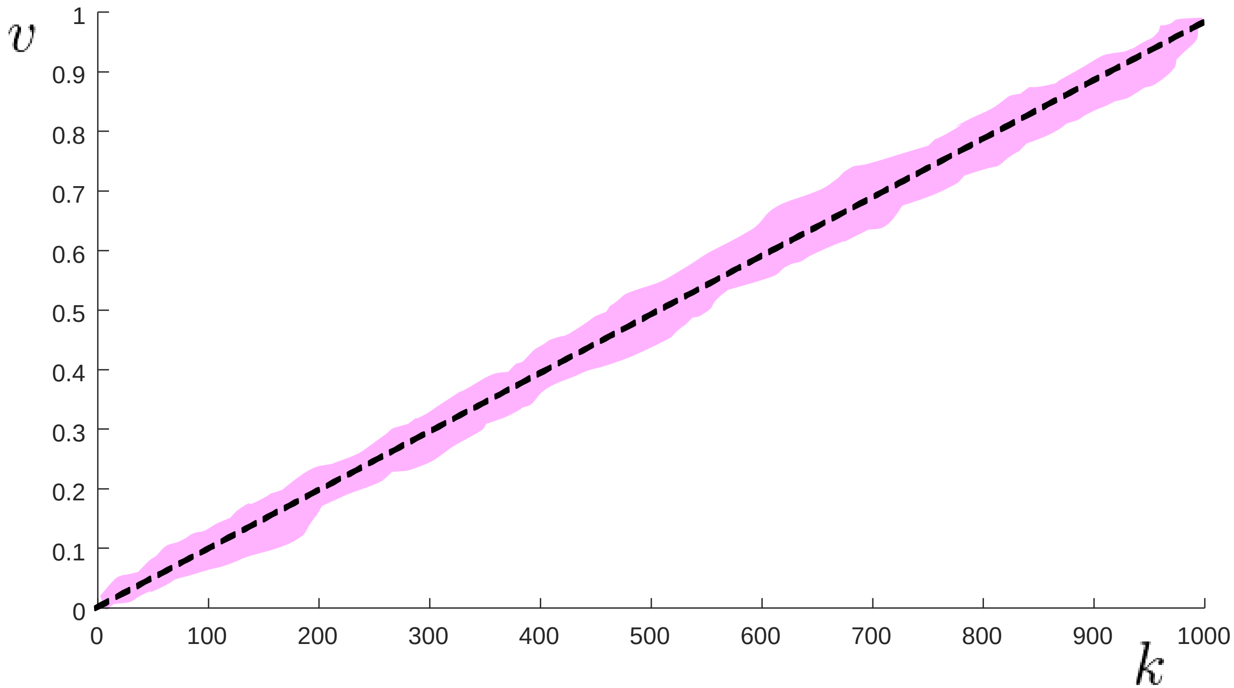

observable!

$V(x^*)$ **can be accurately estimated from** π^*

Main result

Choose $\beta \in (0,1)$ (confidence parameter)

Let $\epsilon^U(k)$ be the unique roots in (0,1) of polynomials

$$\binom{N}{k}(1-\epsilon)^{N-k} - \frac{\beta}{2N}\sum_{m=k}^{N-1}\binom{m}{k}(1-\epsilon)^{m-k}$$

Then, irrespective of $\mathbb{P}$ (distribution-free),

$$\mathbb{P}^N\left\{\delta^{(1)},\ldots,\delta^{(N)} : \quad V(x^*) \leq \epsilon^U(\pi^*)\right\} \geq 1-\beta$$

Main result

Assumption (non-degeneracy): the support set is unique with probability 1 (≅ non-accumulation of constraints in a convex setup)

Choose $\beta \in (0,1)$ (confidence parameter)

Let $\epsilon_L(k), \epsilon^U(k)$ be the unique roots in (0,1) of polynomials

- $$\binom{N}{k}(1-\epsilon)^{N-k} - \frac{\beta}{2N}\sum_{m=k}^{N-1}\binom{m}{k}(1-\epsilon)^{m-k}$$
- $$\binom{N}{k}(1-\epsilon)^{N-k} - \frac{\beta}{2N}\sum_{m=N+1}^{2N}\binom{m}{k}(1-\epsilon)^{m-k}$$

Then, irrespective of $\mathbb{P}$ (distribution-free),

$$\mathbb{P}^N\left\{\delta^{(1)},\ldots,\delta^{(N)}:\ \epsilon_L(\pi^*) \le V(x^*) \le \epsilon^U(\pi^*)\right\} \ge 1-\beta$$

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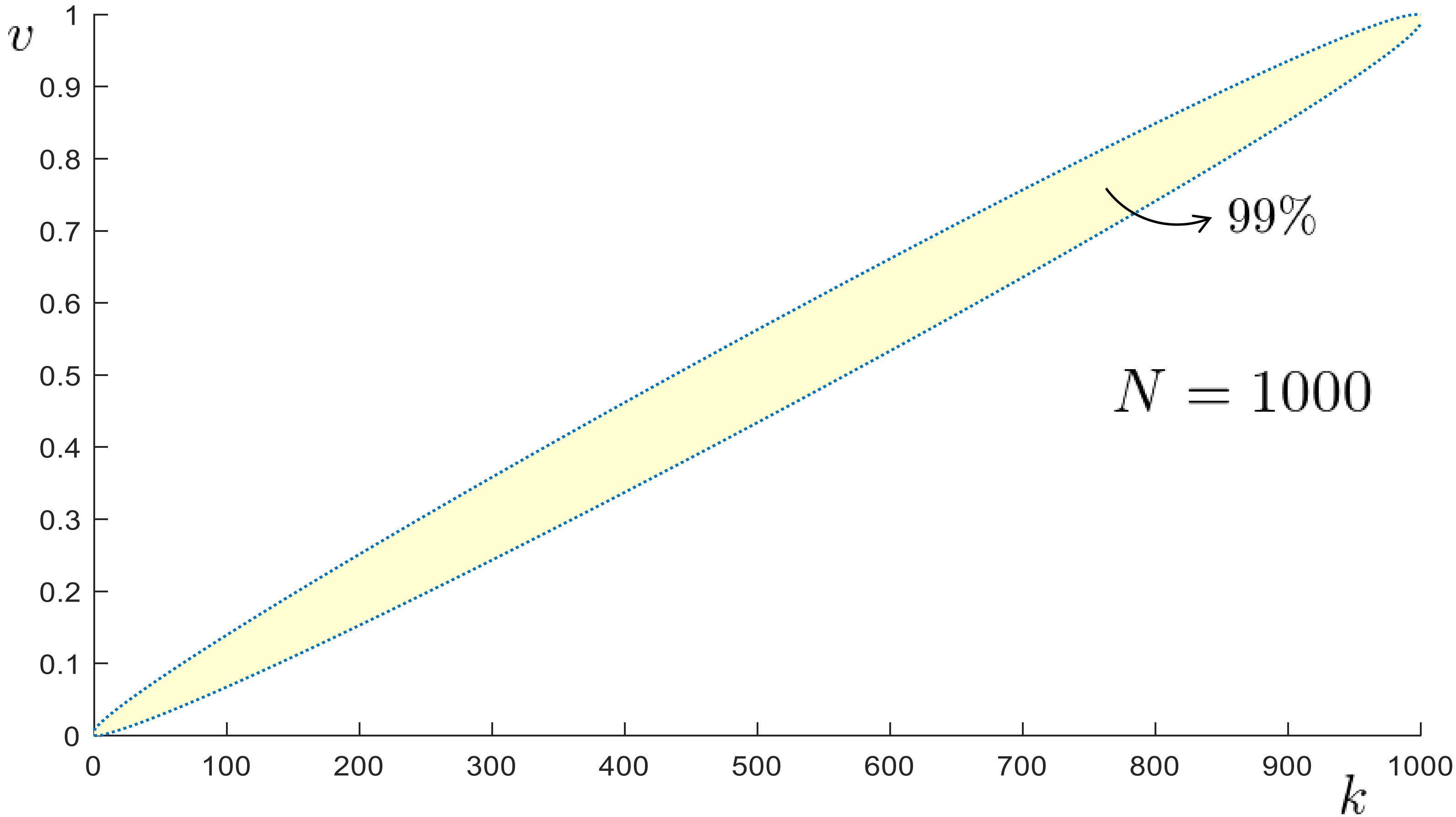

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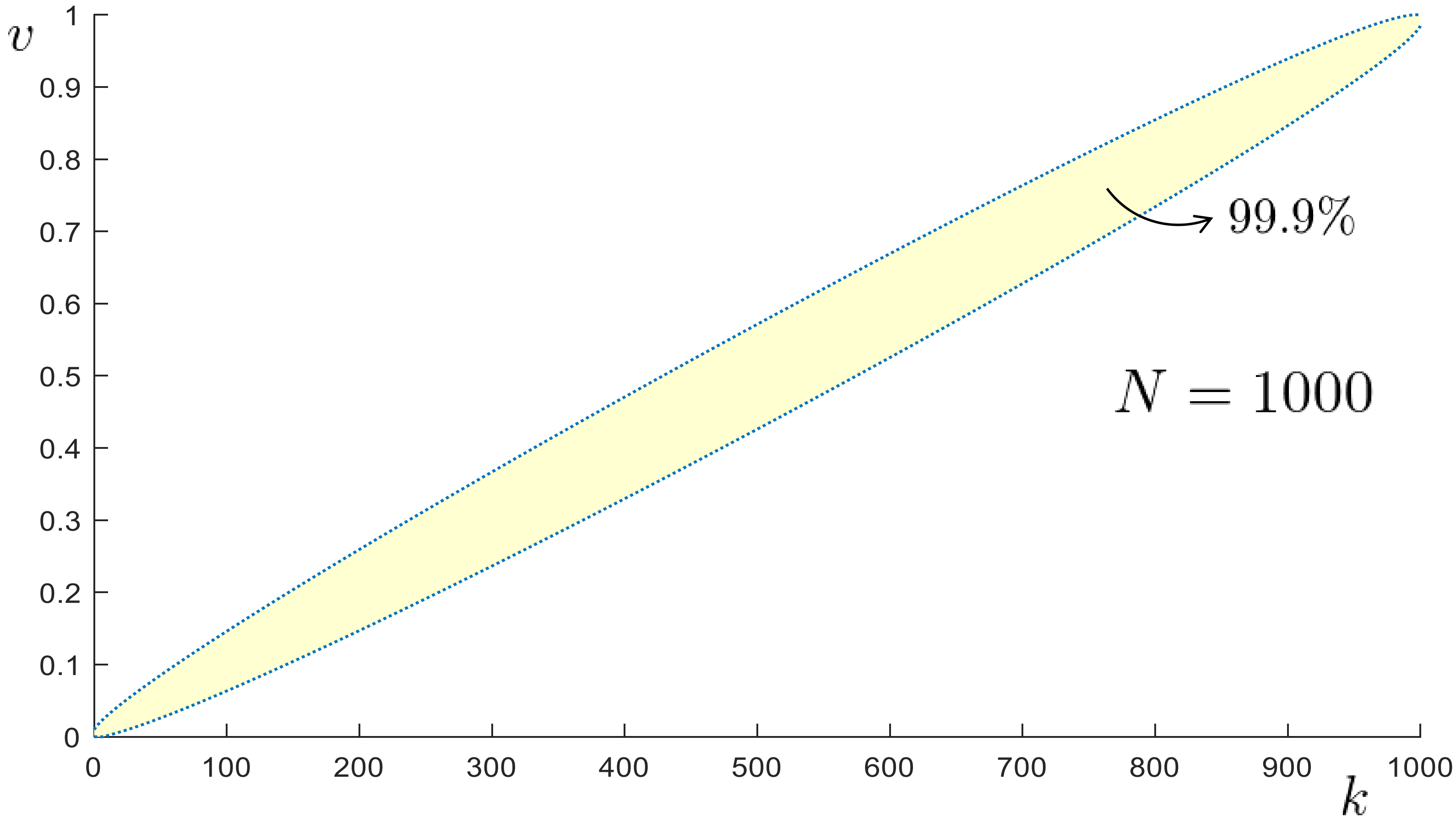

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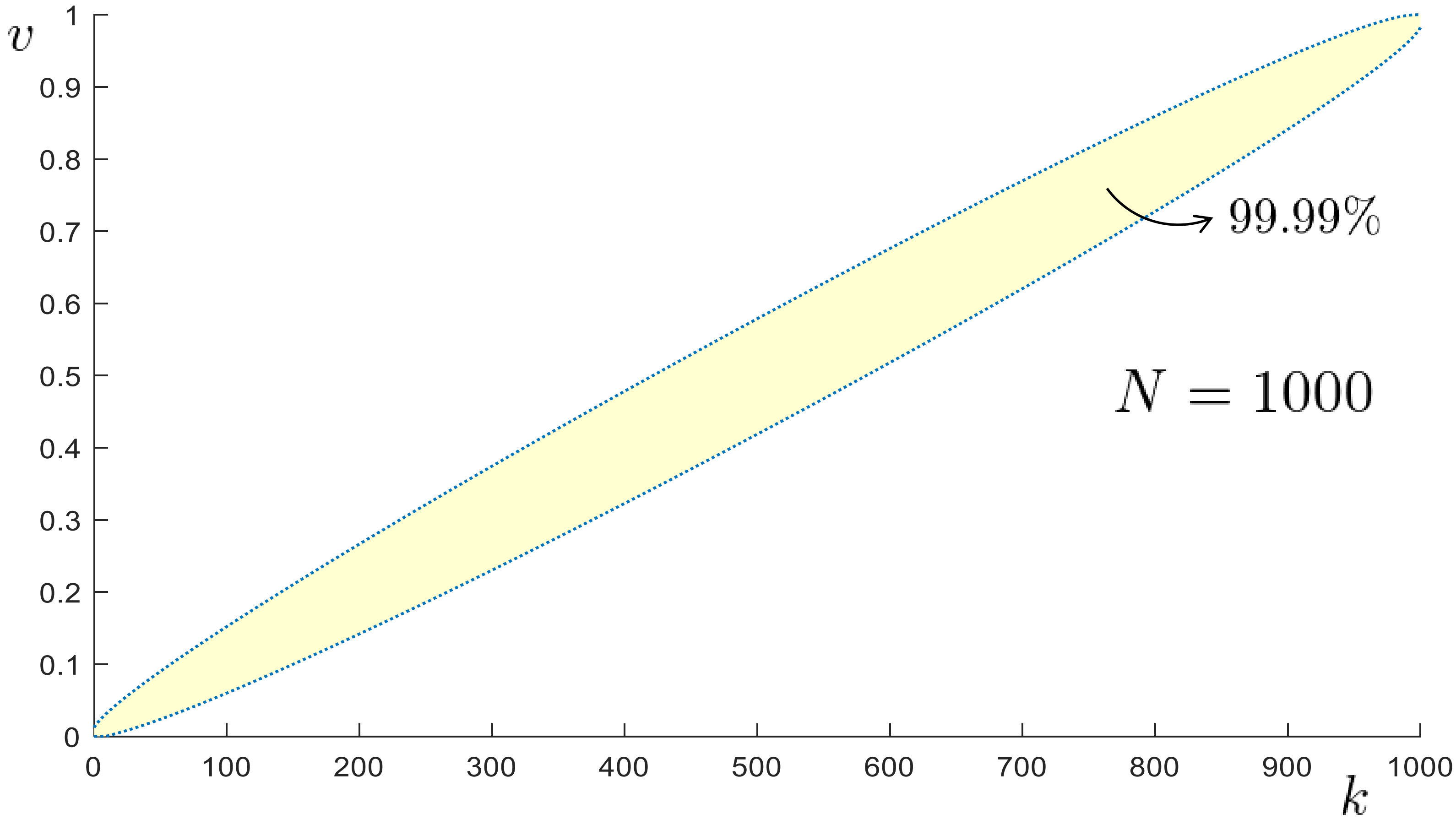

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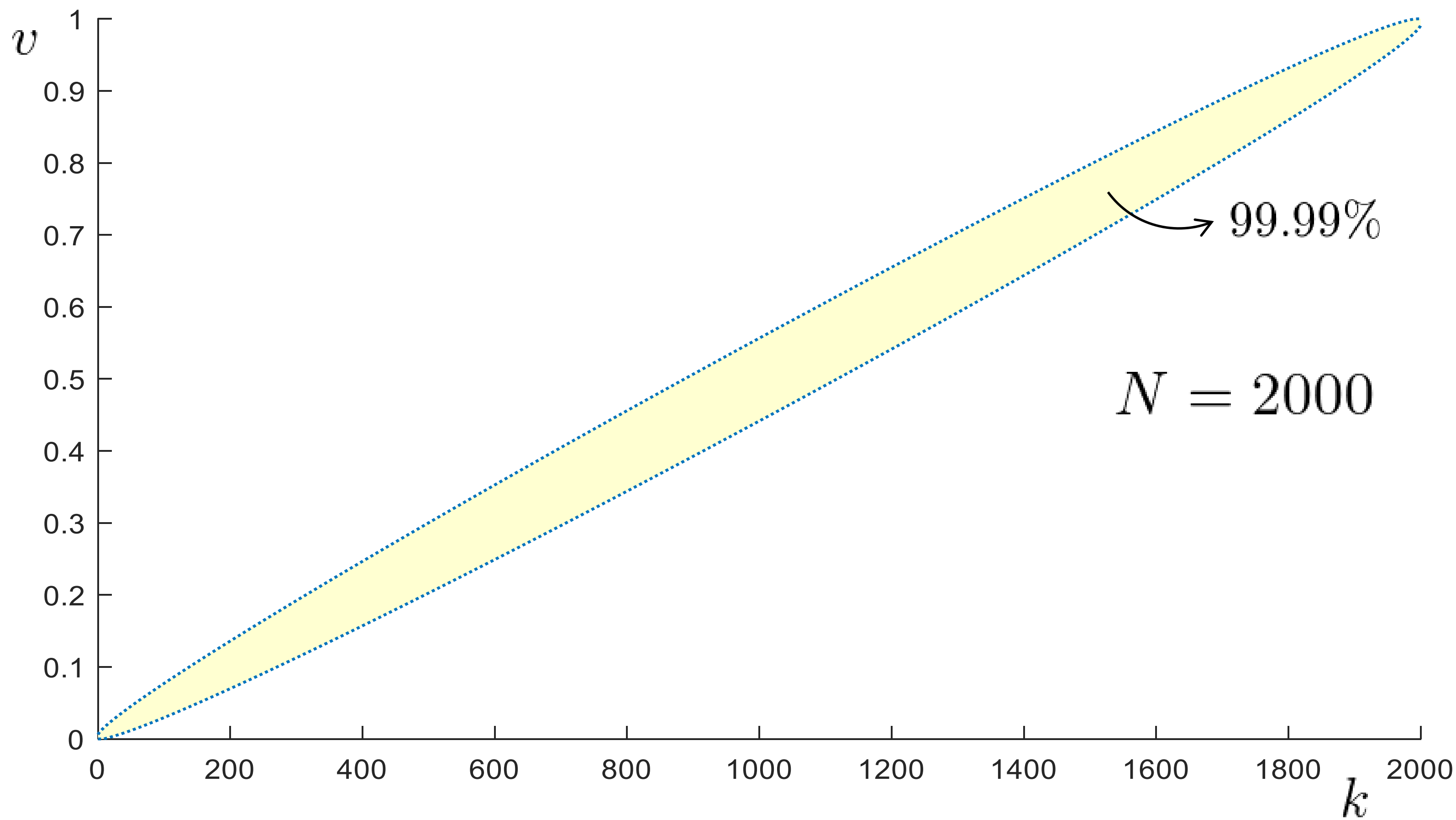

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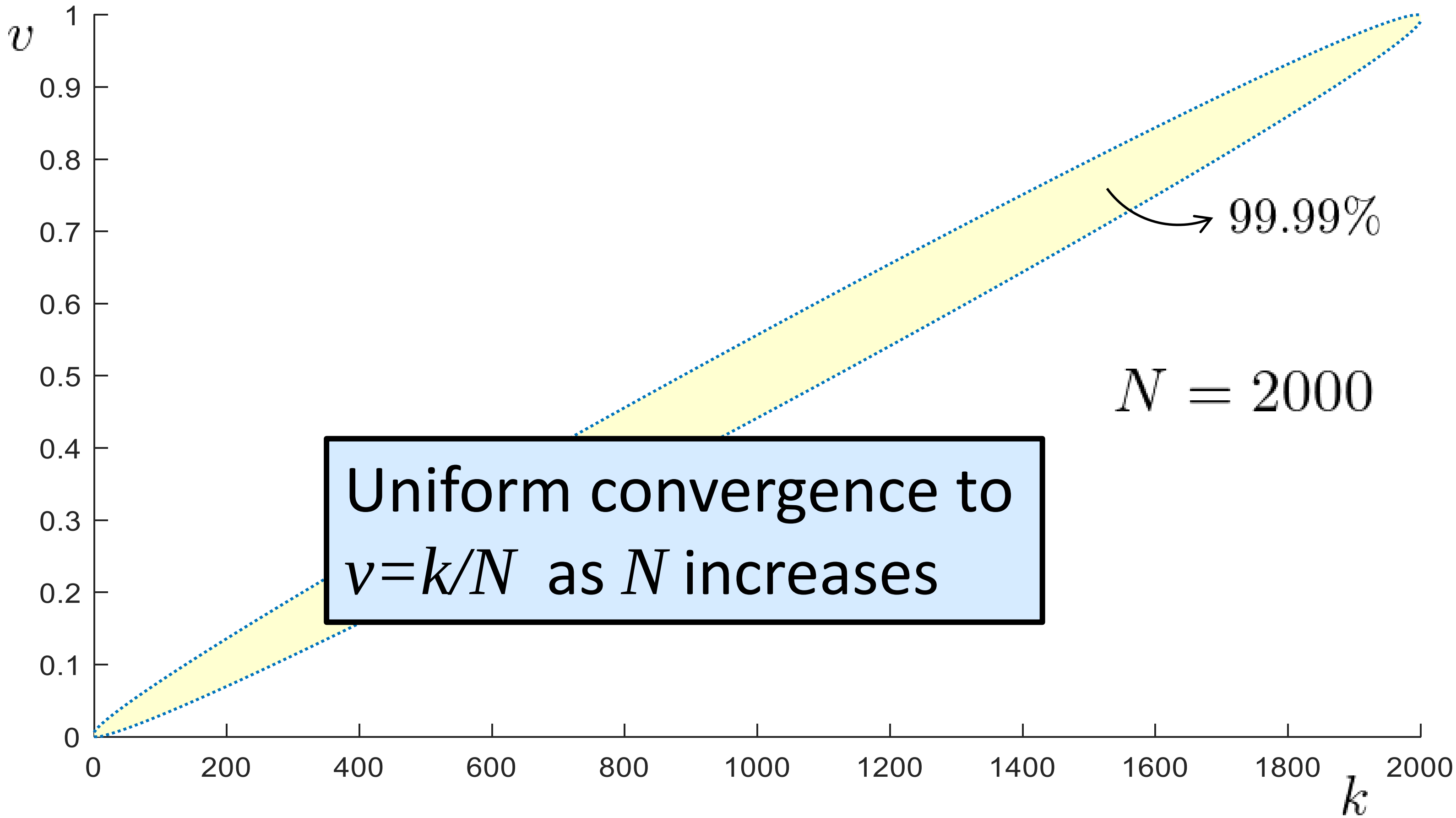

Uniform convergence to $v=k/N$ as N increases

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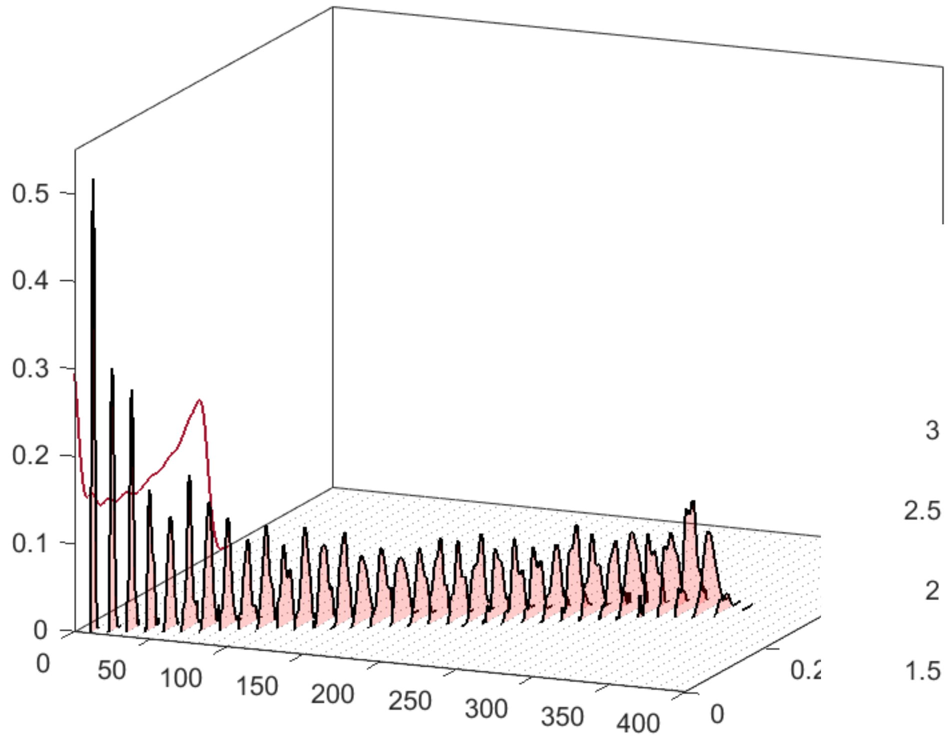

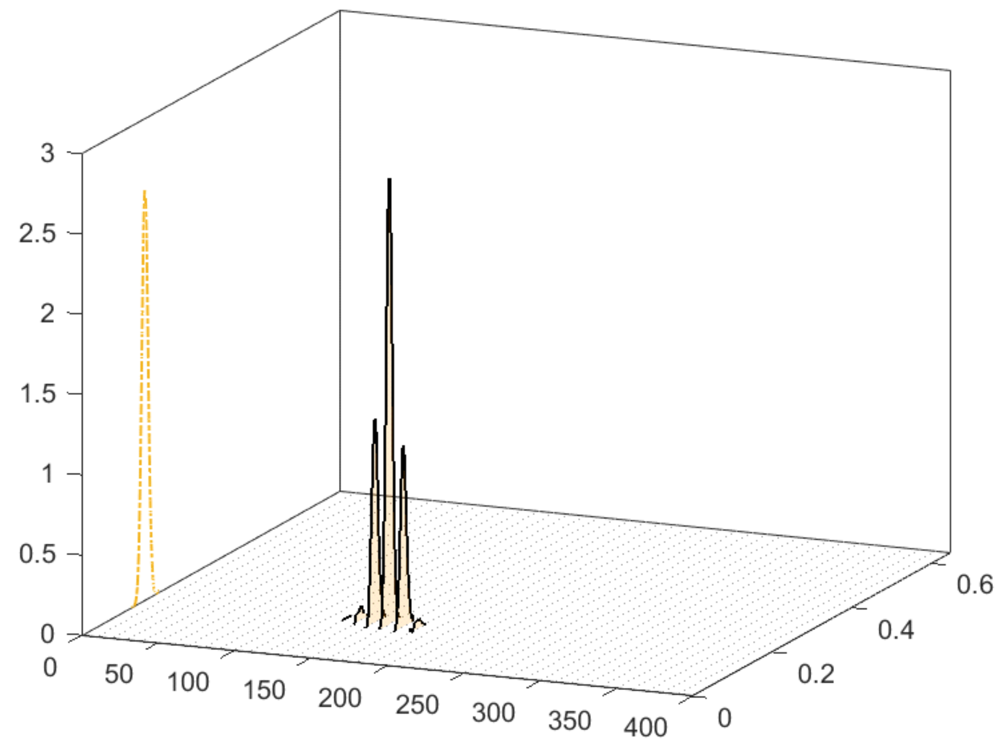

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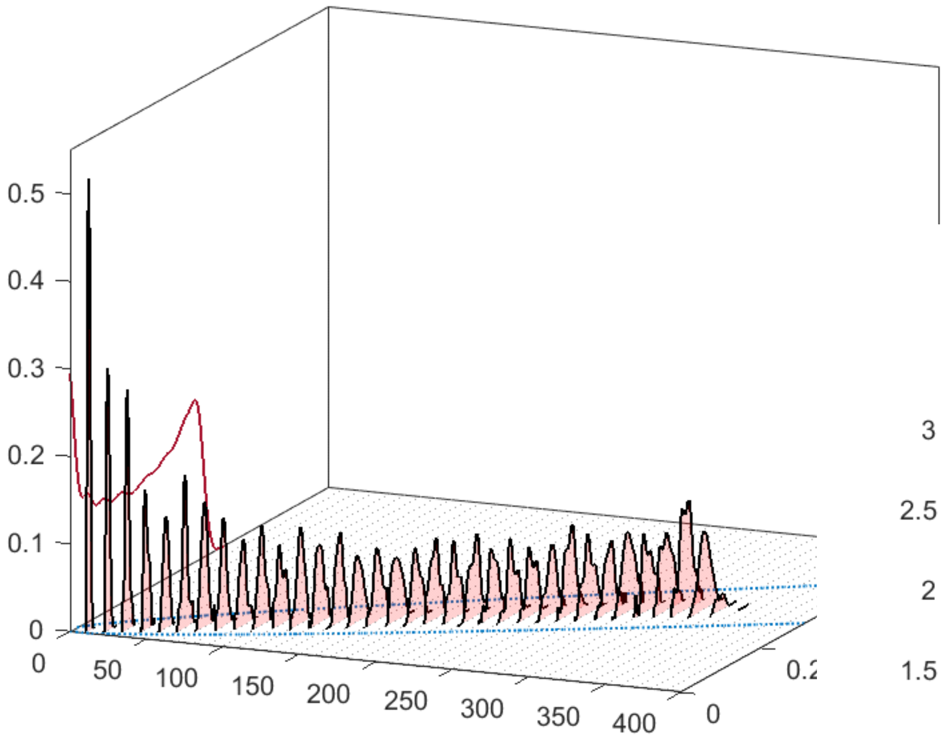
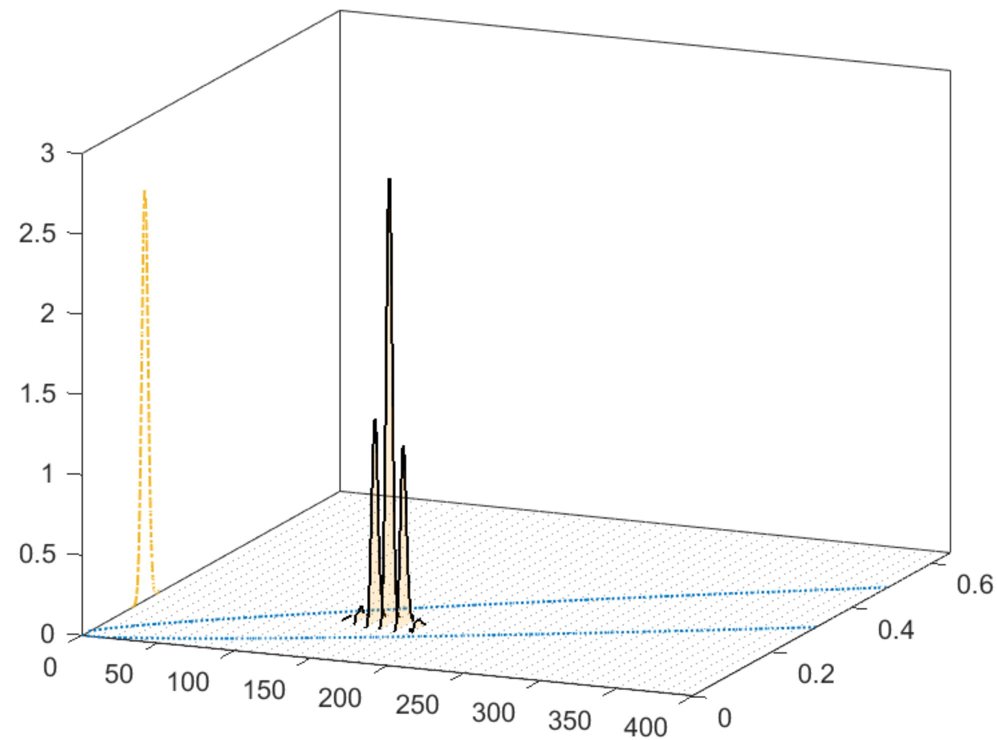
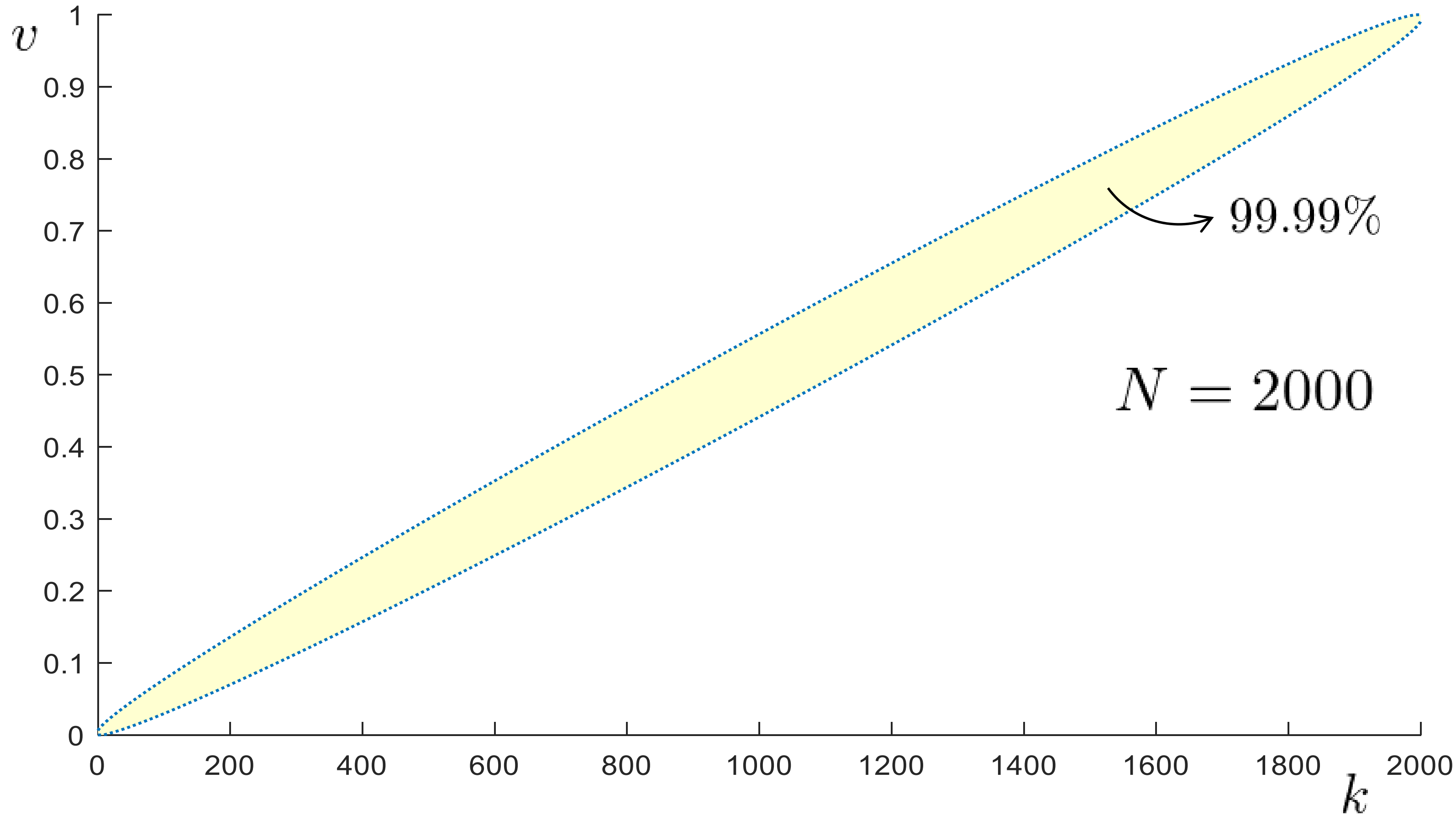




Main result

$\epsilon_L(\pi^*) \leq V(x^*) \leq \epsilon^U(\pi^*)$ **is true with confidence** $1 - \beta$



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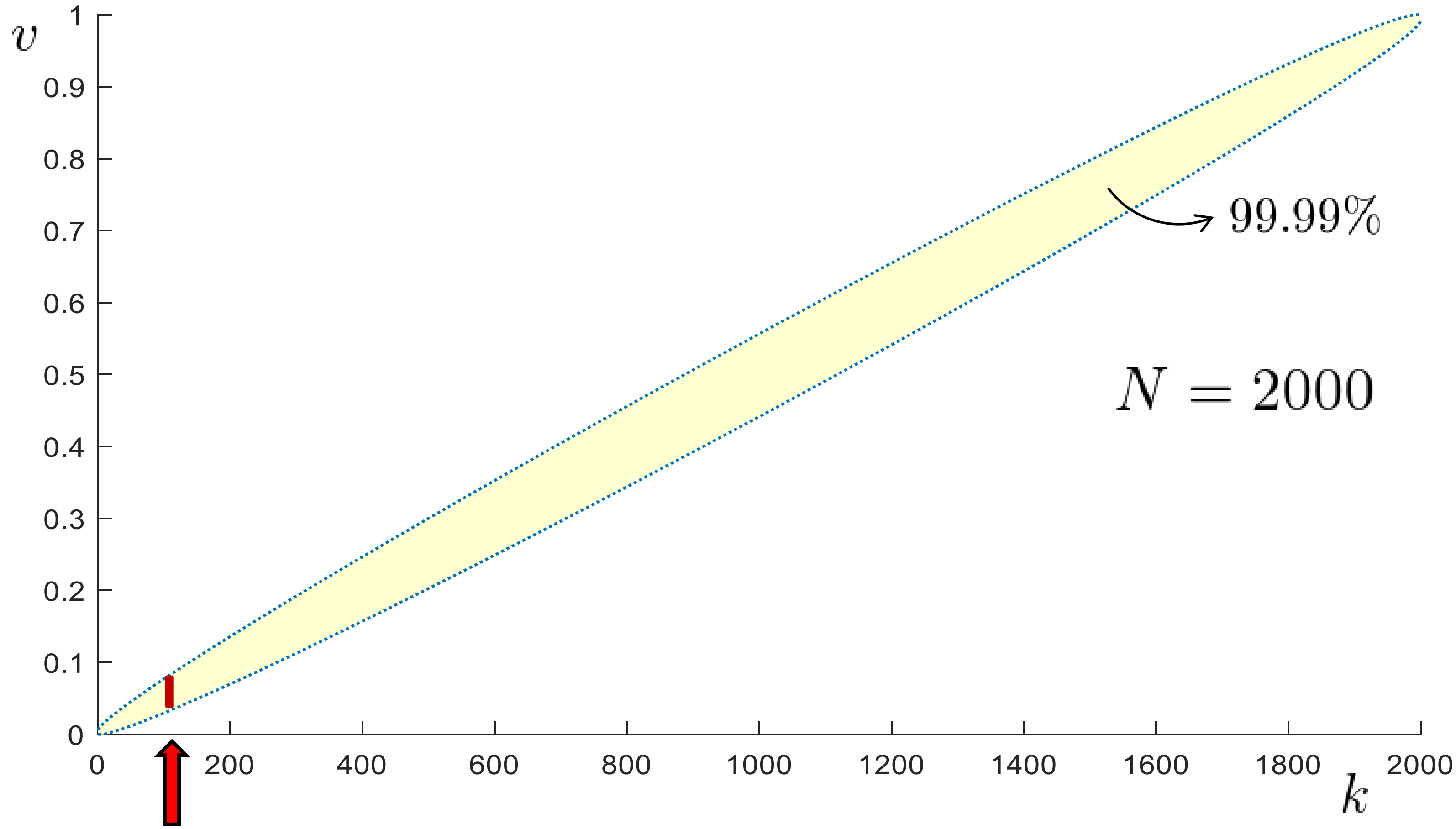
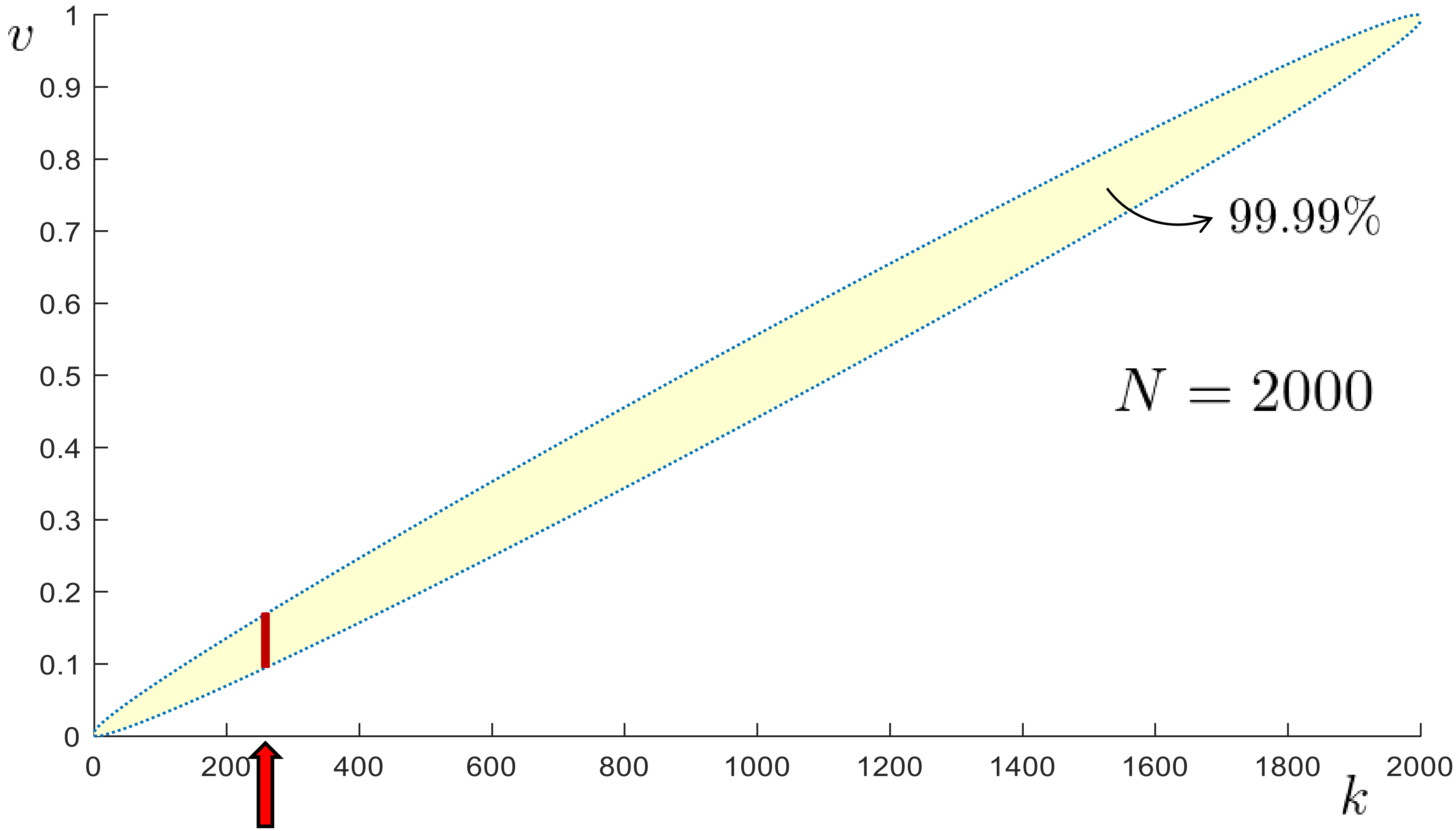


$\pi^* = 90 \rightarrow 0.026 \leq V(x^*) \leq 0.071$

Main result

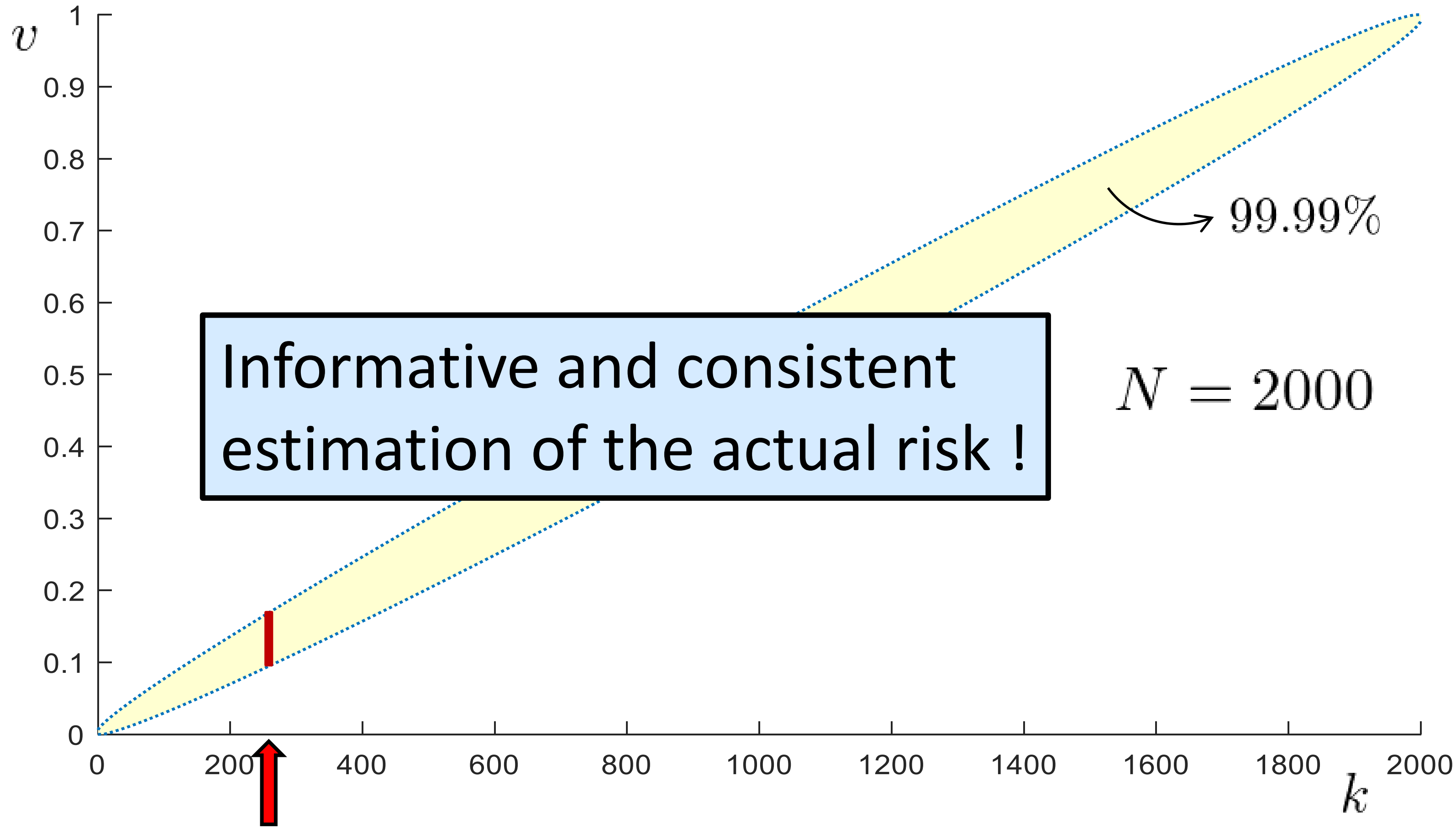
$\epsilon_L(\pi^*) \leq V(x^*) \leq \epsilon^U(\pi^*)$ **is true with confidence** $1-\beta$



$$\pi^* = 260 \rightarrow 0.095 \leq V(x^*) \leq 0.17$$

Main result

$\epsilon_L(\pi^*) \leq V(x^*) \leq \epsilon^U(\pi^*)$ **is true with confidence** $1-\beta$



$$\pi^* = 260 \rightarrow 0.095 \leq V(x^*) \leq 0.17$$

Solution assessment

$c(x^*)$	accessible
$V(x^*)$	not accessible

Solution assessment

$c(x^*)$	accessible
$[\epsilon_L(\pi^*), \epsilon^U(\pi^*)]$	accessible

Solution assessment

$c(x^*)$ accessible

$[\epsilon_L(\pi^*), \epsilon^U(\pi^*)]$ accessible

→ accept/reject the solution

→ make further decisions

→ compare various "solutions"

Cost vs. risk tradeoff

$$\min_{x \in \mathbb{R}^d, \xi_i \geq 0} \quad c(x) + \rho \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.} \quad f(x, \delta^{(i)}) \leq \xi_i,$$

$$i = 1, \ldots, N$$

$$\begin{array}{cccc} \rho_1 & \rho_2 & \rho_3 & \cdots \\ \downarrow & \downarrow & \downarrow & \cdots \\ x_1^*, \pi_1^* & x_2^*, \pi_2^* & x_3^*, \pi_3^* & \cdots \end{array} \Bigg\}$$

cost vs. risk tradeoffs

Cost vs. risk tradeoff

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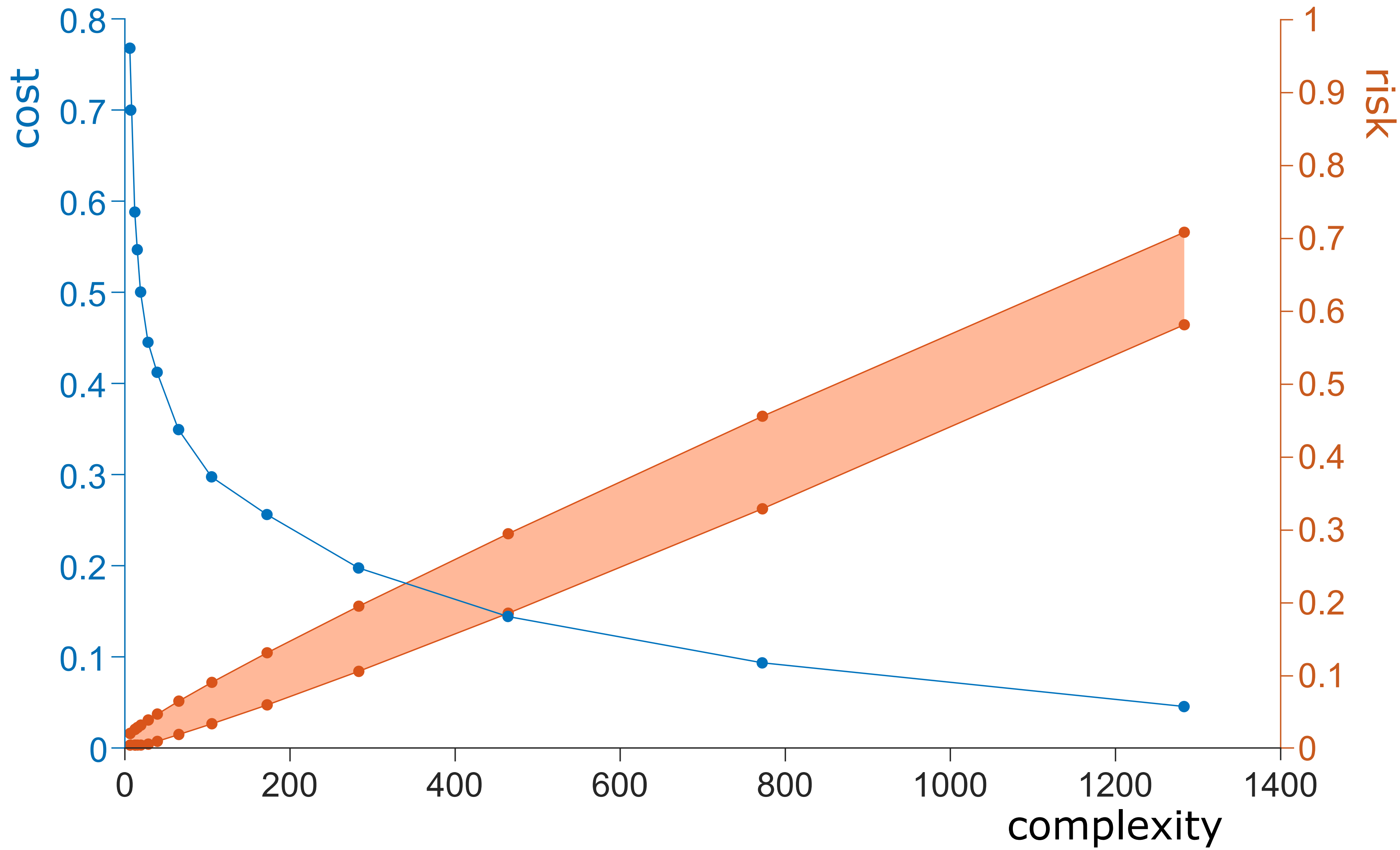
$$\left.\begin{array}{cccc} \rho_1 & \rho_2 & \rho_3 & \cdots \\ \downarrow & \downarrow & \downarrow & \cdots \\ x_1^*, \pi_1^* & x_2^*, \pi_2^* & x_3^*, \pi_3^* & \cdots \end{array}\right\}$$

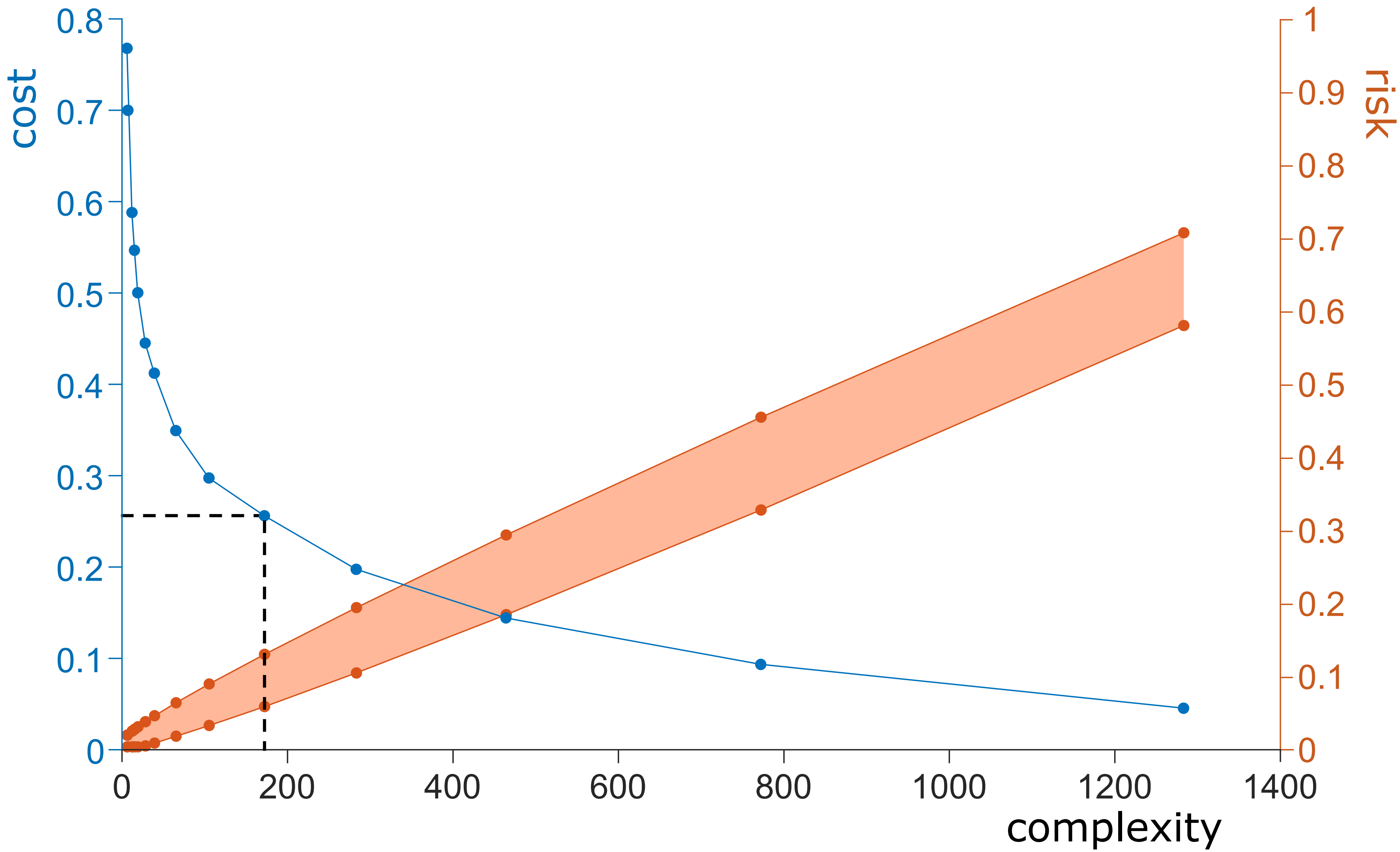
cost vs. risk tradeoffs

quantitative comparison via $c(x_i^*)$ and $[\epsilon_L(\pi_i^*), \epsilon^U(\pi_i^*)]$

Cost vs. risk plot



Cost vs. risk plot



Application to Support Vector Methods

$$\min_{\substack{w \in \mathcal{U}, \gamma \geq 0, b \in \mathbb{R} \\ \xi_i \geq 0, i=1,\ldots,N}} \quad (\gamma + \tau \|w\|^2) + \rho \sum_{i=1}^{N} \xi_i$$

$$\text{subject to:} \quad |y_i - \langle w, \mathbf{u}_i \rangle - b| - \gamma \leq \xi_i, \quad i = 1, \ldots, N$$

Application to Support Vector Methods

$$\min_{\substack{w\in\mathcal{U},\gamma\geq 0,b\in\mathbb{R}\\ \xi_i\geq 0,i=1,\ldots,N}} \quad (\gamma+\tau\|w\|^2)+\rho\sum_{i=1}^{N}\xi_i$$

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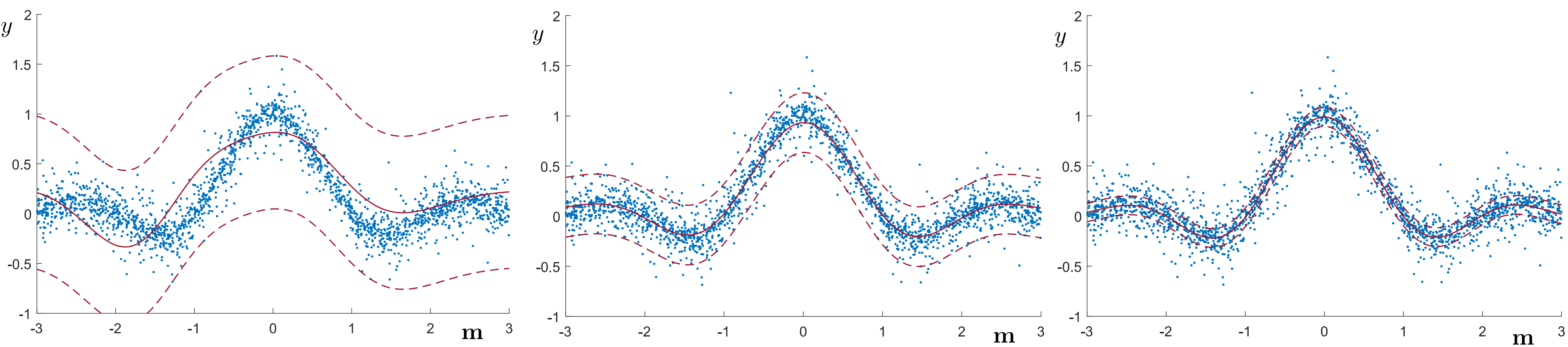

informativeness of prediction vs. probability of misprediction

Conclusions

- Data are a “gold mine” for decision-making, but good theories are needed for a reliable exploitation

- Scenario approach: a flexible and effective setup for data-driven decision making with a good theory to assess the reliability of the solution

- At a very general level, the complexity π^* (visible) carries fundamental information on the risk $V(x^*)$ (hidden), which can be estimated without using any information other the data used to design the solution

- Consistency encompasses many decision schemes; many others yet be discovered!

Thank you !

M.C. Campi, S. Garatti. Wait-and-judge scenario optimization. Mathematical Programming, 167(1):155-189, 2018. https://doi.org/10.1007/s10107-016-1056-9

S. Garatti , M.C. Campi. Risk and complexity in scenario optimization. Mathematical Programming, 191(1): 243-279, 2022. https://doi.org/10.1007/s10107-019-01446-4

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S. Garatti , M.C. Campi. Non-Convex Scenario Optimization. Mathematical Programming – to appear

This research is supported by FAIR (Future Artificial Intelligence Research) project, funded by the NextGenerationEU program within the PNRR-PE-AI scheme (M4C2, Investment 1.3, Line on Artificial Intelligence)

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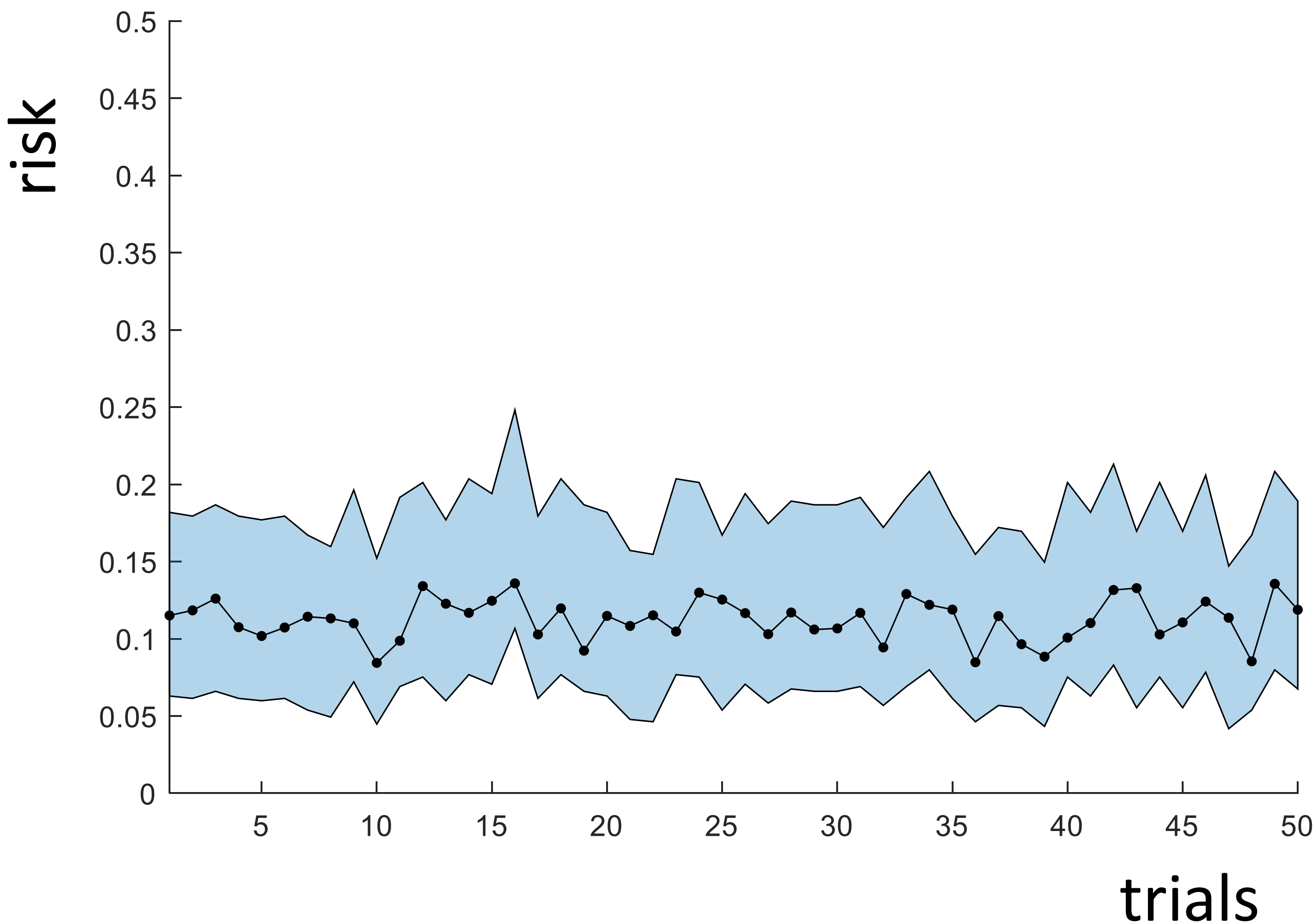
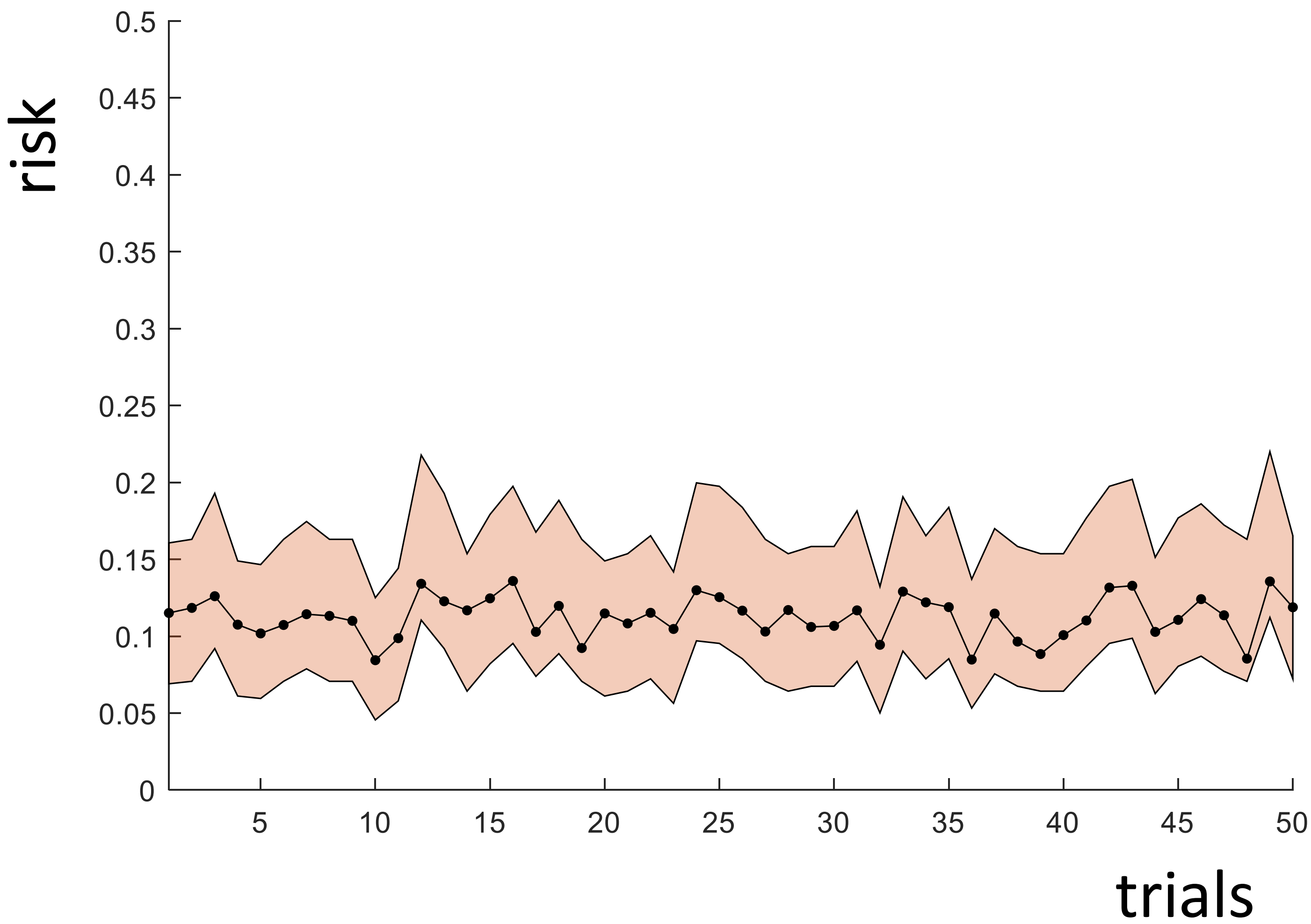
Scenario approach vs. test-set approach

$N = 500$, risk assessment via scenario theory



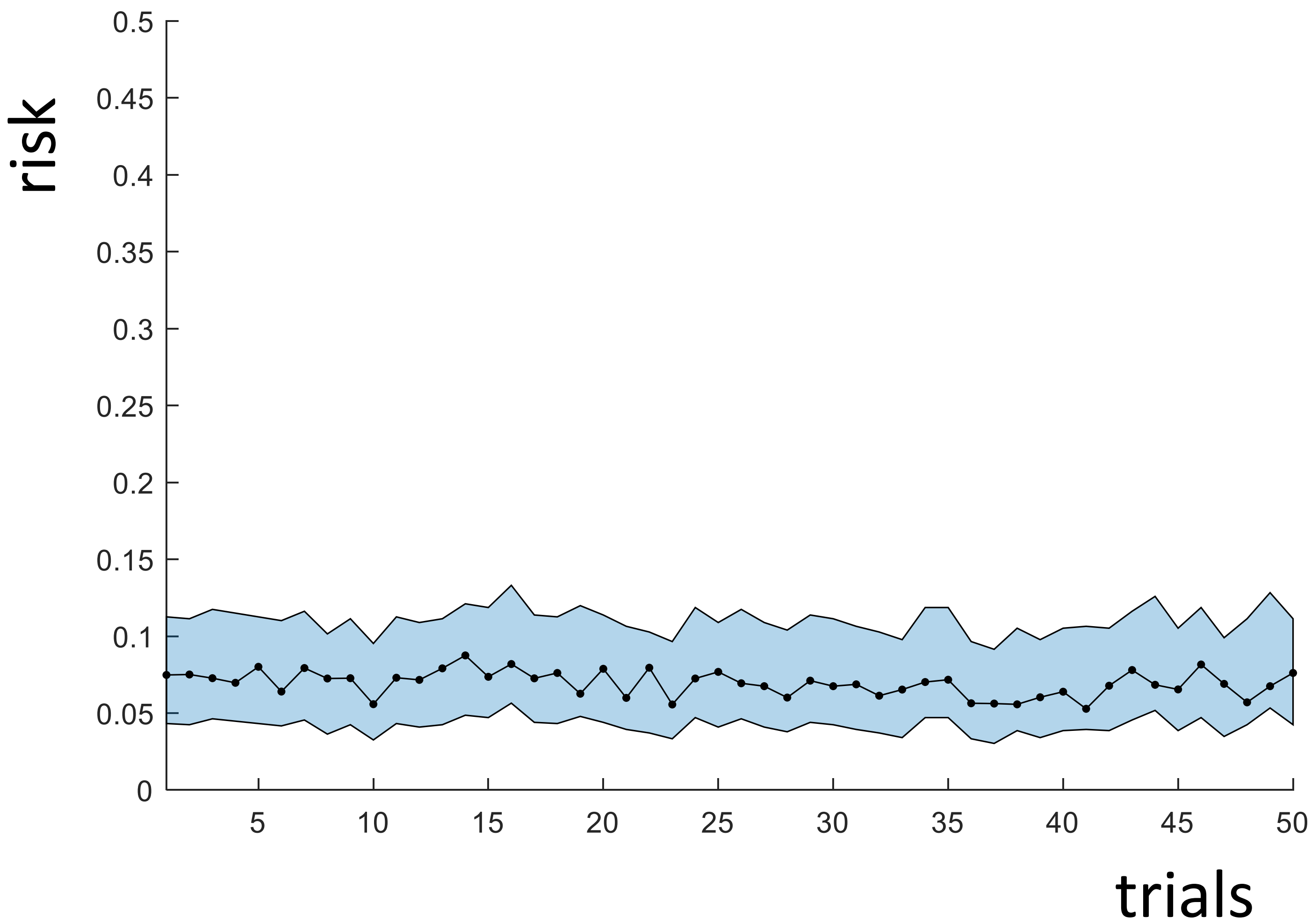
Scenario approach vs. test-set approach

N = 500, risk assessment via validation using new 500 scenarios



Scenario approach vs. test-set approach

$N = 1000$, risk assessment via scenario theory



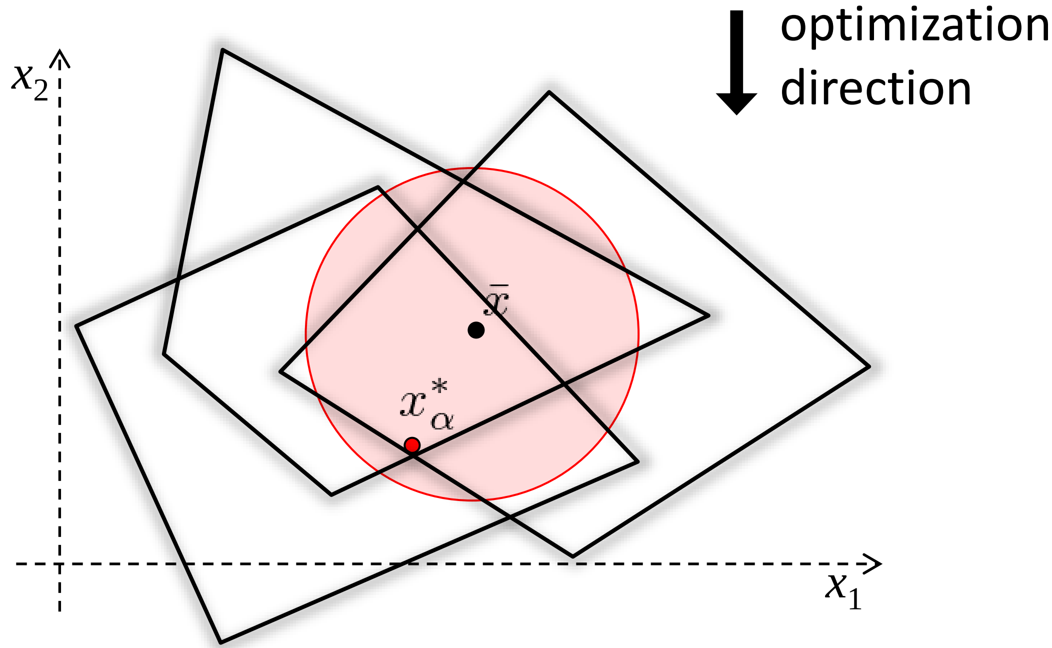
Scenario optimization with regularization

$$\min_x \quad c(x)$$

$$\text{s.t.} \quad x \in \mathcal{X}_{\delta_i}$$

$$i = 1, \ldots, N$$

$$\|x - \bar{x}\| \leq \alpha$$



solution: x^*_α

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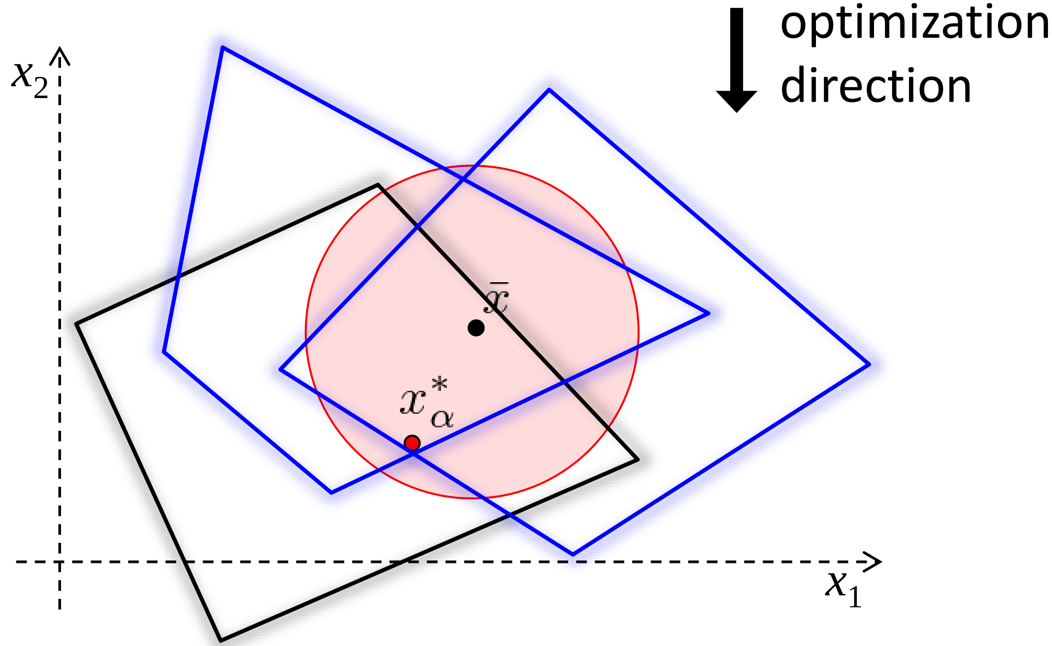

solution: x^*_α

complexity: s^*_α

(support set)

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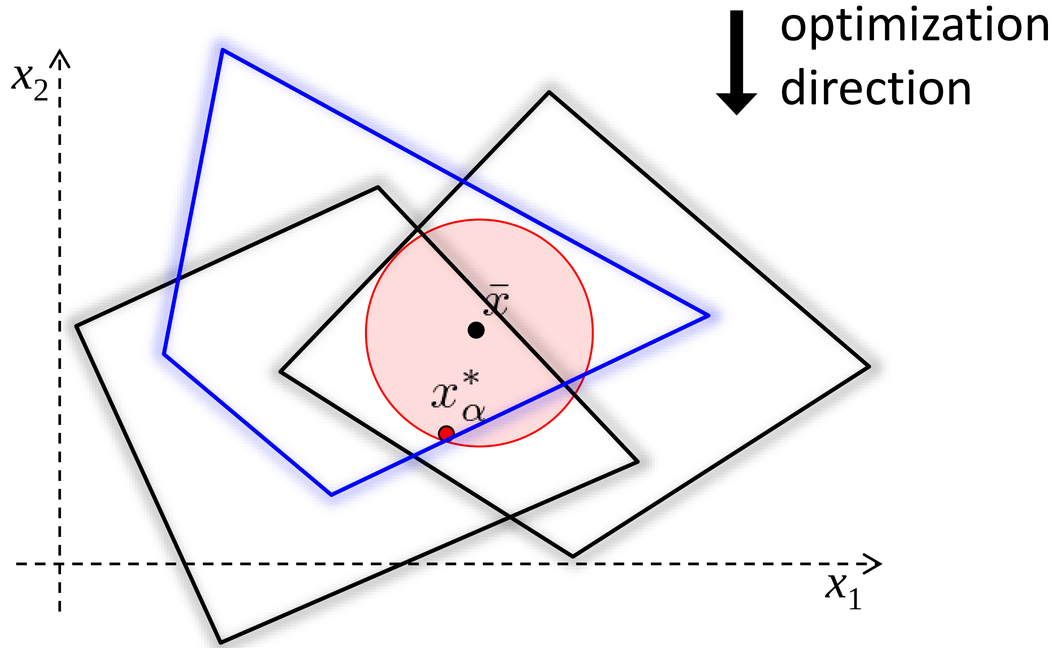

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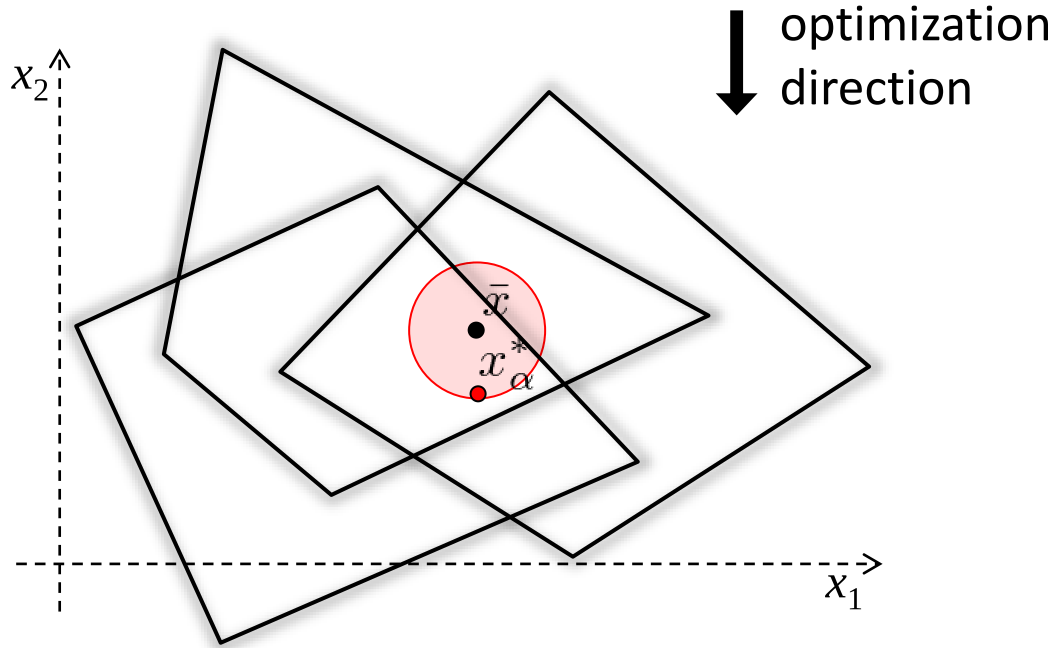

solution: x^*_α

complexity: s^*_α

(support set)

as $\alpha \to 0$

cost $c(x^*_\alpha)$ increasing

risk $\widehat{V}(s^*_\alpha)$ decreasing