

A Unified Machine Learning Framework for Optimization Under Uncertainty

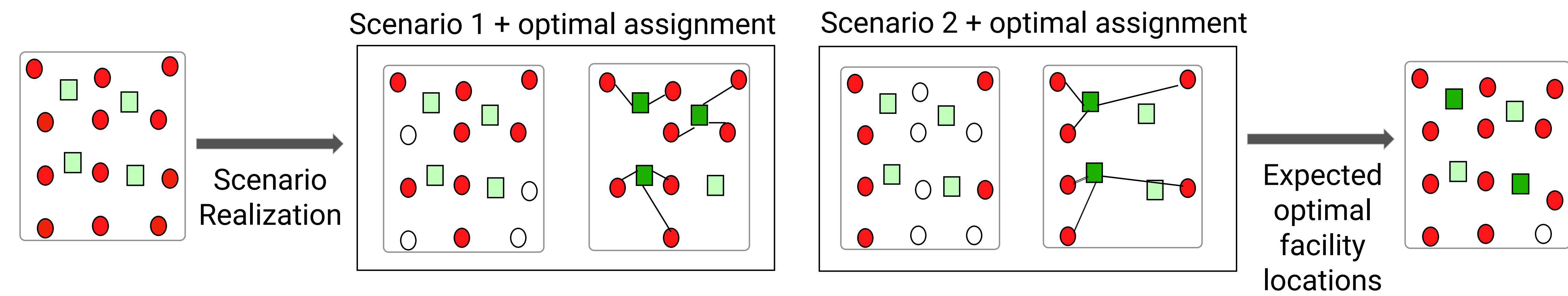
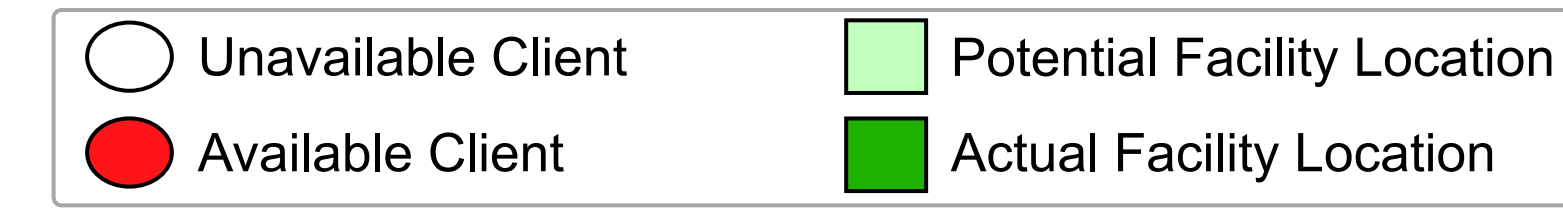
Justin
Dumouchelle

Learning for Two-Stage Stochastic Programming (2SP)

Published at NeurIPS 2022. Joint work with Rahul Patel, Elias Khalil, and Merve Bodur

Stochastic Facility Location Problem

Objective: Determine the optimal set of facilities to construct given uncertainty in client requests.

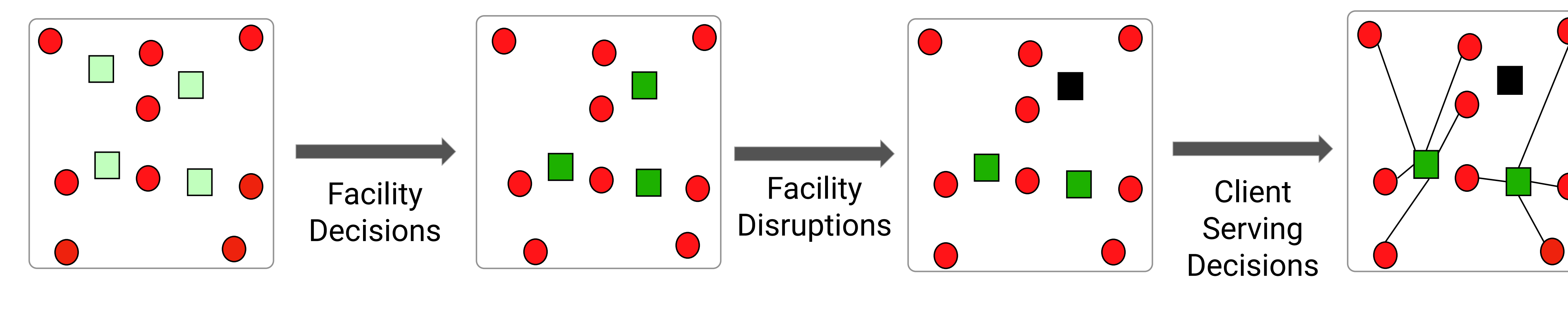


Learning for Two-Stage Robust Optimization (2RO)

Under review. Joint work with Esther Julien, Jannis Kurtz, and Elias Khalil

Robust Facility Location Problem

Objective: Determine the optimal set of facilities to open under the worst-case facility disruption.



Overall framework

Data Collection

- Sample decisions + uncertainty.
- Solve subproblems with off-the-shelf solvers.



Evaluation on new instances

- Solve the surrogate MILP with an off-the-shelf solver.



Supervised Learning

- Train an NN using off-the-shelf ML packages.



Optimization Formulation

Objective: Determine optimal **first-stage decisions** that minimize sum of the **first-stage cost** and **expected second-stage cost**.

Challenge: Exact optimization becomes exponentially harder with the number of observed scenarios, K . Integer decision further aggravates intractability.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \sum_{k=1}^K p_k Q(\mathbf{x}, \xi_k) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions (blue box), Expected second-stage cost (orange box)

Second-Stage Problem

$$Q(\mathbf{x}, \xi) := \min_{\mathbf{y}} \{ F(\mathbf{y}, \xi) : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \}$$

Second-stage cost (blue box), Second-stage decisions (green box)

Objective: Determine optimal **first-stage decisions** that minimize the sum of the **first-stage cost** and **worst-case cost**.

Challenge: Solving the nested optimization problem is intractable and specialized algorithms only exists for a limited classes of problems.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + Q(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions (blue box), Worst-case cost (orange box)

Second-Stage Problem

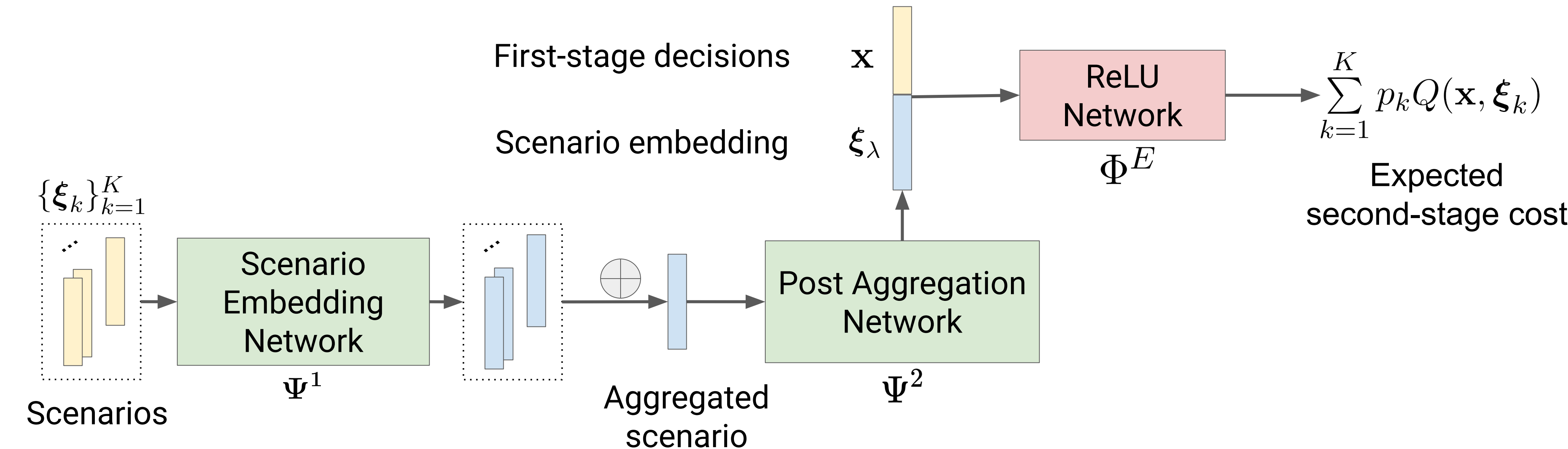
$$Q(\mathbf{x}) := \max_{\xi \in \Xi} \min_{\mathbf{y}} \{ \mathbf{d}(\xi)^T \mathbf{y} : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \}$$

Worst-case uncertainty (orange box), Second-stage cost (blue box), Second-stage decisions (green box)

Machine Learning Methodology

ML Solution: Replace the expected stage-cost value function with a neural network approximation.

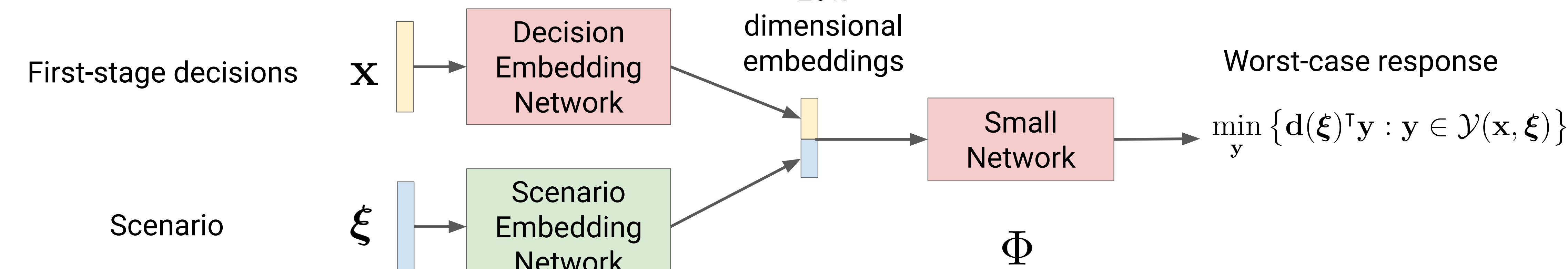
Neural Network Architecture:



Surrogate Optimization Model: $\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \text{NN}(\mathbf{x}, \{\xi_k\}_{k=1}^K) : \mathbf{x} \in \mathcal{X} \}$

ML Solution: Replace the worst-case response optimization problem with a neural network approximation.

Neural Network Architecture:



Surrogate Optimization Model: $\min_{\mathbf{x}, \mathbf{y}, \xi_a} \{ \mathbf{c}^T \mathbf{x} + \mathbf{d}(\xi_a)^T \mathbf{y} : \mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi_a), \xi_a \in \arg \max_{\xi \in \Xi} \{ \text{NN}(\mathbf{x}, \xi) \} \}$

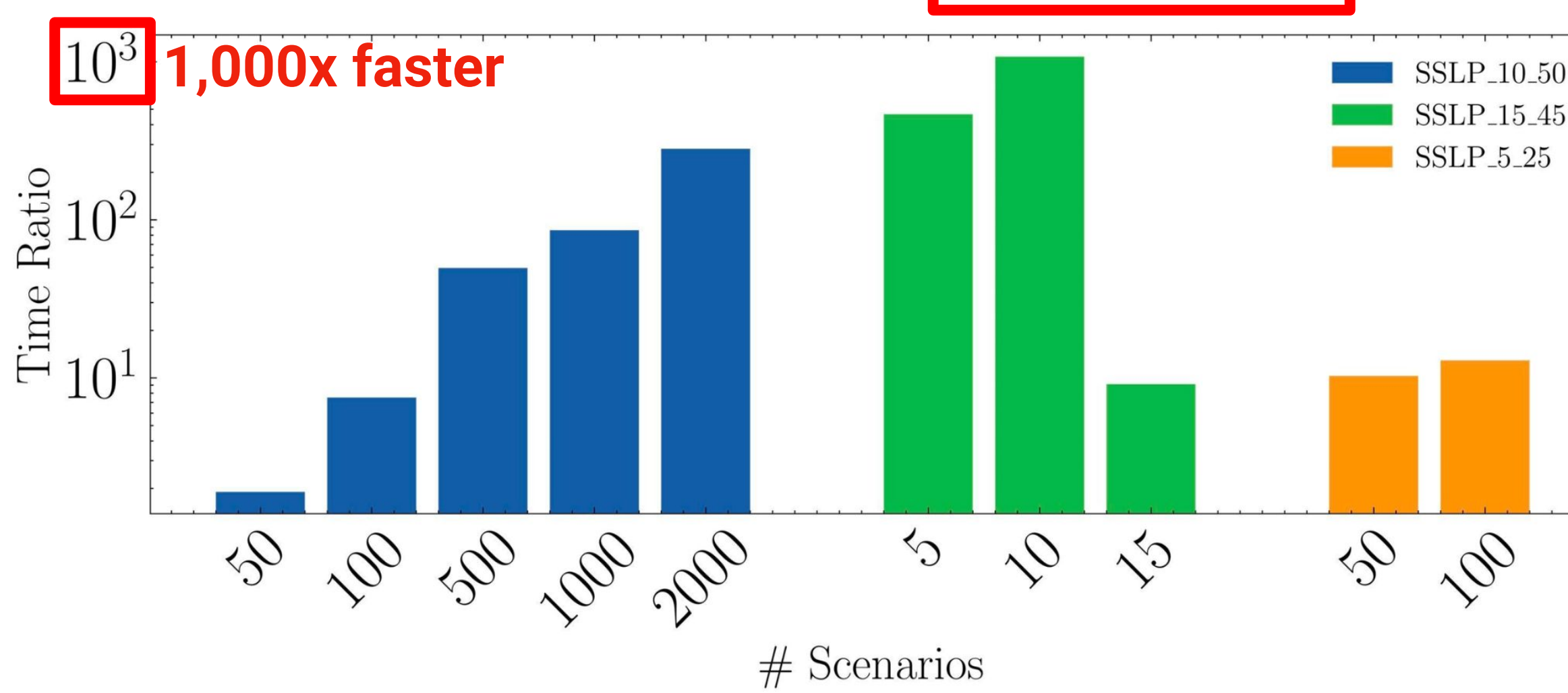
- Optimization problem solved via constraint generation of small networks.
- Worst-case scenarios determined via adversarial problem ($\max_{\xi \in \Xi} \text{NN}(\hat{\mathbf{x}}, \xi)$).

Experimental Results

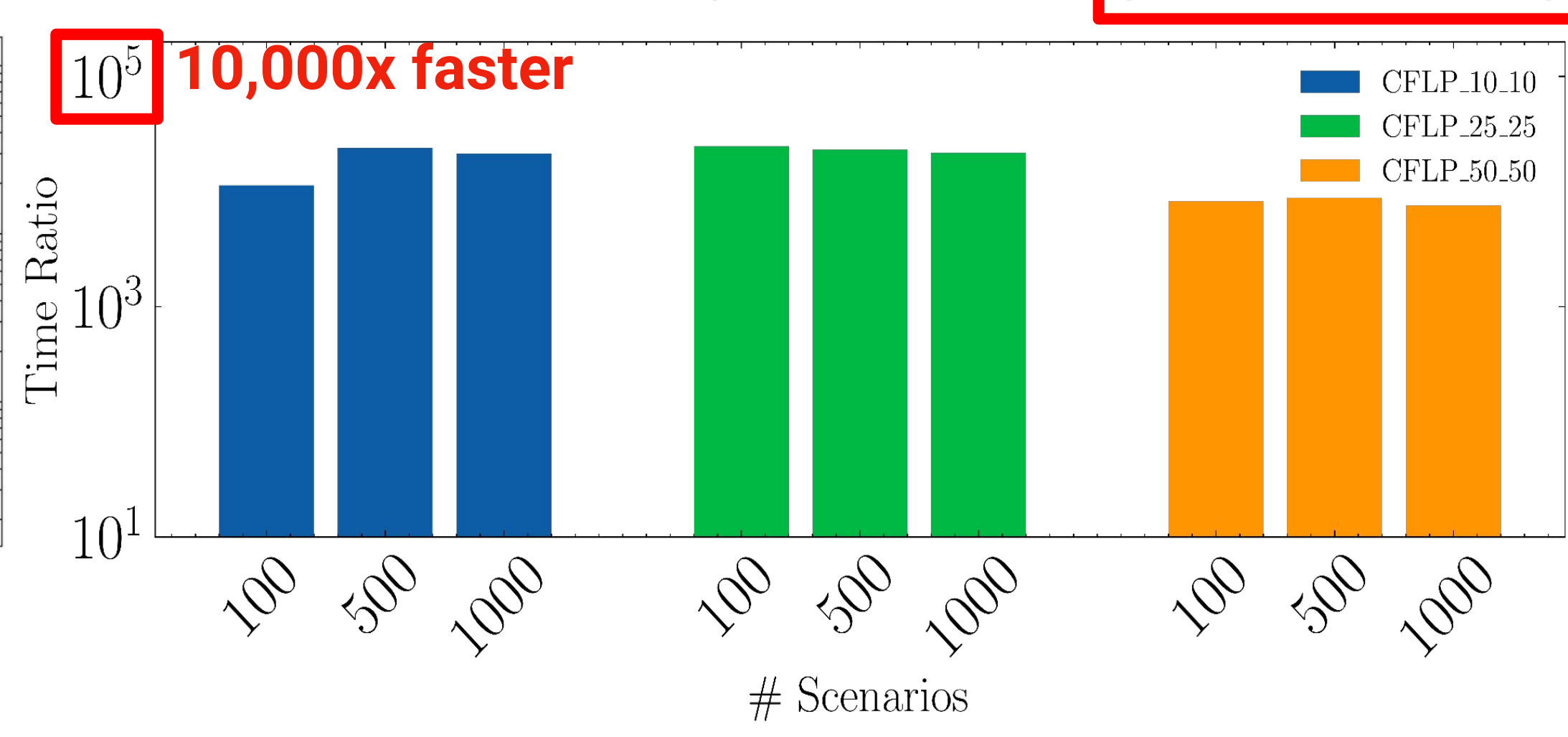
Stochastic Programming

Reduction factor in solving time over baseline (Integer L-shaped/EF) (higher is better).

Stochastic Server Location (Gap: 0.87%)



Capacitated Facility Location (Gap: -2.93%)

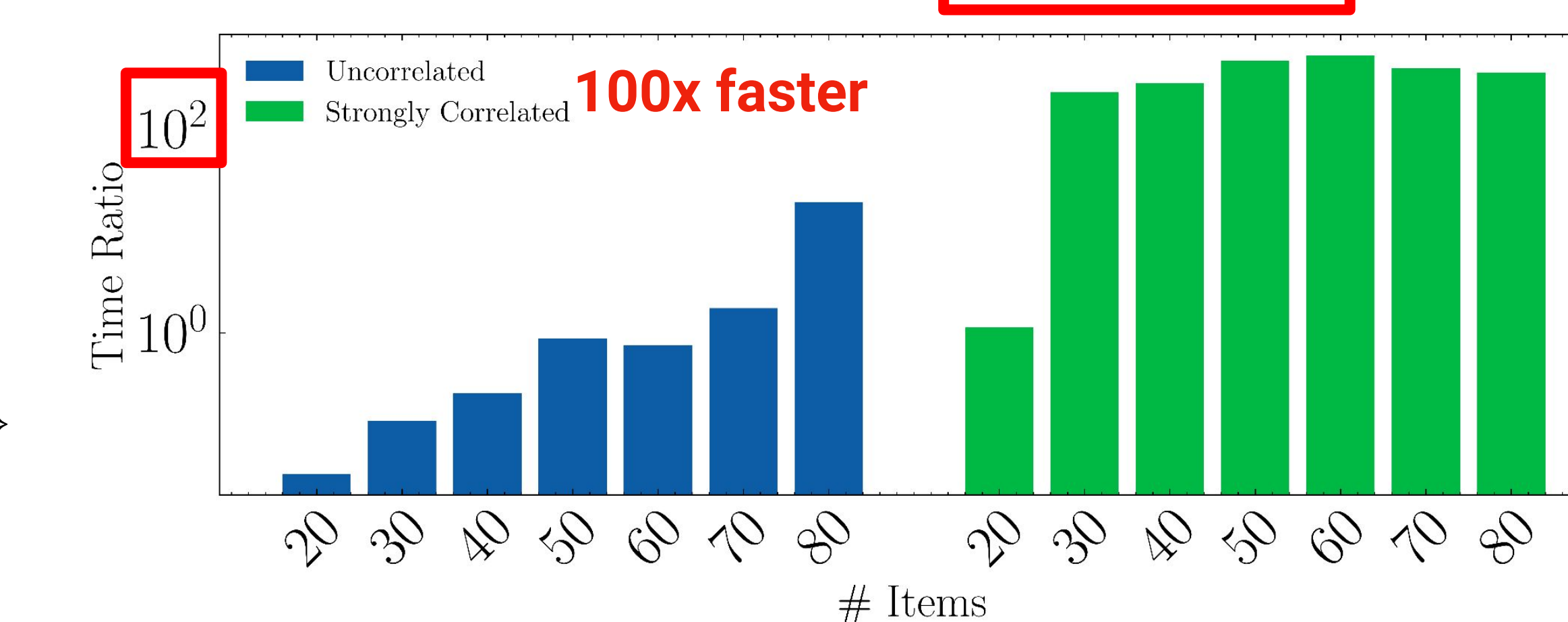


- ML finds OPT on most SSLP instances and best known solutions on most CFLP instances.

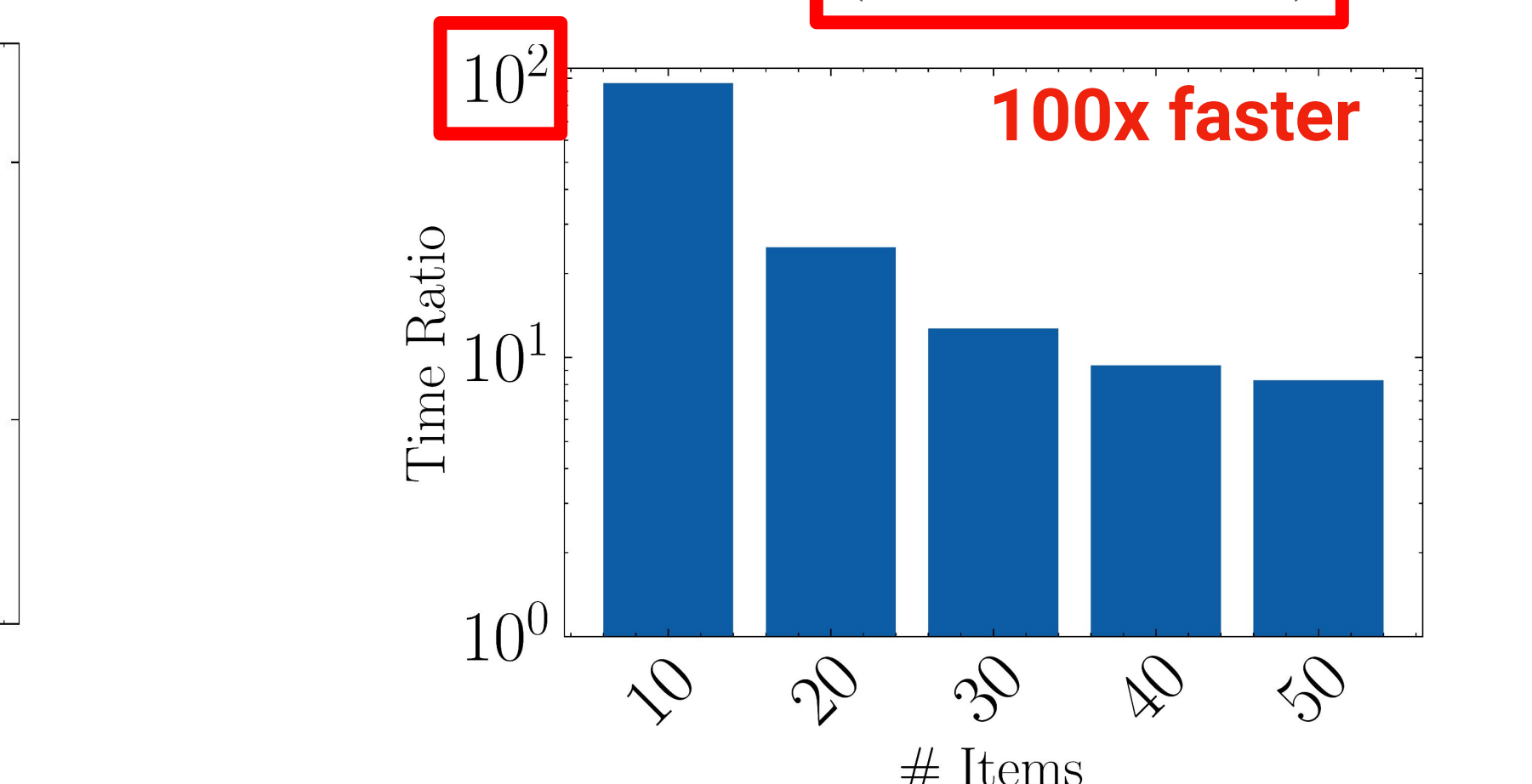
Robust Optimization

Reduction factor in solving time over baseline (branch-and-price/k-adaptability) (higher is better).

Robust Knapsack Problem (Gap: 1.30%)



Capital Budgeting (Gap: 0.33%)



- ML finds best solutions on difficult instances; near OPT on easy instances.

2SP

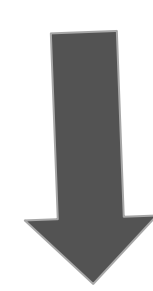


2RO

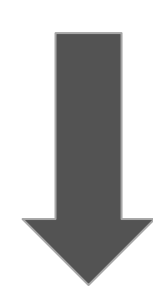


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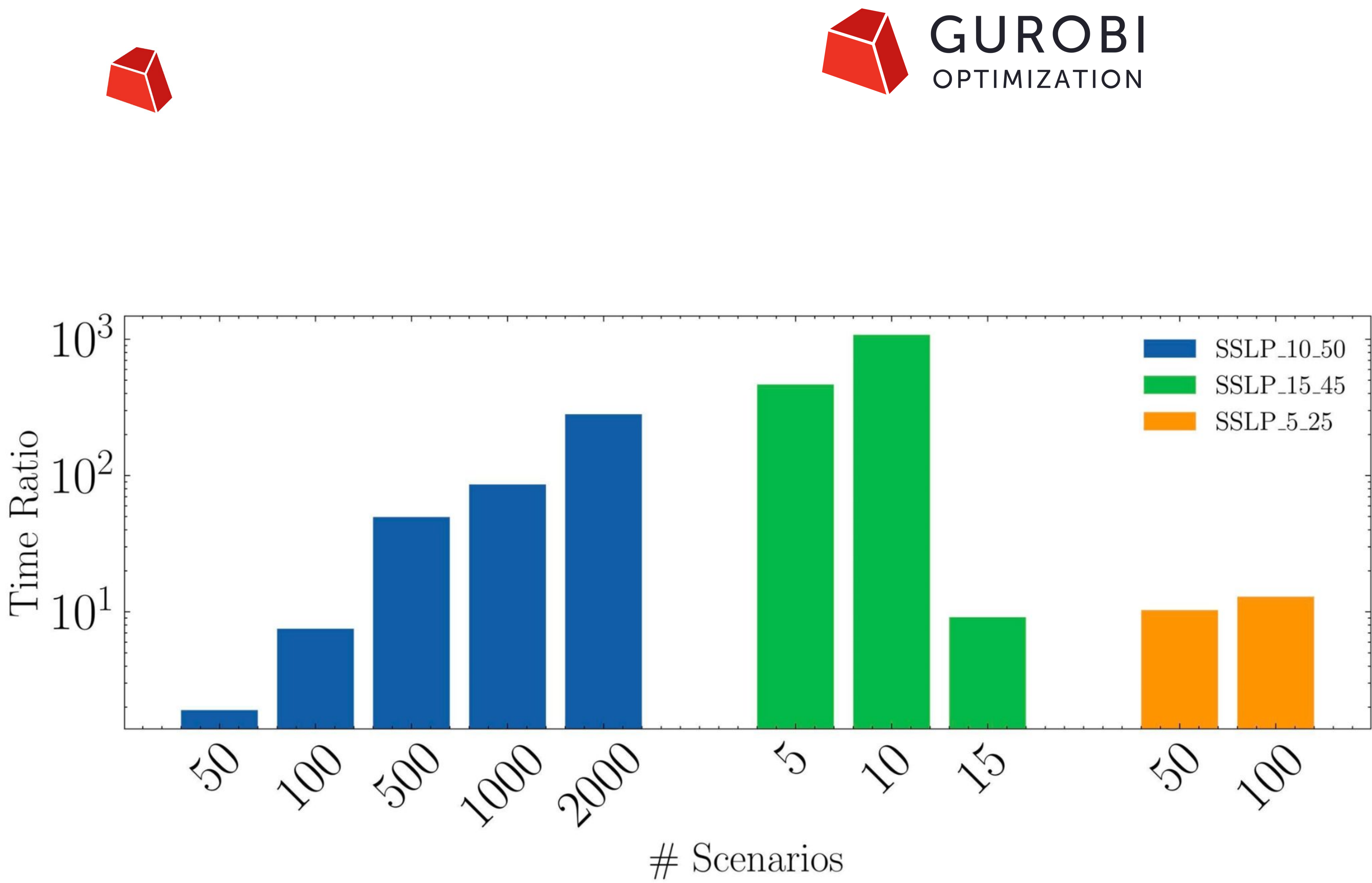
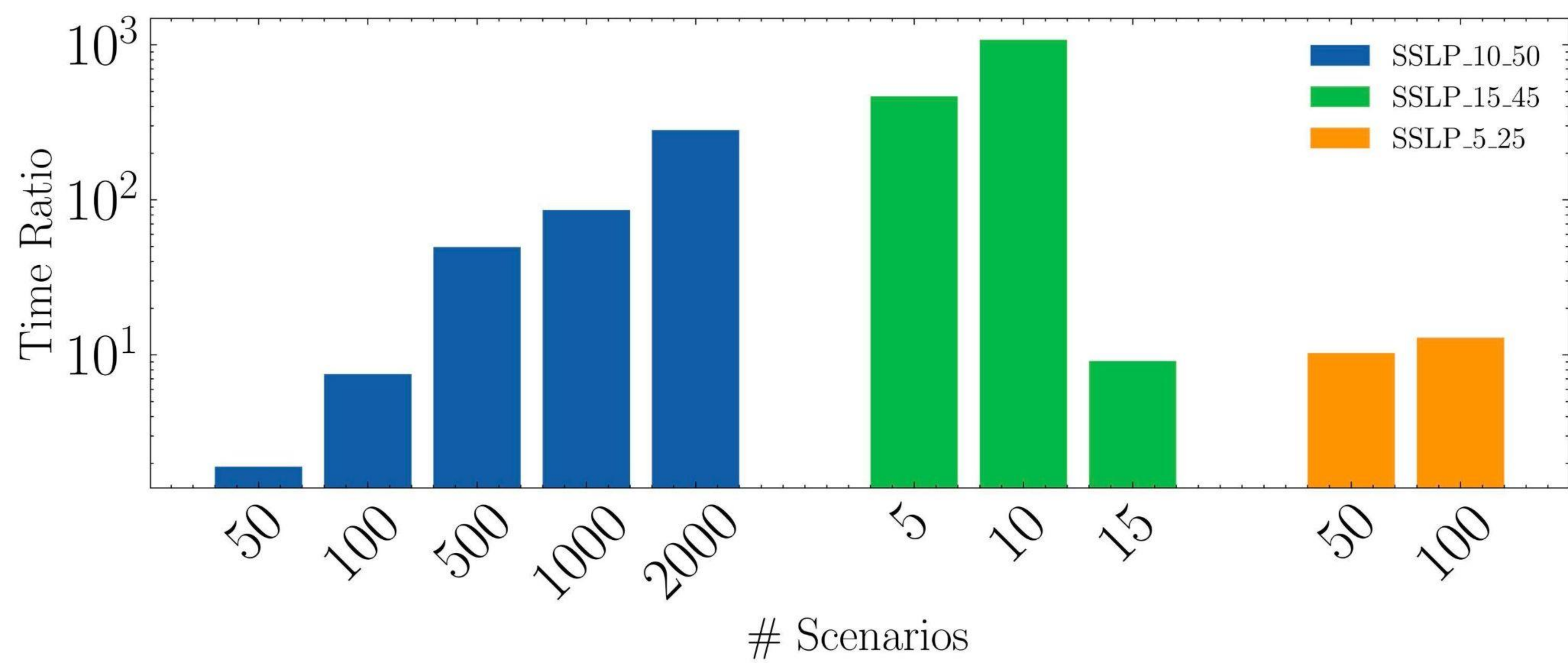
Data Collection:
1. Sample decision + uncertainty
2. Solve subproblems with off-the-shelf solvers



Supervised Learning:
Train an NN using off-the-shelf ML packages



Evaluation on new instances:
Solve the surrogate MILP with an off-the-shelf solver



(these can be presented visually using a flowchart and logos for Gurobi/PyTorch to make it more concrete)

1. Data collection using off-the-shelf solvers
2. Supervised training of NN using off-the-shelf ML packages
3. Given a new instance: solving the surrogate MILP with an off-the-shelf solver



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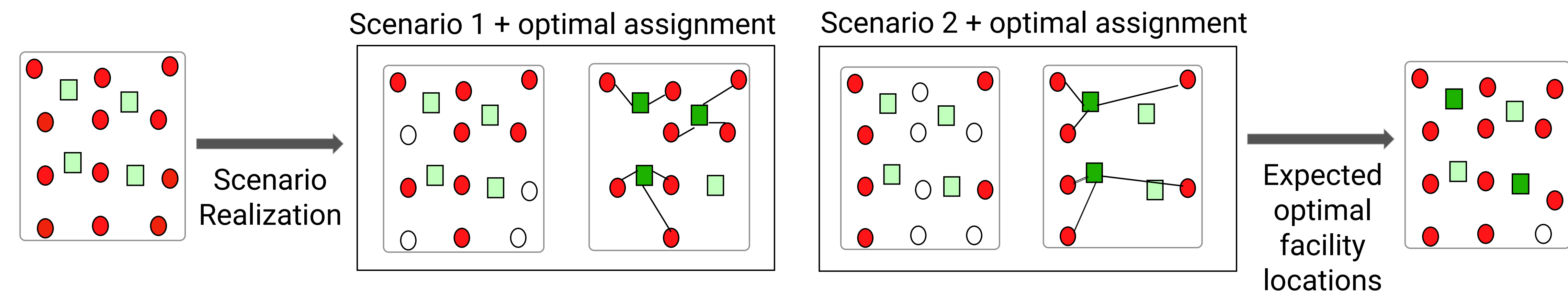
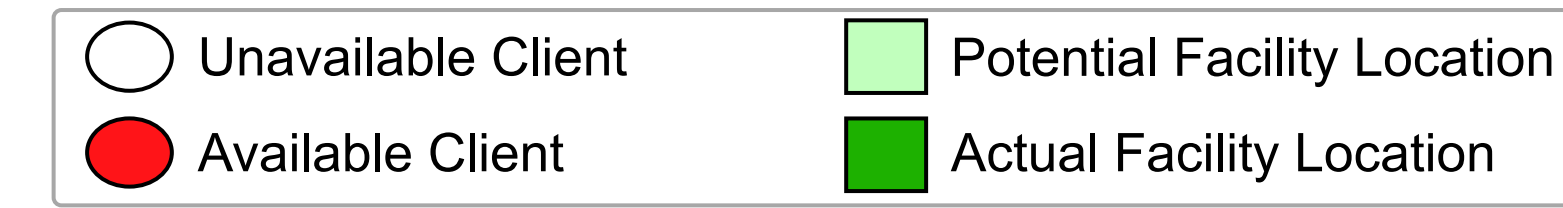
Learning for Two-Stage Stochastic Programming (2SP)

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Stochastic Facility Location Problem

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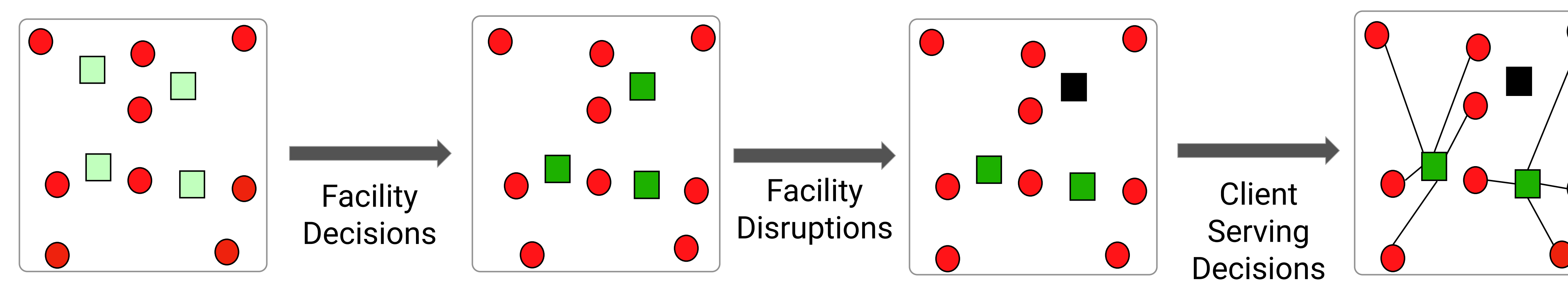
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Robust Facility Location Problem

Objective: Determine the optimal set of facilities to open under the worst-case facility disruption.



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First-Stage Problem

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Second-Stage Problem

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Second-stage cost (blue box), Second-stage decisions (green box)

Objective: Determine optimal **first-stage decisions** that minimize the sum of the **first-stage cost** and **worst-case cost**.

Challenge: Solving the nested optimization problem is intractable and specialized algorithms only exists for a limited classes of problems.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + Q(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \}$$

First-stage cost (blue box), First-stage decisions (green box), Worst-case cost (orange box)

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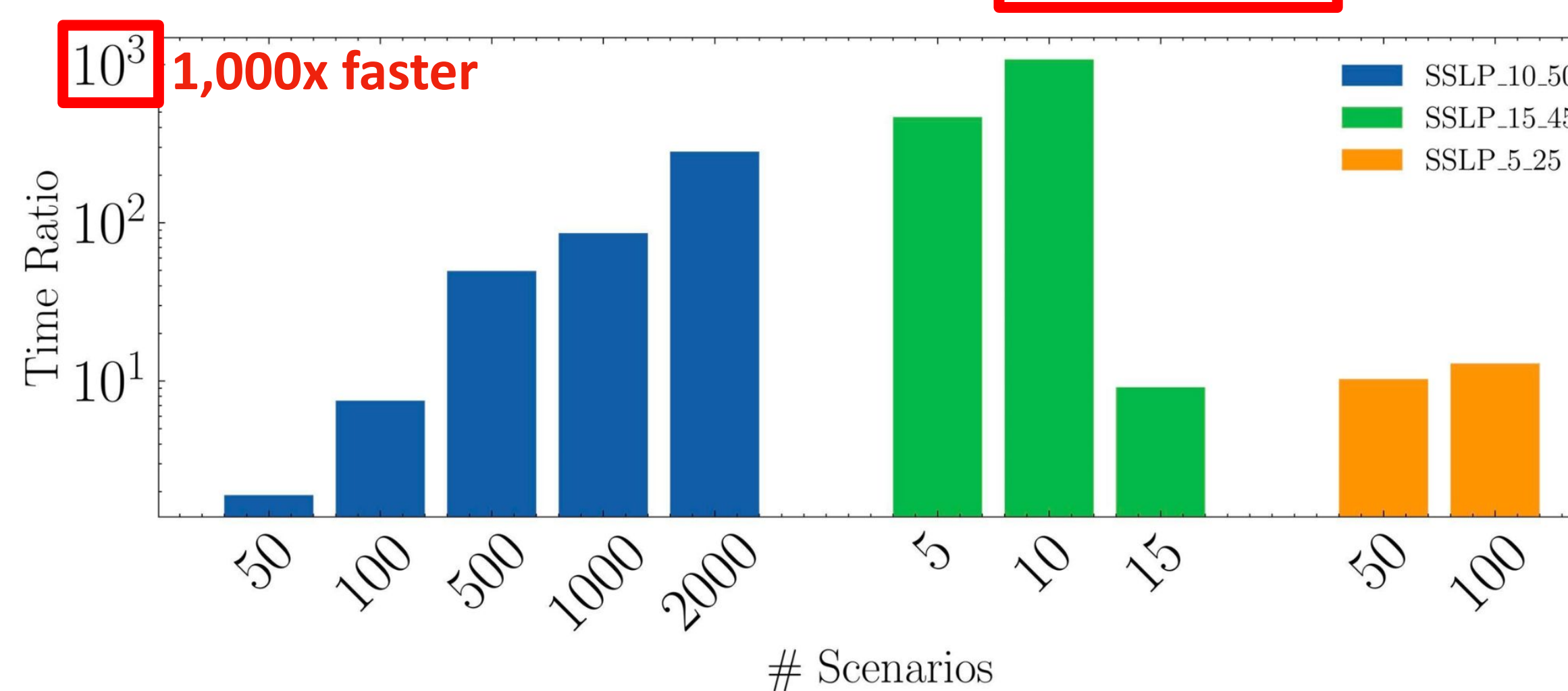
Worst-case uncertainty (orange box), Second-stage cost (blue box), Second-stage decisions (green box)

Experimental Results

Stochastic Programming

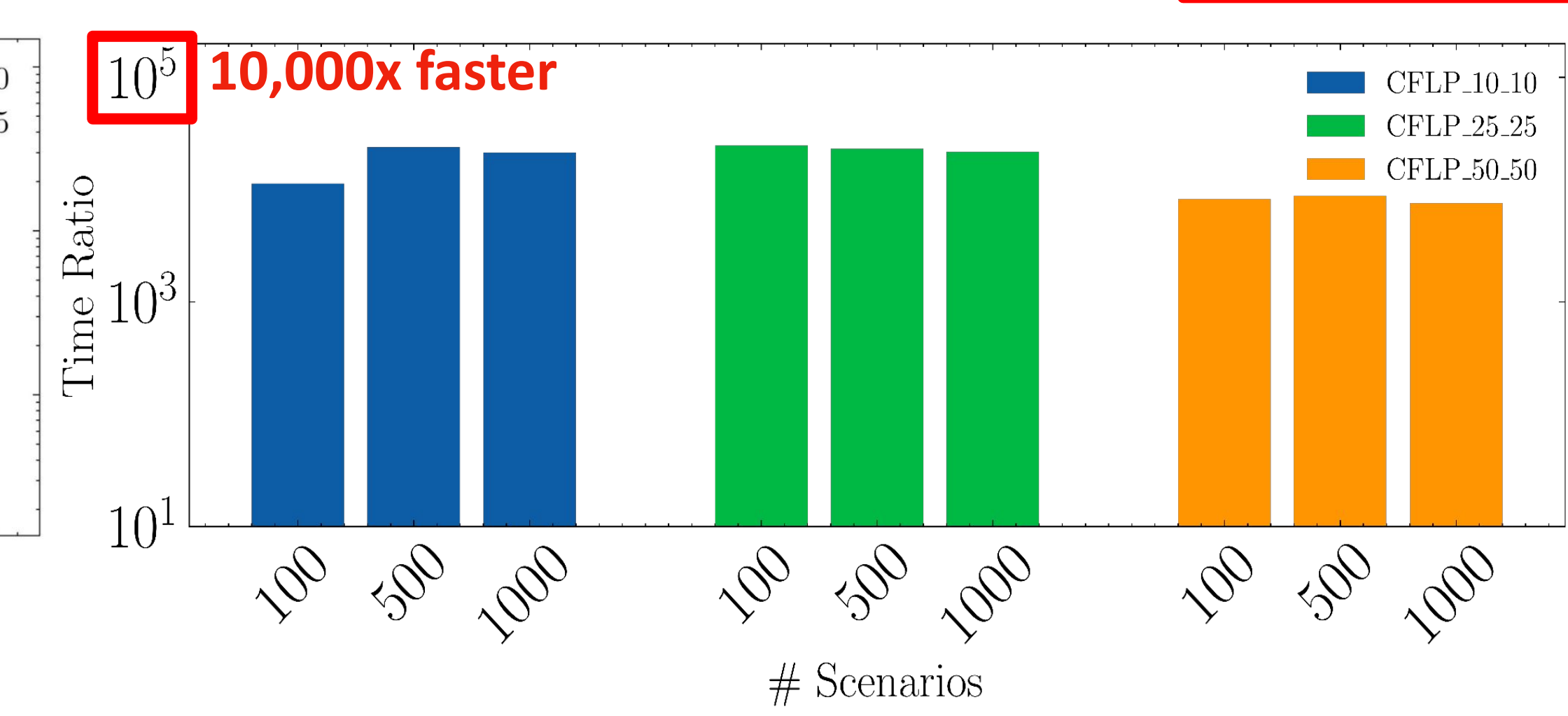
Reduction factor in computing time over baseline (Integer L-shaped/EF) (higher is better).

Stochastic Server Location Problem (Gap: 0.87%)



- ML finds OPT on most instances.

Capacitated Facility Location Problem (Gap: -2.93%)

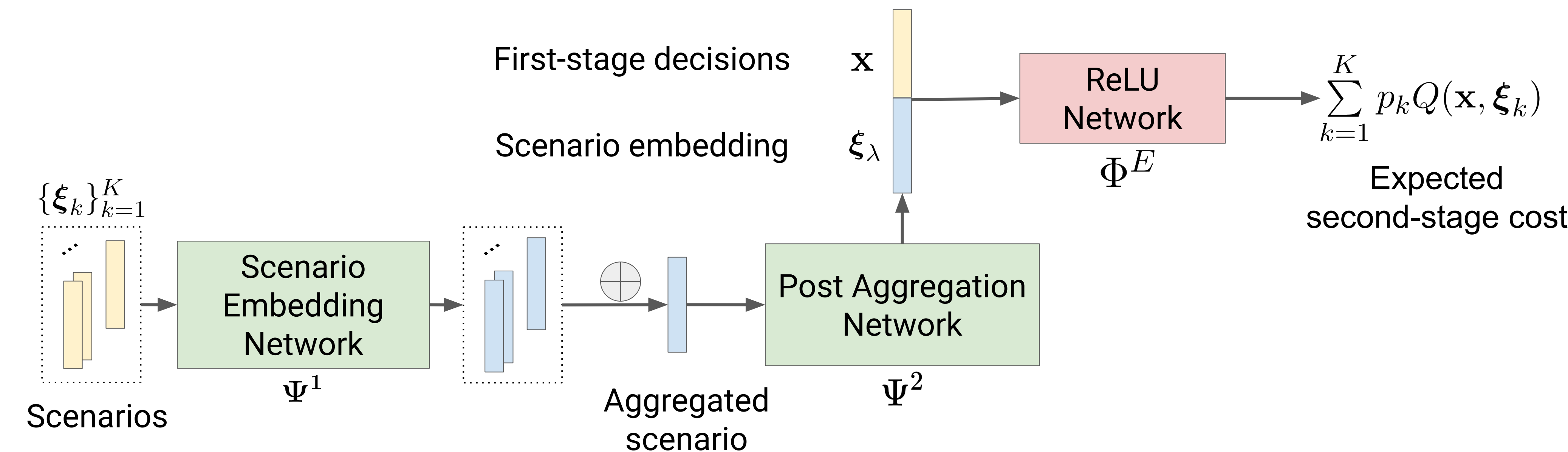


- ML finds best solutions on most instances.

Machine Learning Methodology

ML Solution: Replace the expected stage-cost value function with a neural network approximation.

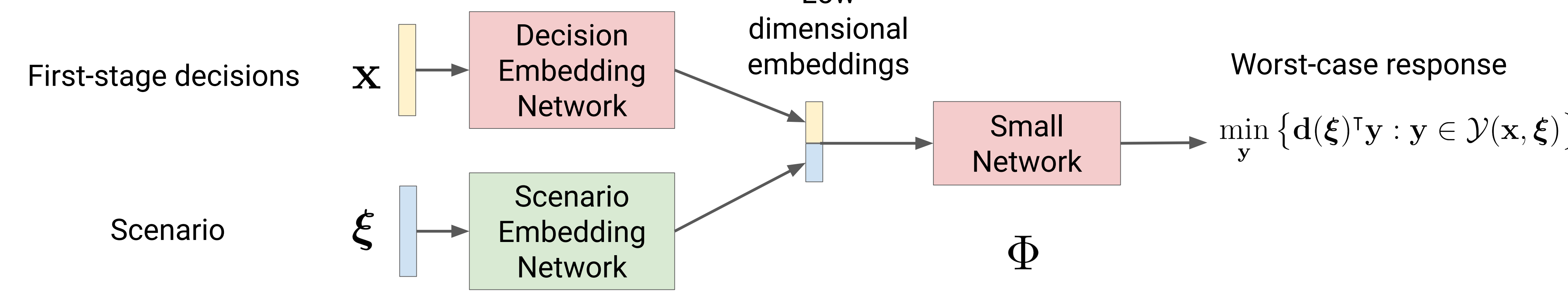
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Surrogate Optimization Model: $\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \text{NN}(\mathbf{x}, \{\xi_k\}_{k=1}^K) : \mathbf{x} \in \mathcal{X} \}$

ML Solution: Replace the worst-case response optimization problem with a neural network approximation.

Neural Network Architecture:



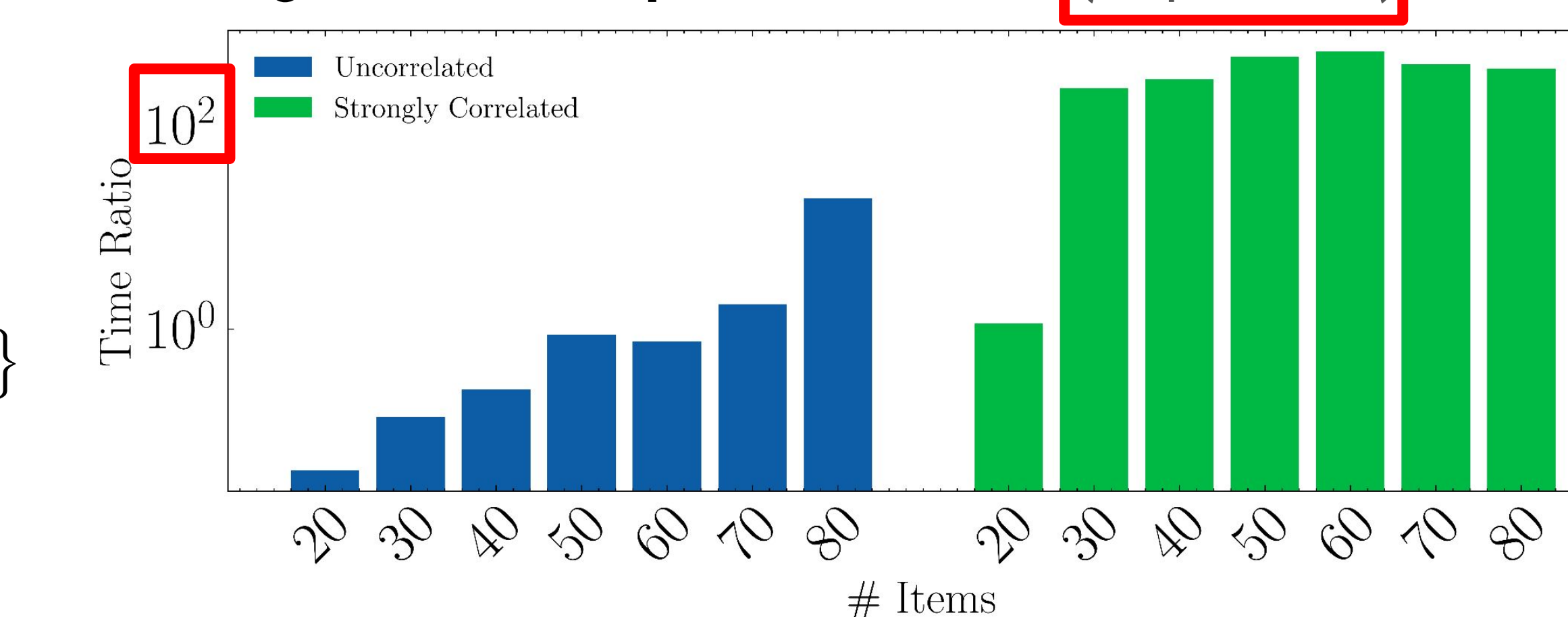
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Robust Optimization

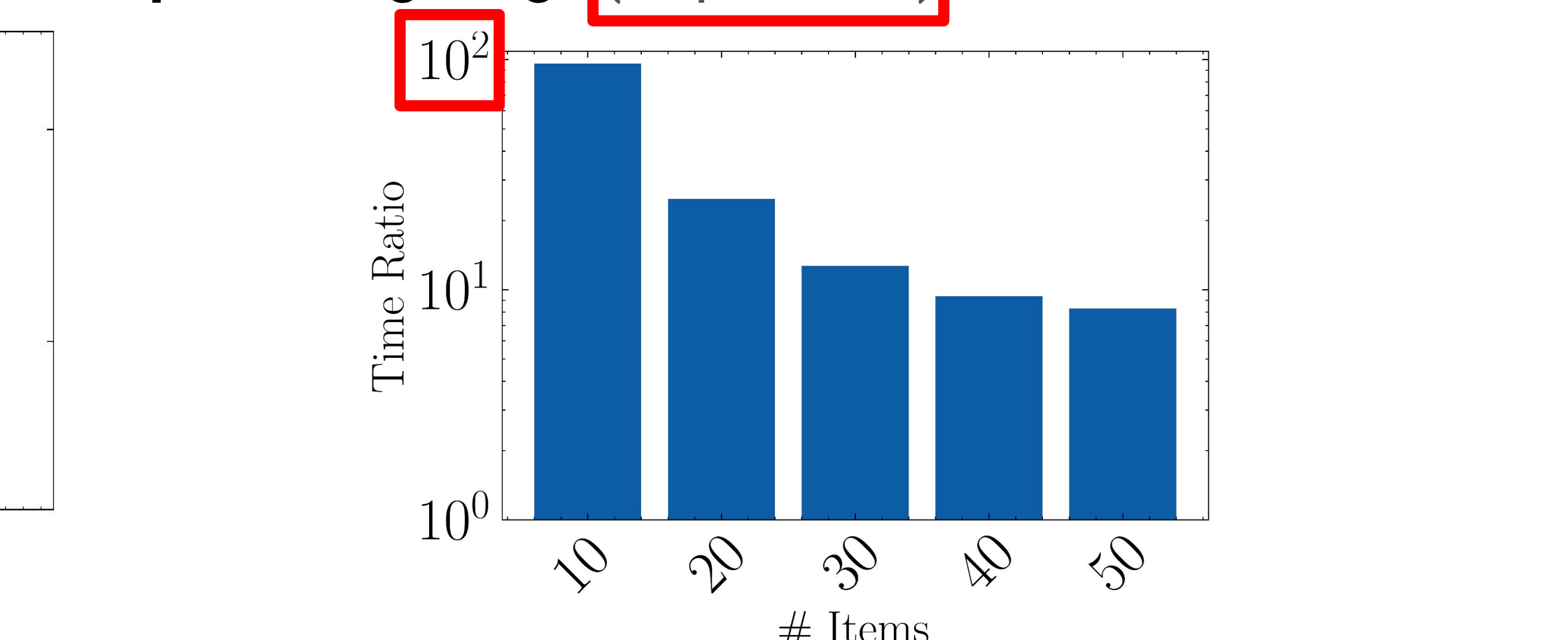
Reduction factor in computing time over baseline (branch-and-price/k-adaptability) (higher is better).

Two-Stage Robust Knapsack Problem (Gap: 1.30%)



- ML finds best solutions on difficult instances; near optimal on easy instances.
- Time reductions on the order of 10-100x the state-of-the-art baselines.

Capital Budgeting (Gap: 0.33%)



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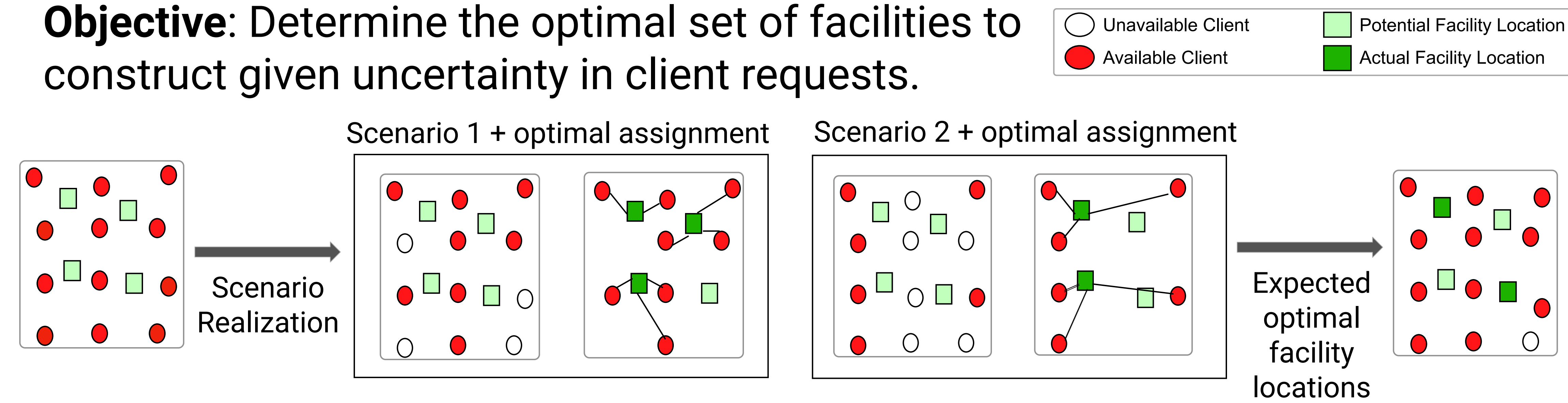
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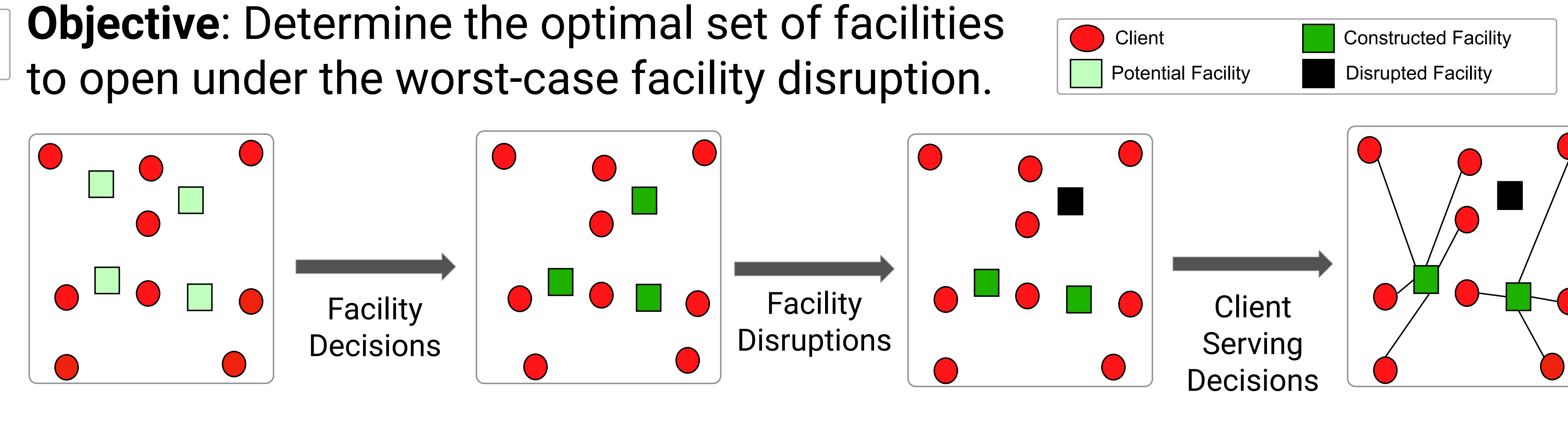


Learning for Adjustable Robust Optimization (2RO)

Under review

Robust Facility Location Problem

Objective: Determine the optimal set of facilities to open under the worst-case facility disruption.



Overall framework

Data Collection

- Sample decisions + uncertainty.
- Solve subproblems with off-the-shelf solvers.

Evaluation on new instances

- Solve the surrogate MILP with an off-the-shelf solver.

Supervised Learning

- Train an NN using off-the-shelf ML packages.

PyTorch

Optimization Formulation

Objective: Determine optimal **first-stage decisions** that minimize sum of the **first-stage cost** and **expected second-stage cost**.

Challenge: Exact optimization becomes exponentially harder with the number of observed scenarios, K . Integer decision further aggravates intractability.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \sum_{k=1}^K p_k Q(\mathbf{x}, \xi_k) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions
 Expected second-stage cost

Second-Stage Problem

$$Q(\mathbf{x}, \xi) := \min_{\mathbf{y}} \{ F(\mathbf{y}, \xi) : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \}$$

Second-stage decisions

Objective: Determine optimal **first-stage decisions** that minimize the sum of the **first-stage cost** and **worst-case cost**.

Challenge: Solving the nested optimization problem is intractable and specialized algorithms only exists for a limited classes of problems.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + Q(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions
 Worst-case cost

Second-Stage Problem

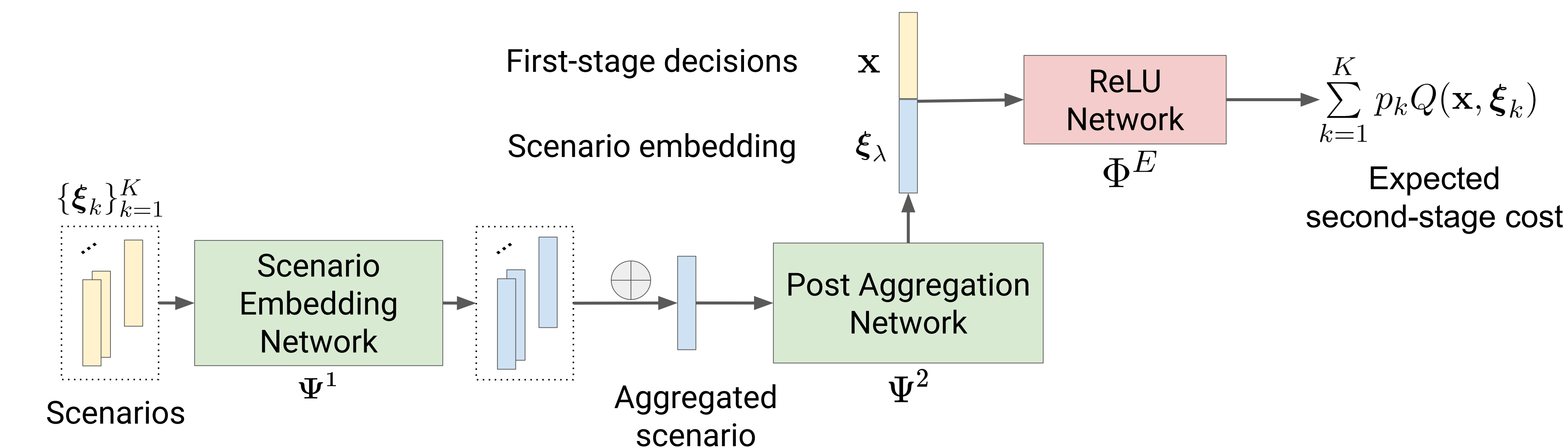
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Worst-case uncertainty
 Second-stage decisions

Machine Learning Methodology

ML Solution: Replace the expected stage-cost value function with a neural network approximation.

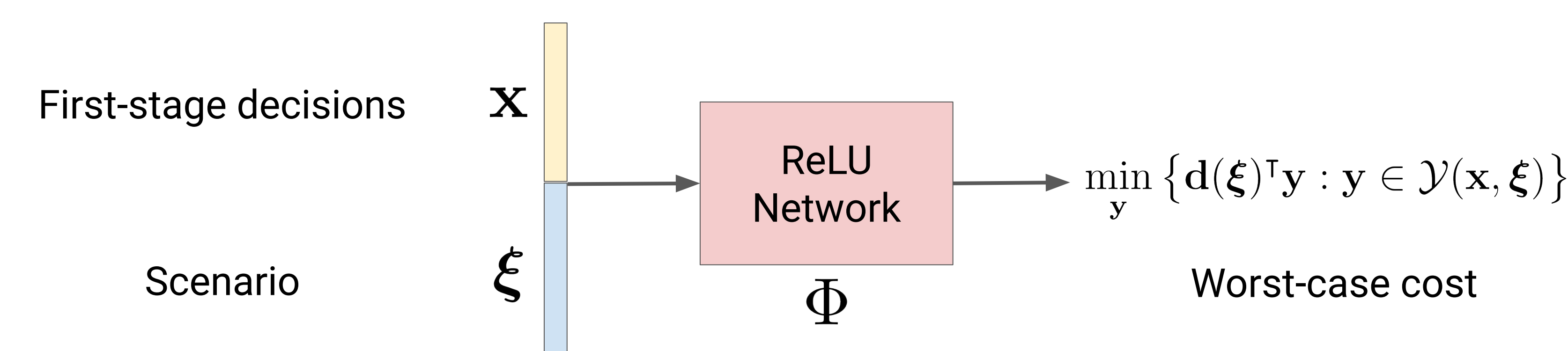
Neural Network Architecture:



Surrogate Optimization Model: $\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \text{NN}(\mathbf{x}, \{\xi_k\}_{k=1}^K) : \mathbf{x} \in \mathcal{X} \}$

ML Solution: Replace the worst-case cost with a neural network approximation.

Neural Network Architecture:



Surrogate Optimization Model: $\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \eta : \mathbf{x} \in \mathcal{X}, \eta \geq \text{NN}(\mathbf{x}, \xi), \forall \xi \in \Xi \}$

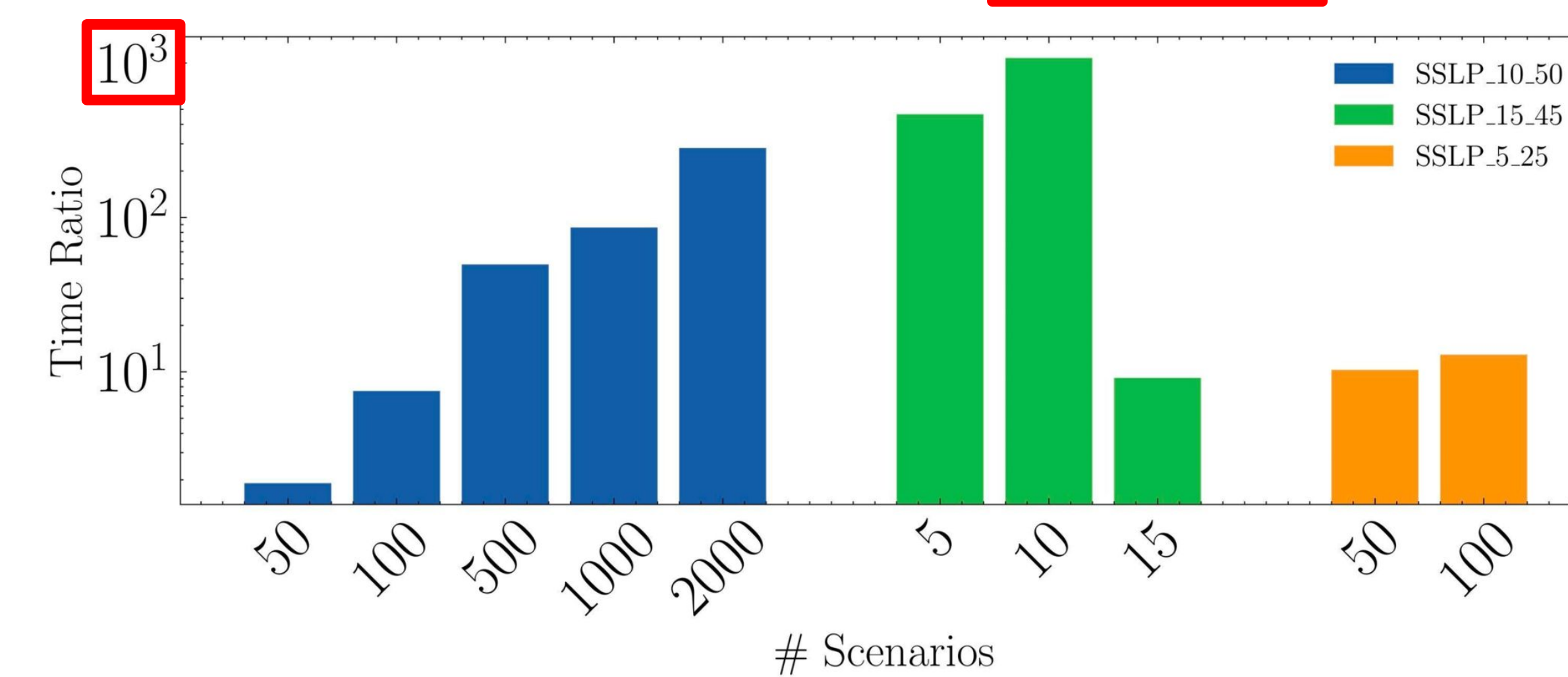
- Optimization problem solved with row generation.
- Worst-case scenarios determined by sampling or adversarial problem.

Experimental Results

Stochastic Programming

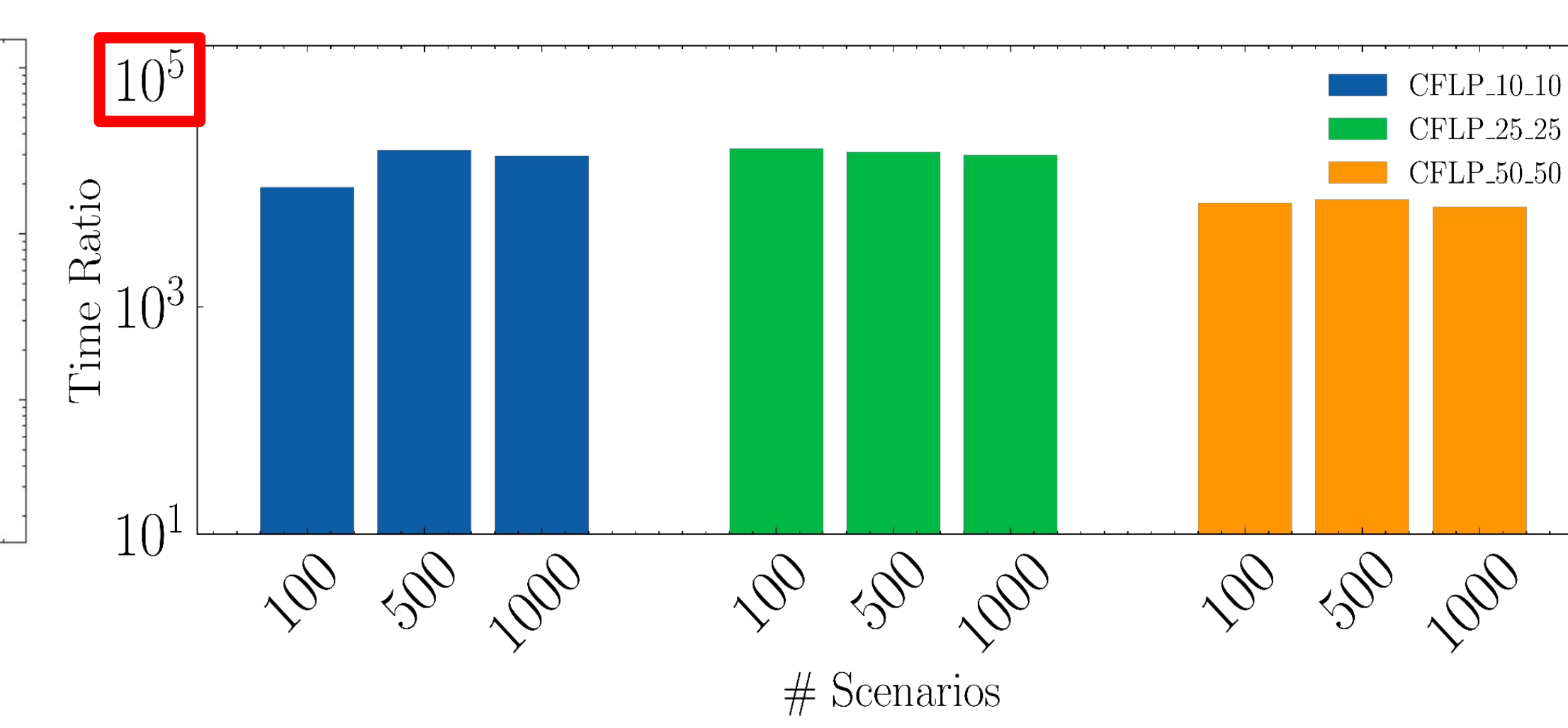
Reduction factor in computing time over baseline (Integer L-shaped/EF) (higher is better).

Stochastic Server Location Problem (Gap: 0.87%)



- NN is up to 1,000x faster than baseline.
- Approximation finds optimal solutions on most instances.

Capacitated Facility Location Problem (Gap: -2.93%)

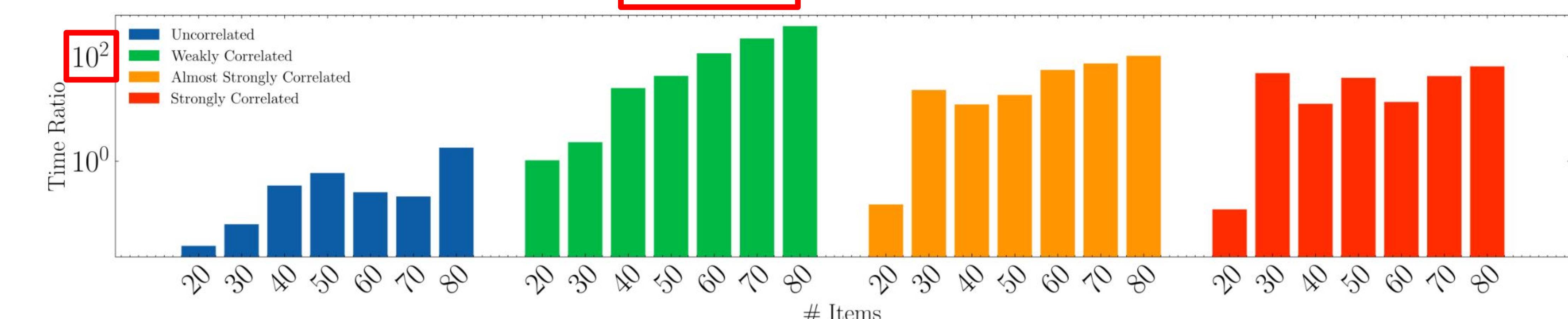


- NN is up to 10,000x faster than baseline.
- Approximation finds better solutions than baseline.

Robust Optimization

Reduction factor in computing time over problem specific decomposition (higher is better).

Adjustable Robust Knapsack Problem (Gap: 5.39%)



- Time ratio and relative solution quality improve as problem sizes increase or correlation increases difficult of problem.

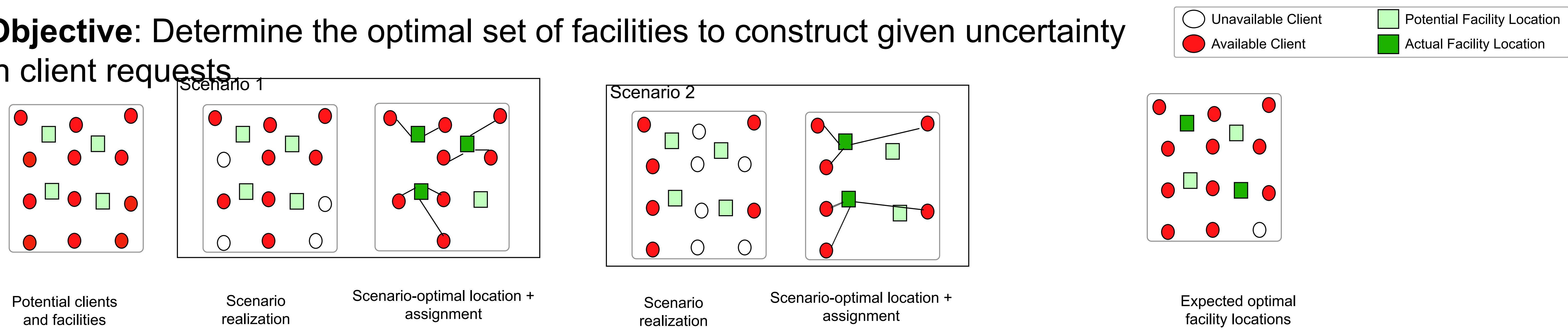


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Learning for Two-Stage Stochastic Programming (2SP)

Stochastic Facility Location Problem

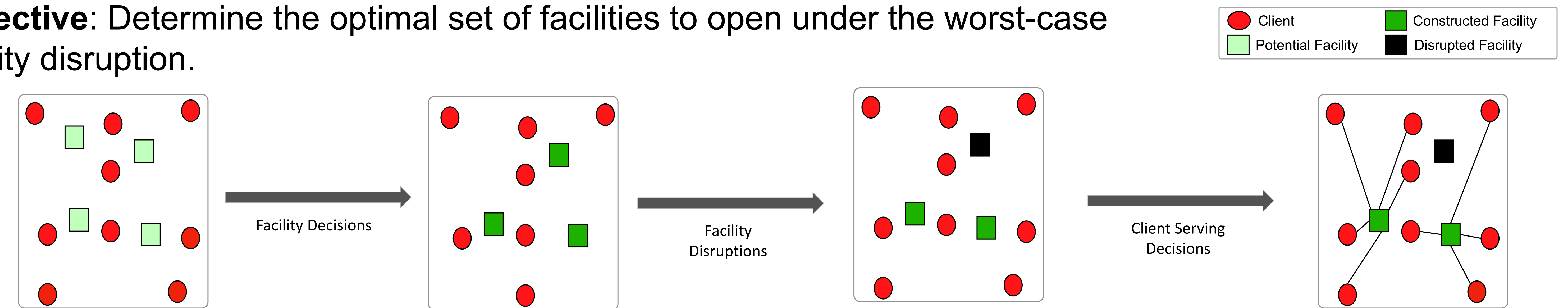
Objective: Determine the optimal set of facilities to construct given uncertainty in client requests.



Learning for Adjustable Robust Optimization (ARO)

Robust Facility Location Problem

Objective: Determine the optimal set of facilities to open under the worst-case facility disruption.



Formulation

Objective: Determine optimal **first-stage decisions** that minimize sum of **first-stage cost** and **expected second-stage cost**.

Challenge: Exact optimization becomes exponentially harder with the number of observed scenarios, K . Integer decision further aggravates intractability.

First-Stage Problem

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First-stage cost
Expected second-stage cost
First-stage decisions

Second-Stage Problem

$$Q(\mathbf{x}, \xi) := \min_{\mathbf{y}} \left\{ F(\mathbf{y}, \xi) : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \right\}$$

Second-stage cost
Second-stage decisions

Objective: Determine optimal **first-stage decisions** that minimize sum of **first-stage cost** and **worst-case scenario**.

Challenge: Exact optimization becomes exponentially harder with the number of observed scenarios, K . Integer decision further aggravates intractability.

First-Stage Problem

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First-stage cost
Worst-case cost
First-stage decisions

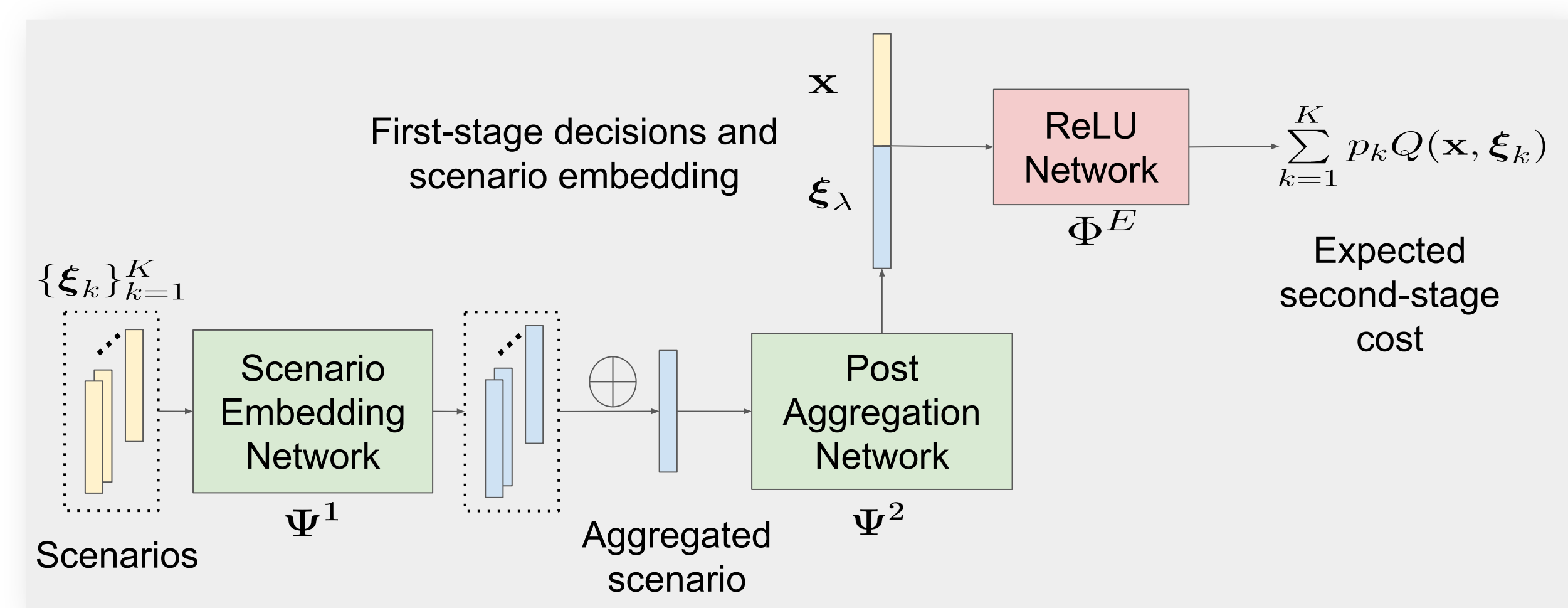
Second-Stage Problem

$$Q(\mathbf{x}) := \max_{\xi \in \Xi} \min_{\mathbf{y}} \left\{ \mathbf{d}(\xi)^T \mathbf{y} : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \right\}$$

Second-stage cost
Second-stage decisions

Methodology

Learning Model

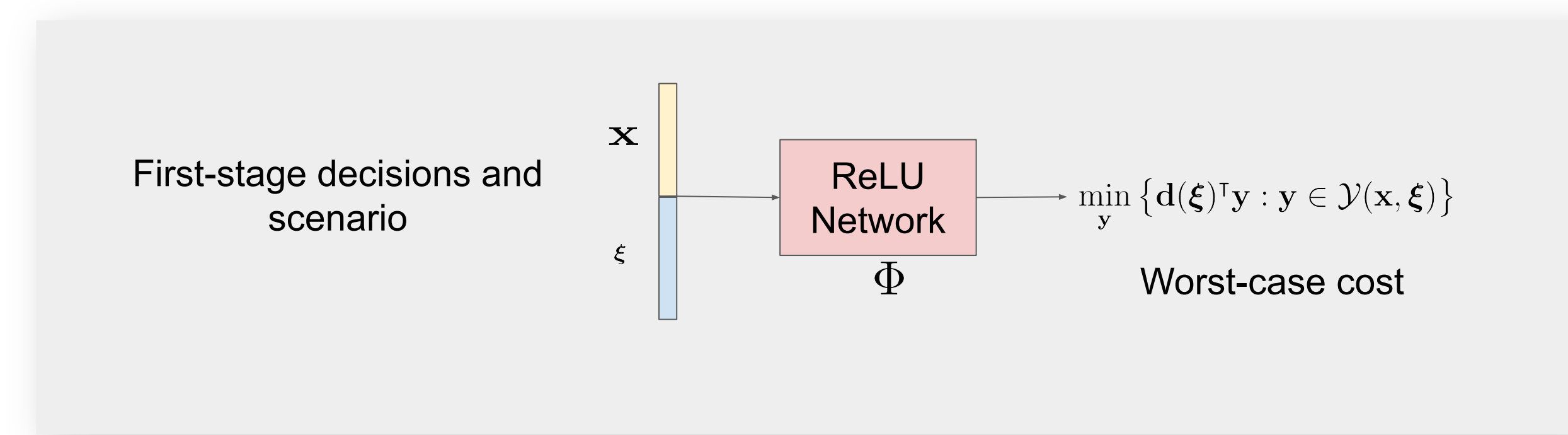


Surrogate Optimization Model

$$\min_{\mathbf{x}} \left\{ \mathbf{c}^T \mathbf{x} + \text{NN}(\mathbf{x}, \{\xi_k\}_{k=1}^K) : \mathbf{x} \in \mathcal{X} \right\}$$

Add details about how optimization problem is solved and pros/cons

Learning Model



Surrogate Optimization Model

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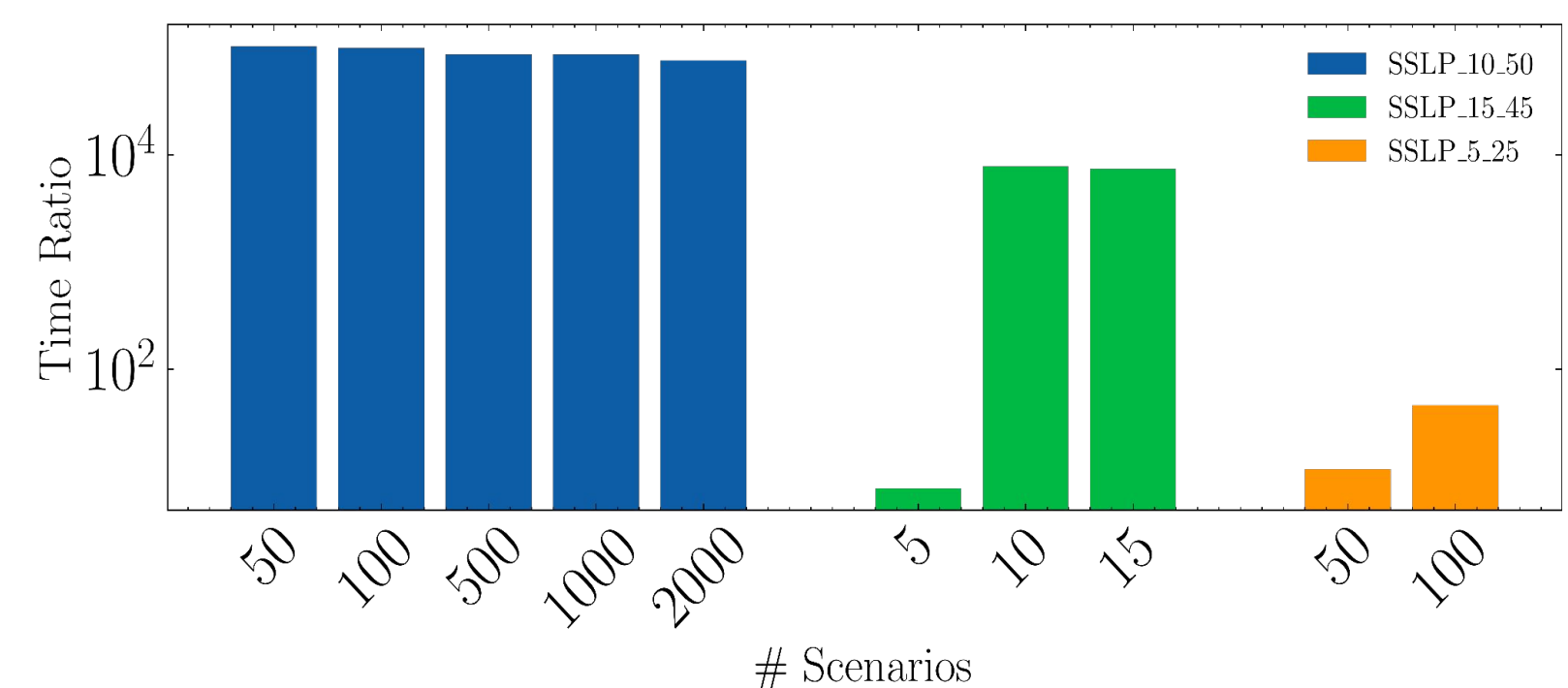
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Experimental Results

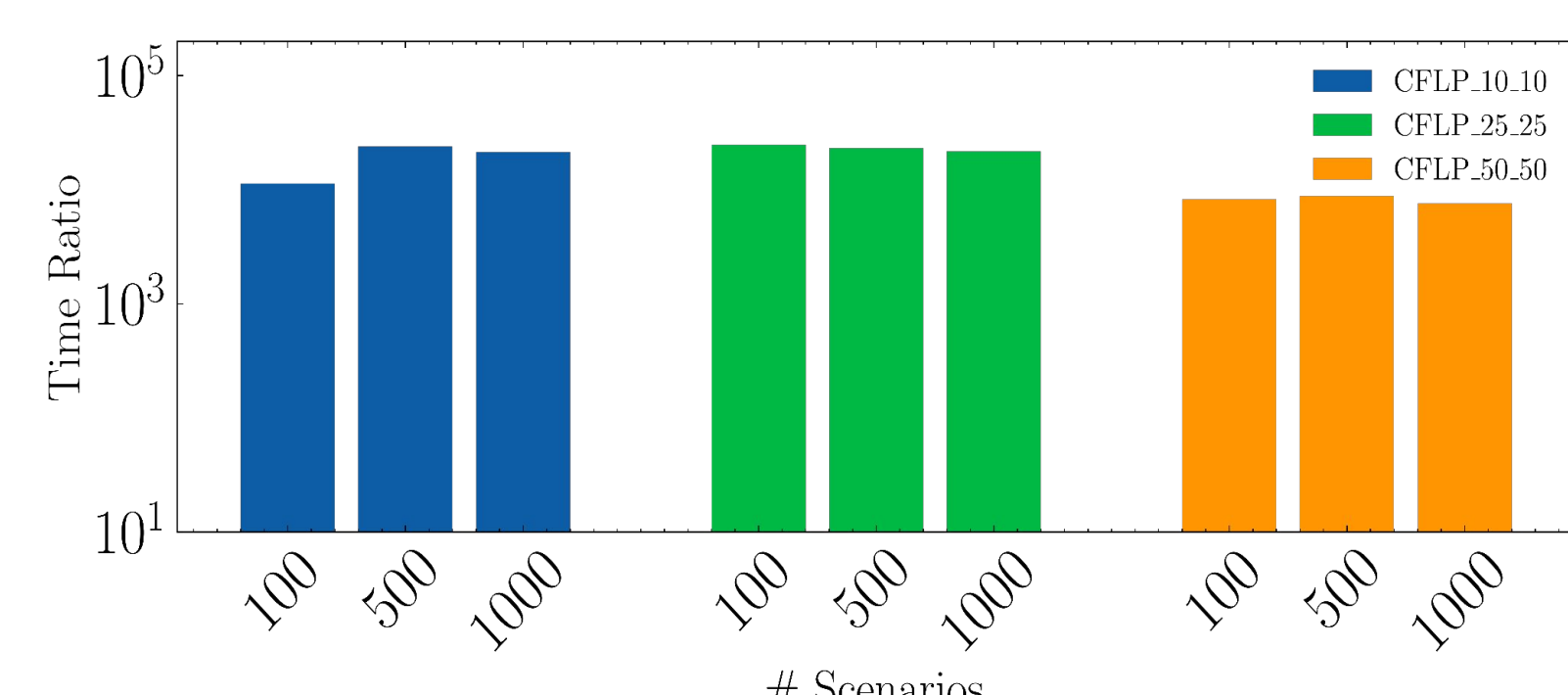
Gap: Mean % difference in solution quality relative to baseline (lower is better).

Bars: Reduction in computing time over baseline (higher is better).

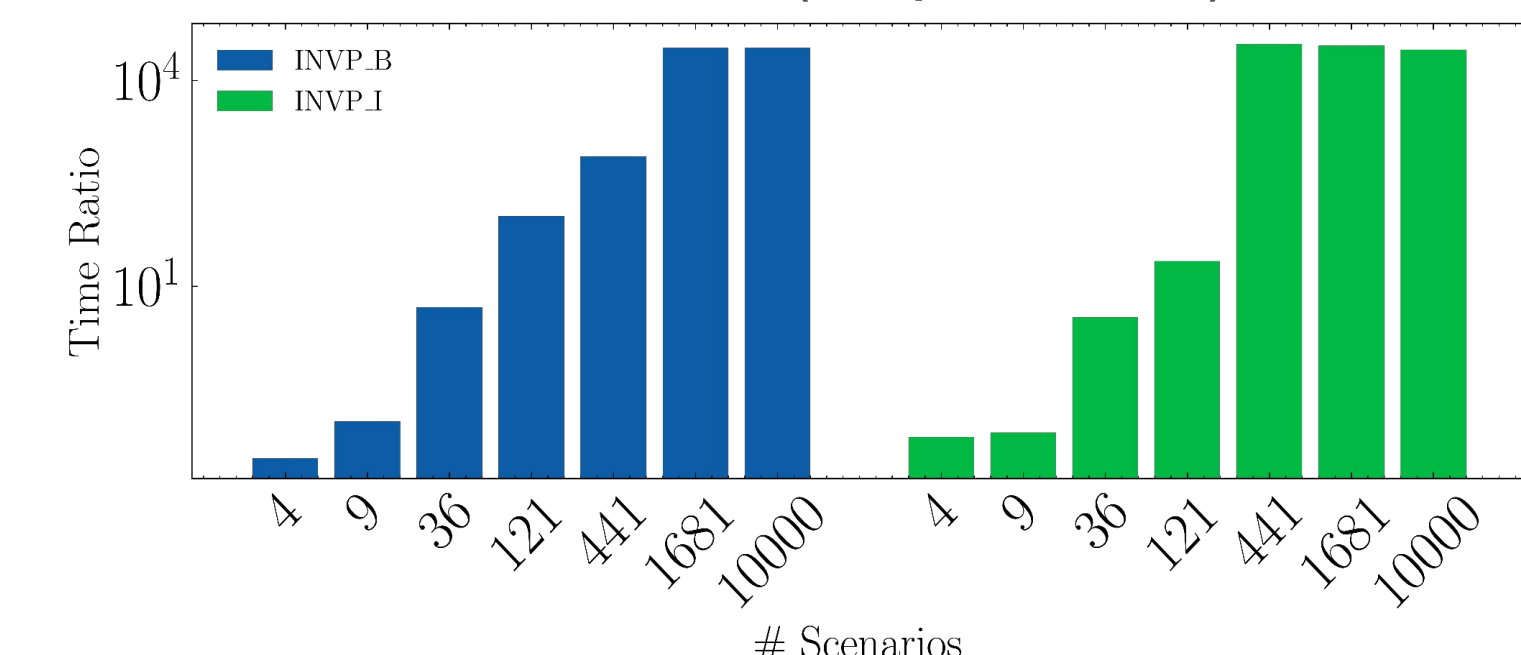
Stochastic Server Location Problem (Gap: -14.91%)



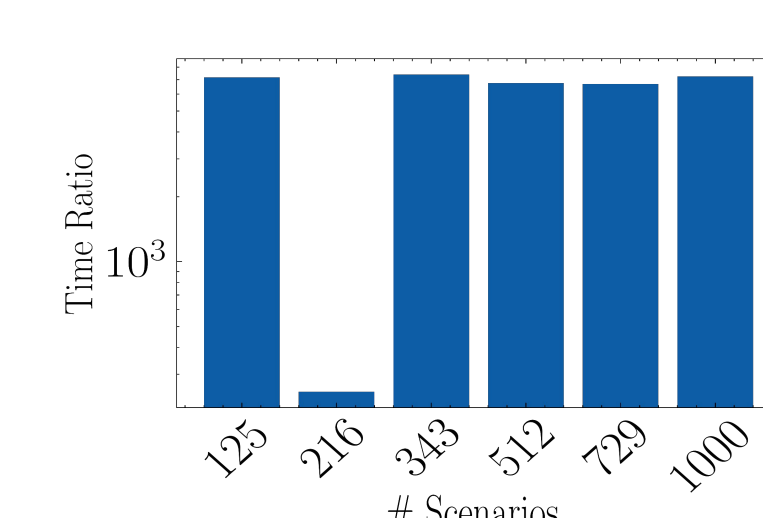
Capacitated Facility Location Problem (Gap: -2.93%)



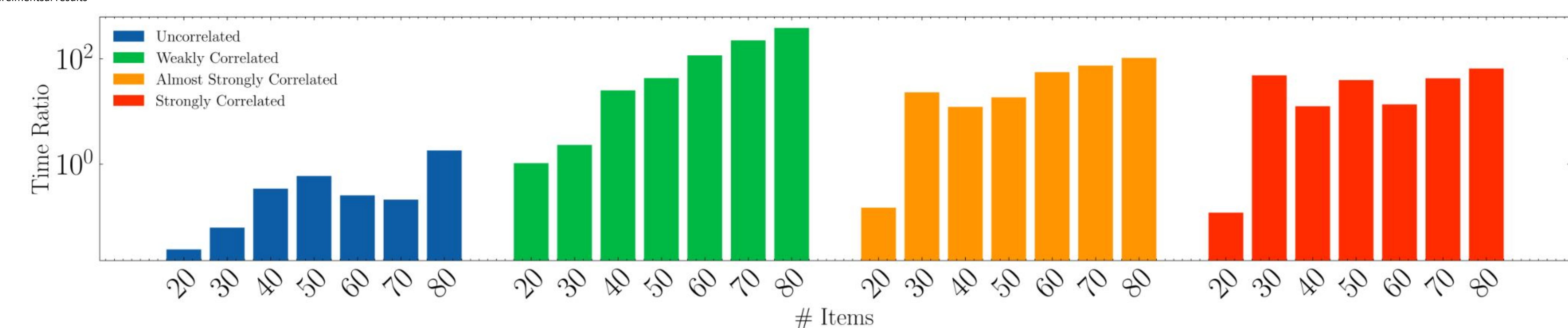
Investment Problem (Gap: 3.82%)



Pooling Problem (Gap: 4.82%)

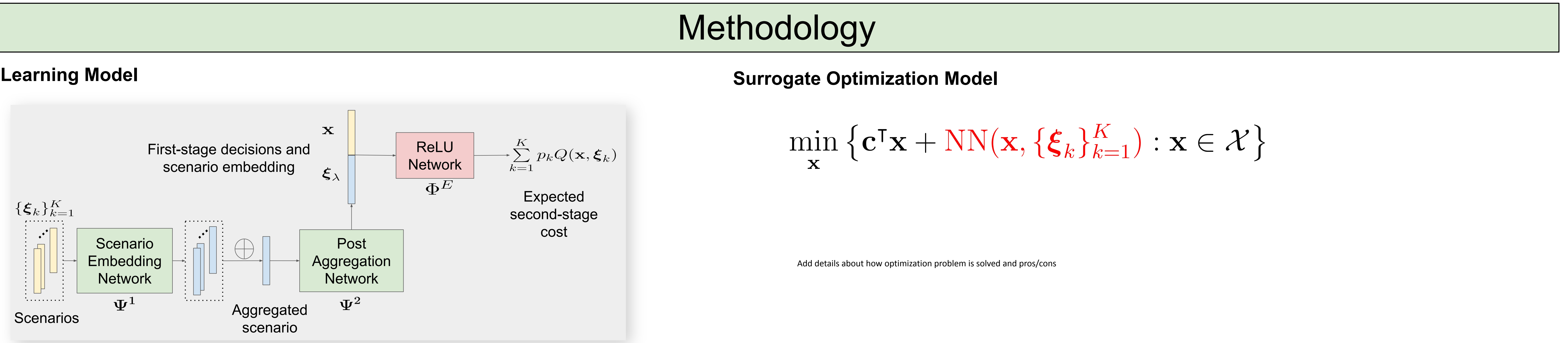
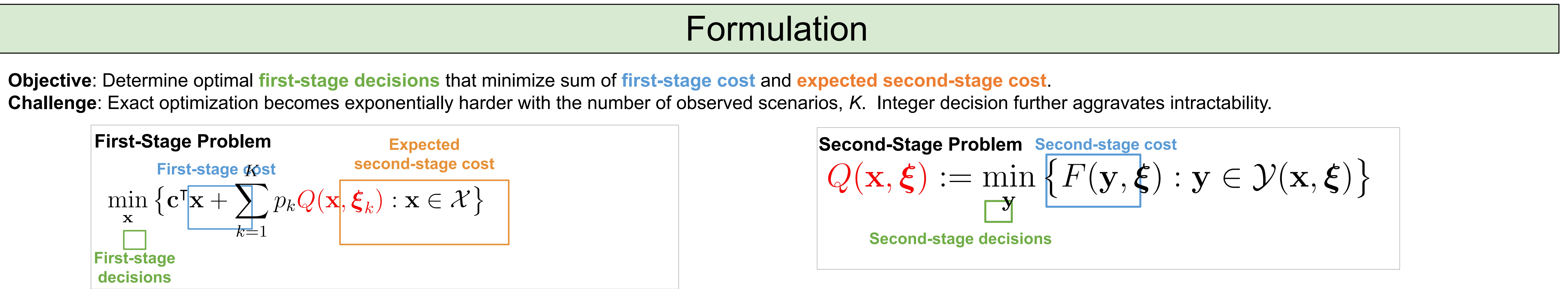
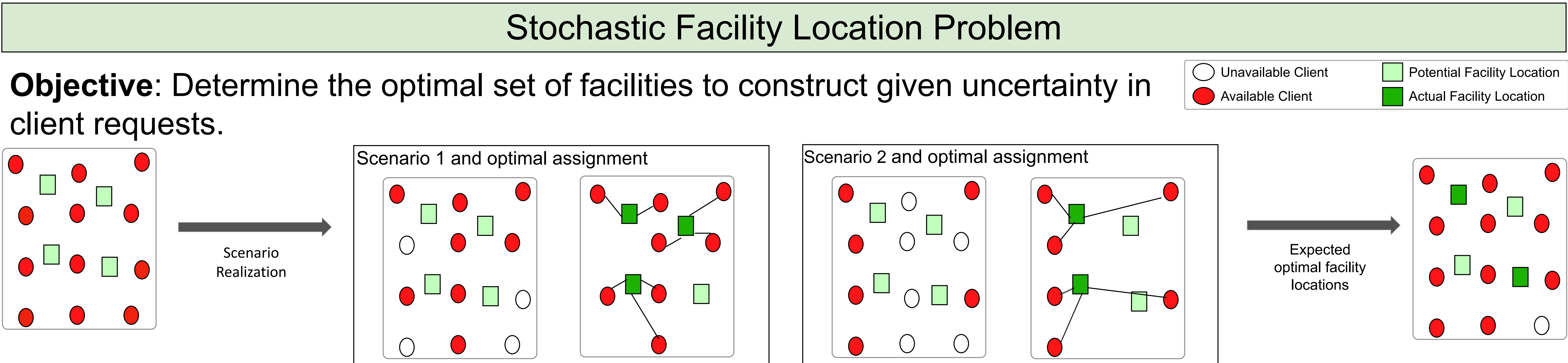


Add experimental results



Average Optimality Gaps:
Uncorrelated: 3.96%
Weakly Correlated: 7.25%
Almost Strongly Correlated: 5.63%
Strongly Correlated: 4.69%

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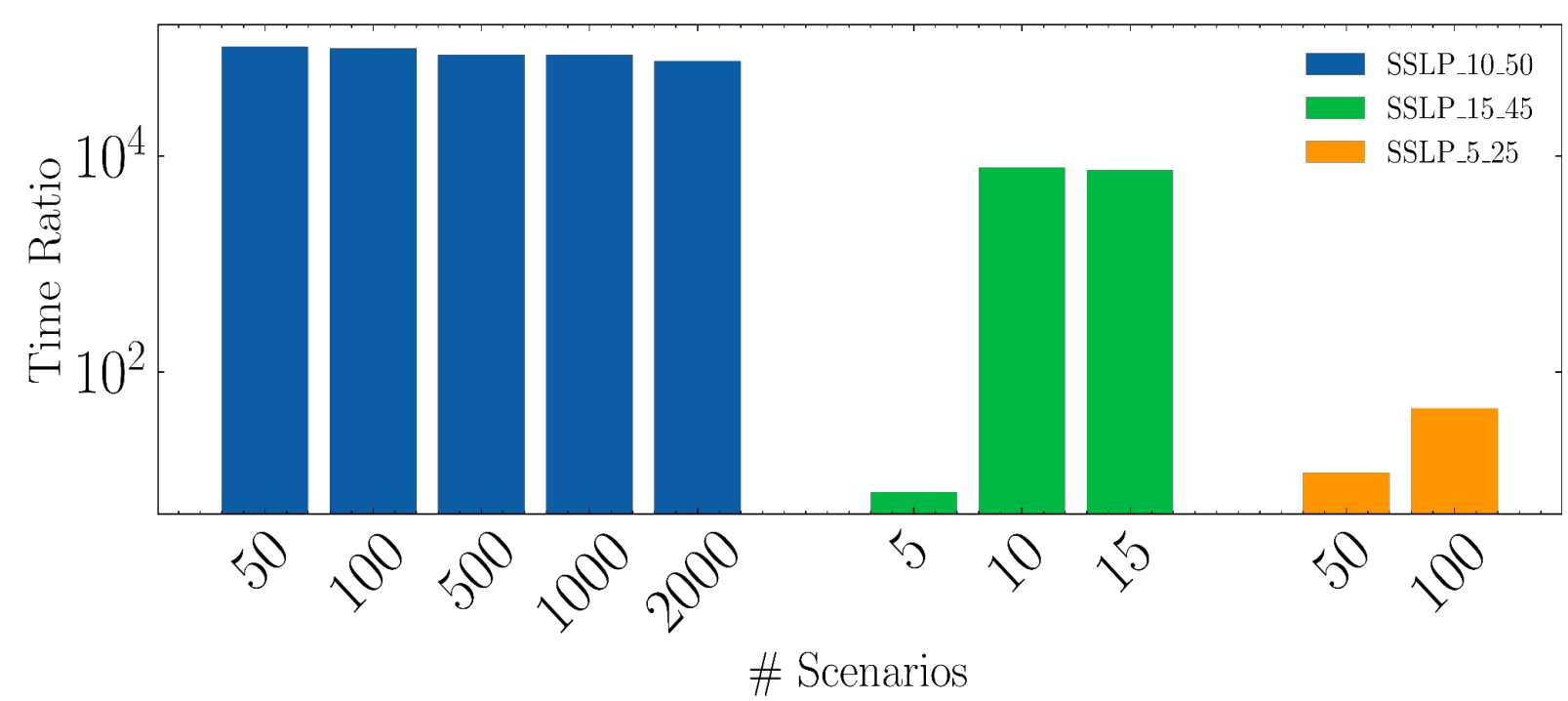


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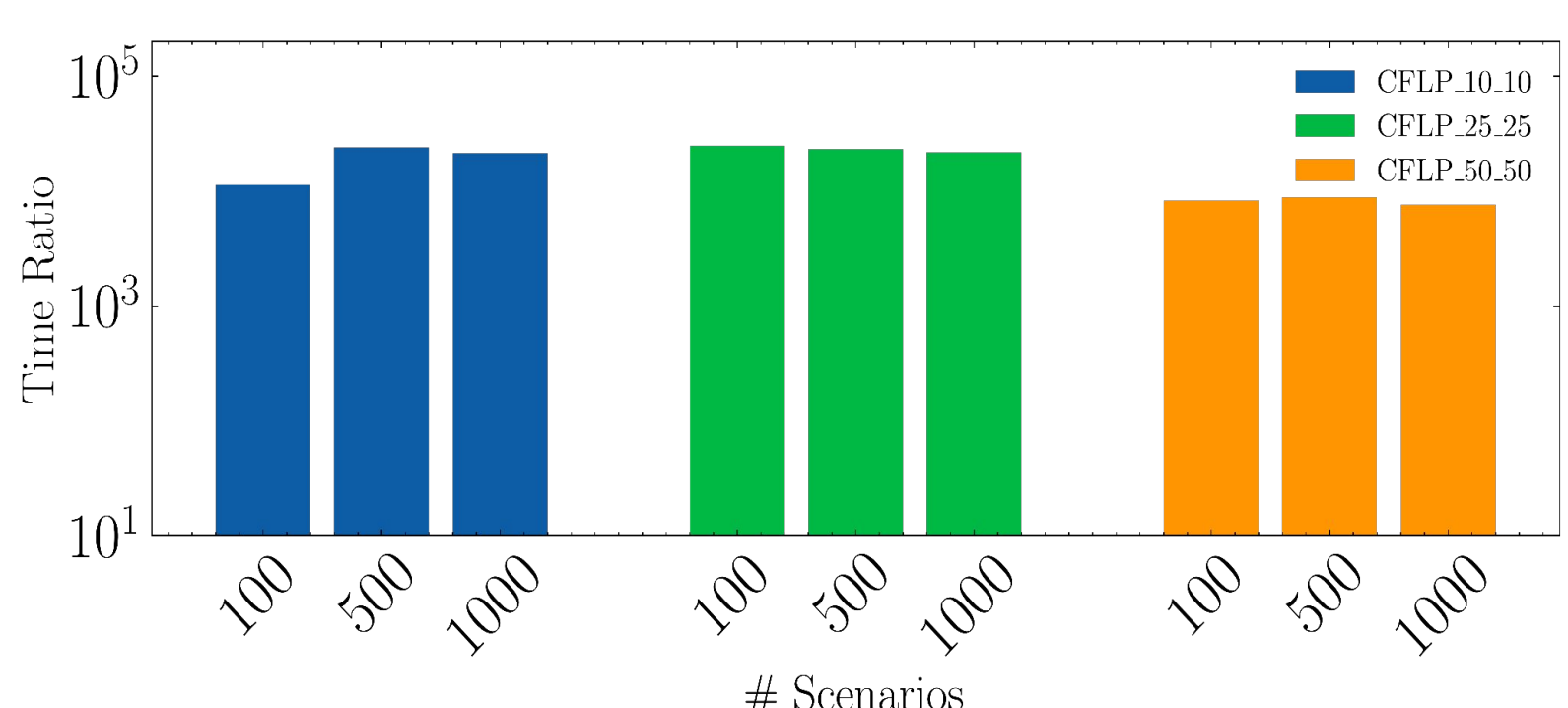
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Bars: Reduction in computing time over baseline (higher is better).

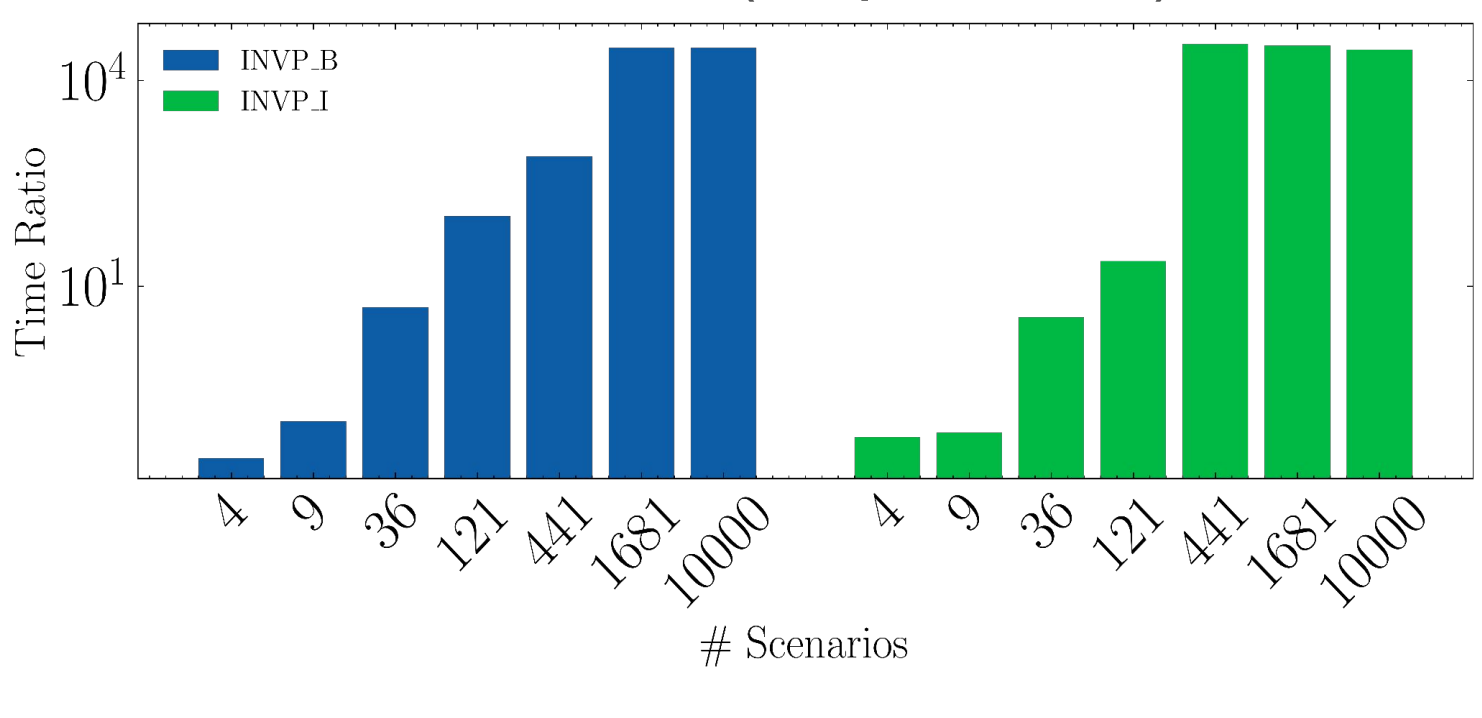
Stochastic Server Location Problem (Gap: -14.91%)



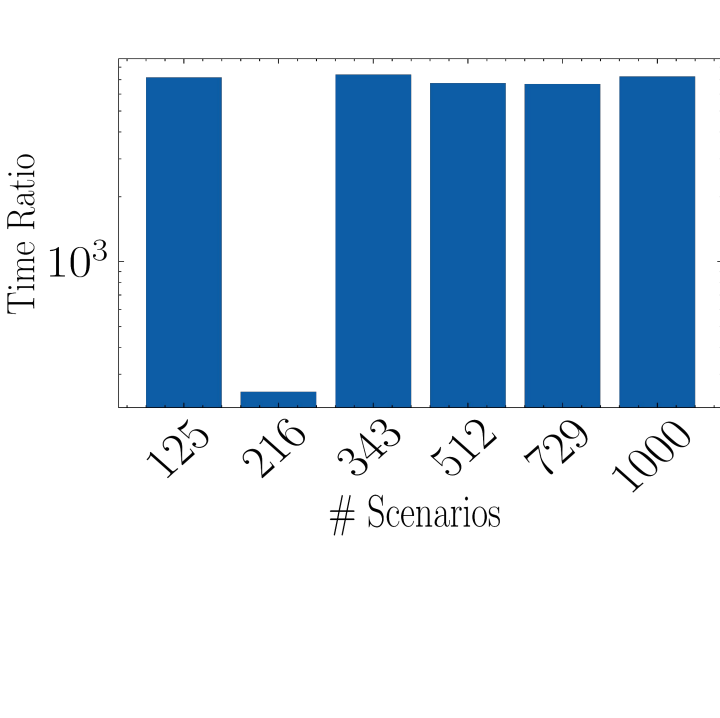
Capacitated Facility Location Problem (Gap: -2.93%)



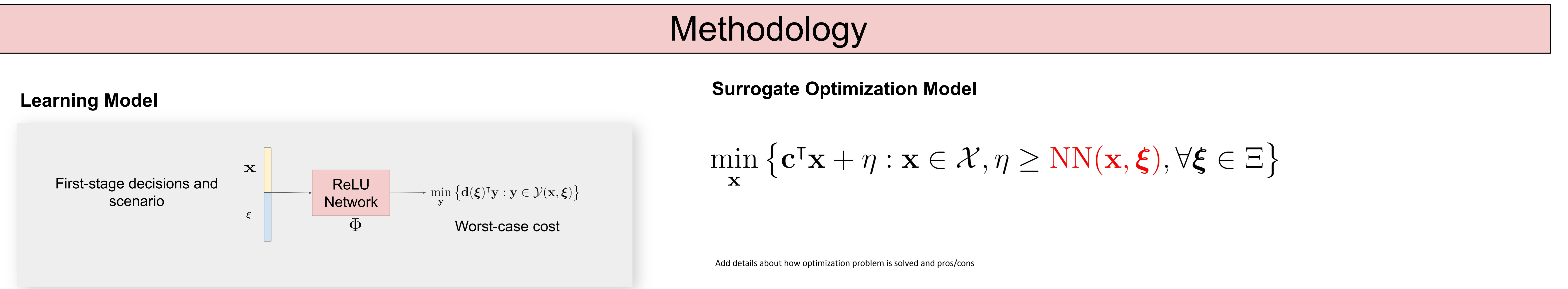
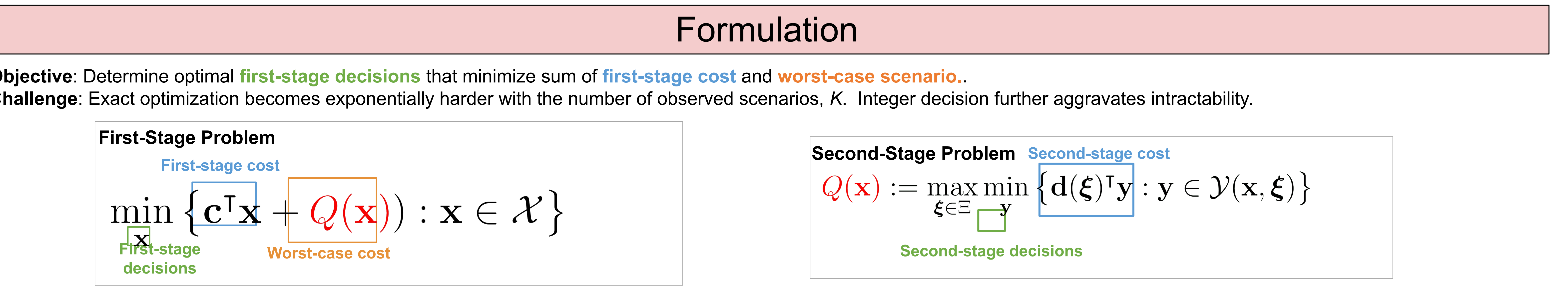
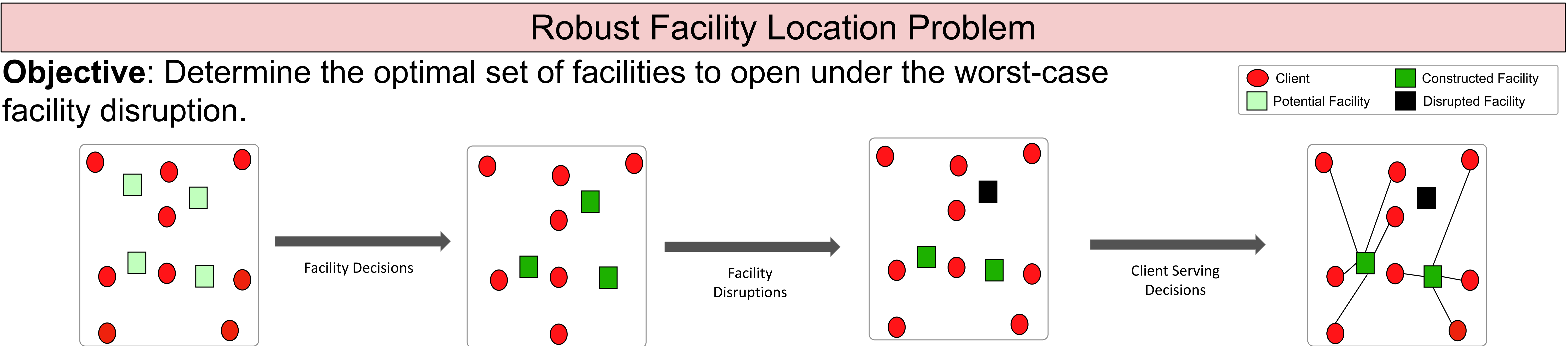
Investment Problem (Gap: 3.82%)



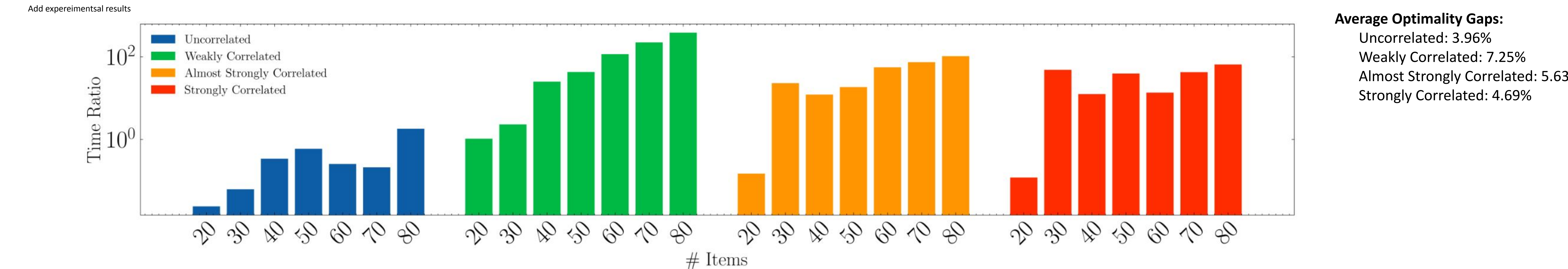
Pooling Problem (Gap: 4.82%)



Learning for Adjustable Robust Optimization (ARO)



Experimental Results



A Unified Machine Learning Framework for Optimization Under Uncertainty

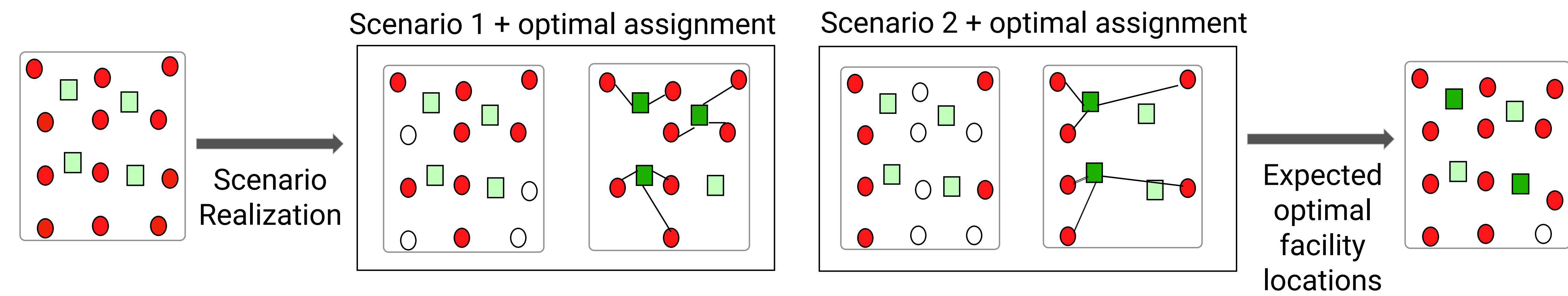
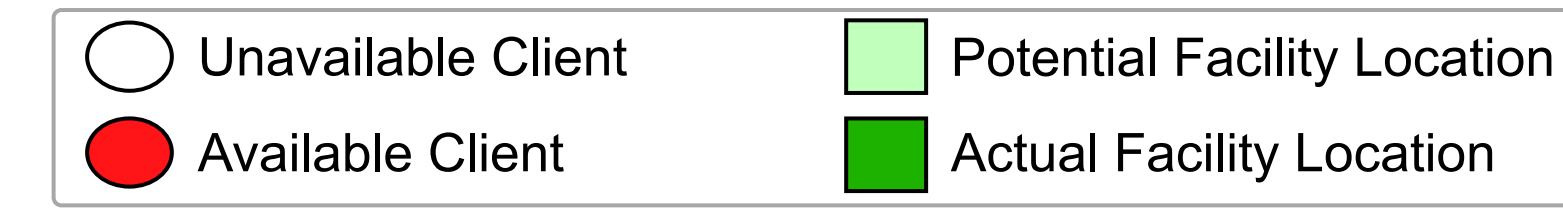
Justin Dumouchelle

Learning for **Two-Stage Stochastic Programming (2SP)**

Published at NeurIPS 2022. Joint work Elias Khalil, Merve Bodur, and Rahul Patel

Stochastic Facility Location Problem

Objective: Determine the optimal set of facilities to construct given uncertainty in client requests.

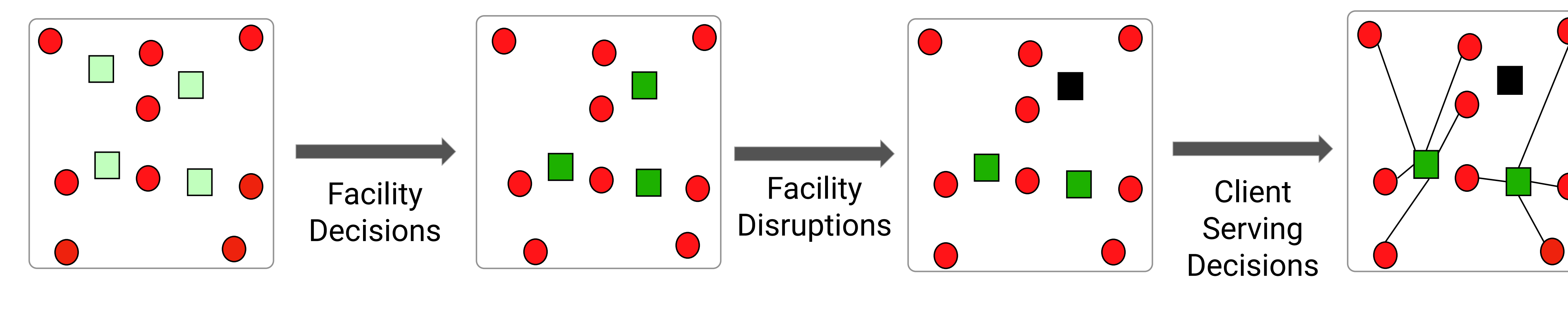


Learning for **Adjustable Robust Optimization (ARO)**

Under review (you can updated this to an arxiv link for the conference)

Robust Facility Location Problem

Objective: Determine the optimal set of facilities to open under the worst-case facility disruption.



Overall framework

Data Collection:

- Sample decisions + uncertainty
- Solve subproblems with off-the-shelf solvers

Evaluation on new instances:

- Solve the surrogate MILP with an off-the-shelf solver

Supervised Learning:

- Train an NN using off-the-shelf ML packages

Optimization Formulation

Objective: Determine optimal **first-stage decisions** that minimize sum of **first-stage cost** and **expected second-stage cost**.

Challenge: Exact optimization becomes exponentially harder with the number of observed scenarios, K . Integer decision further aggravates intractability.

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \sum_{k=1}^K p_k Q(\mathbf{x}, \xi_k) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions (x), Expected second-stage cost (Q)

Second-Stage Problem

$$Q(\mathbf{x}, \xi) := \min_{\mathbf{y}} \{ F(\mathbf{y}, \xi) : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \}$$

Second-stage decisions (y)

Objective: Determine optimal **first-stage decisions** that minimize **first-stage cost** and under the **worst-case cost**.

Challenge:

First-Stage Problem

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + Q(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \}$$

First-stage decisions (x), Worst-case cost (Q)

Second-Stage Problem

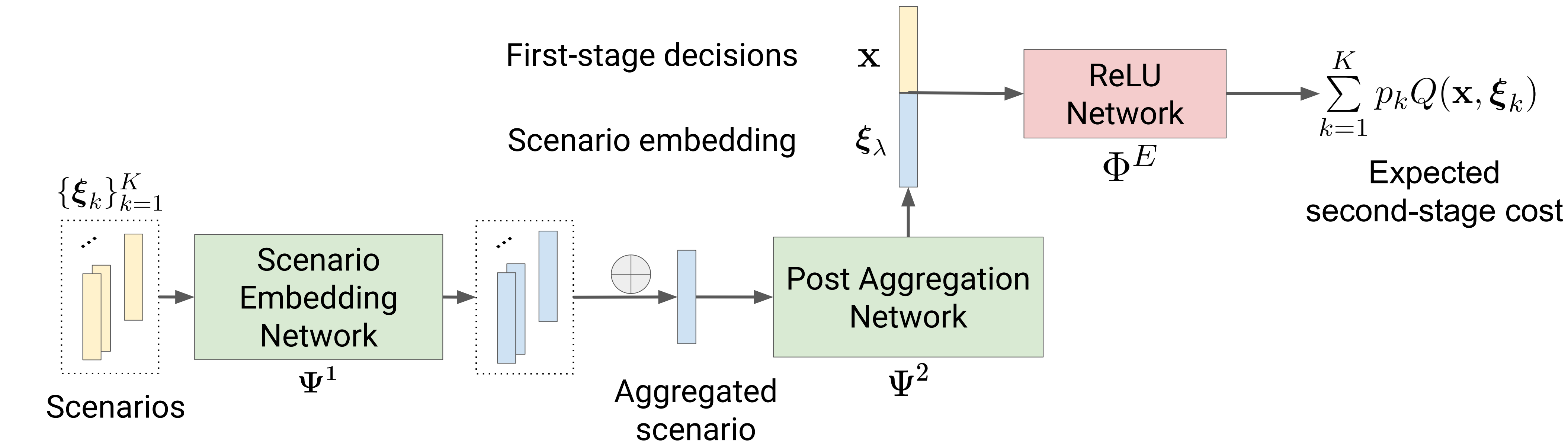
$$Q(\mathbf{x}) := \max_{\xi \in \Xi} \min_{\mathbf{y}} \{ \mathbf{d}(\xi)^T \mathbf{y} : \mathbf{y} \in \mathcal{Y}(\mathbf{x}, \xi) \}$$

Worst-case uncertainty (xi), Second-stage decisions (y)

Machine Learning Methodology

ML Solution: Replace the expected stage-cost value function with a neural network approximation.

Neural Network Architecture:

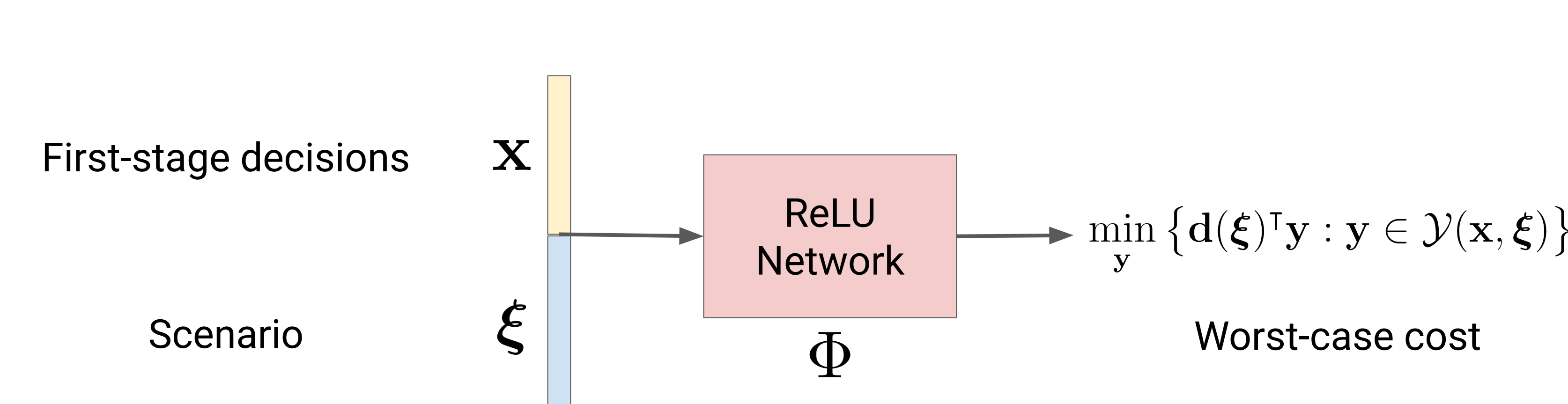


Surrogate Optimization Model:

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \text{NN}(\mathbf{x}, \{\xi_k\}_{k=1}^K) : \mathbf{x} \in \mathcal{X} \}$$

ML Solution: Replace the worst-case cost with a neural network approximation.

Neural Network Architecture:



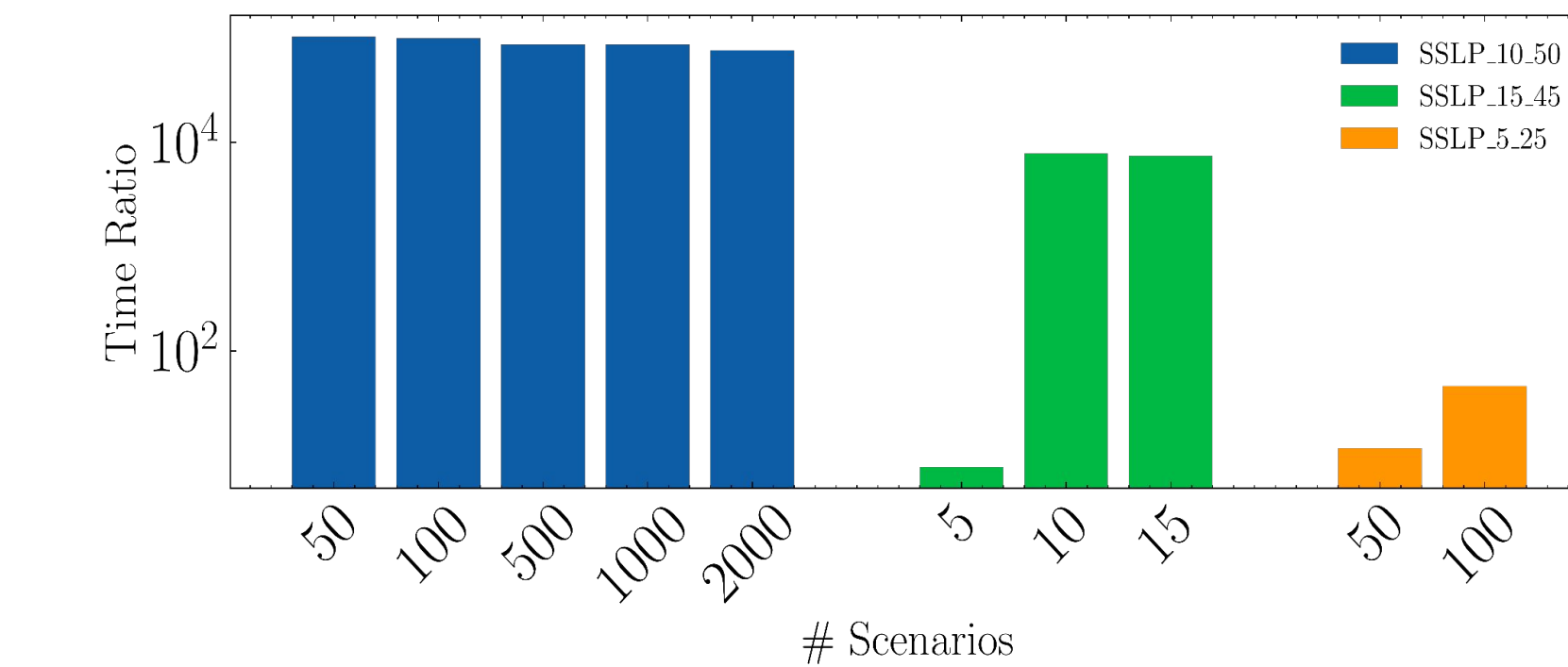
Surrogate Optimization Model:

$$\min_{\mathbf{x}} \{ \mathbf{c}^T \mathbf{x} + \eta : \mathbf{x} \in \mathcal{X}, \eta \geq \text{NN}(\mathbf{x}, \xi), \forall \xi \in \Xi \}$$

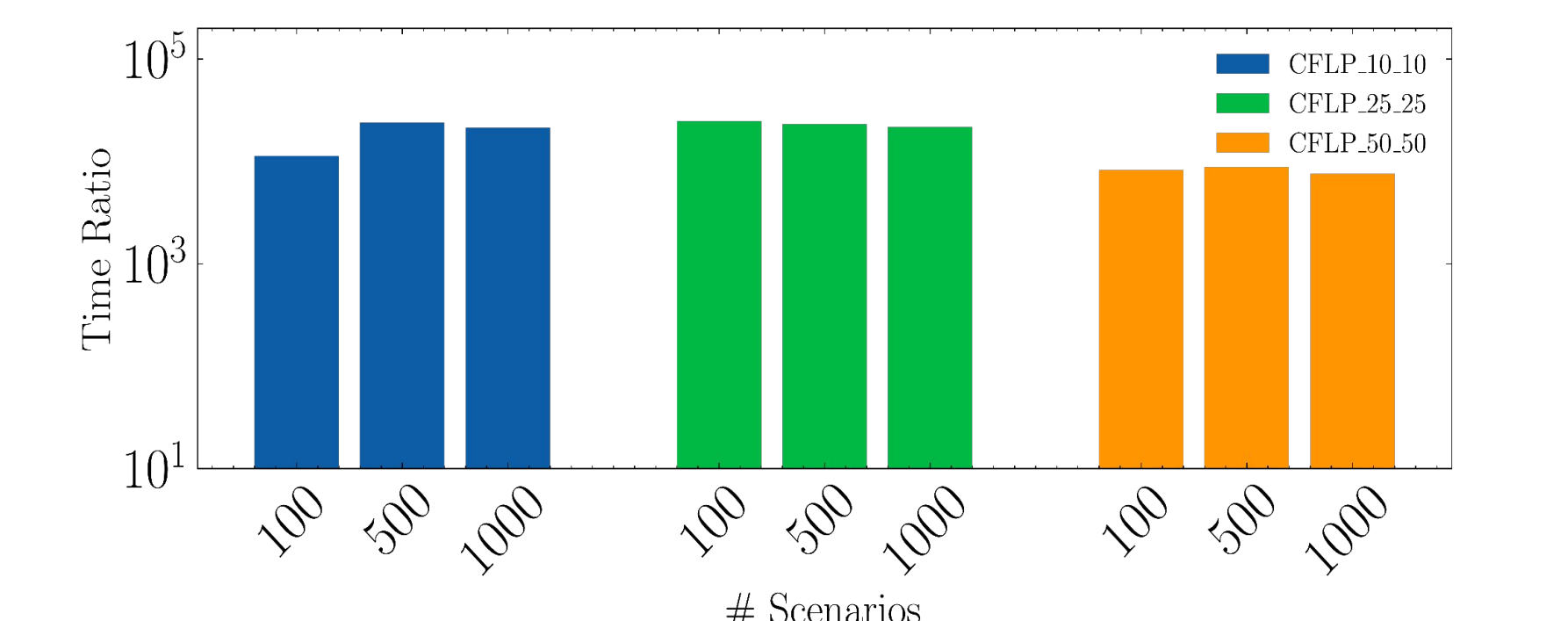
Experimental Results

Stochastic Programming

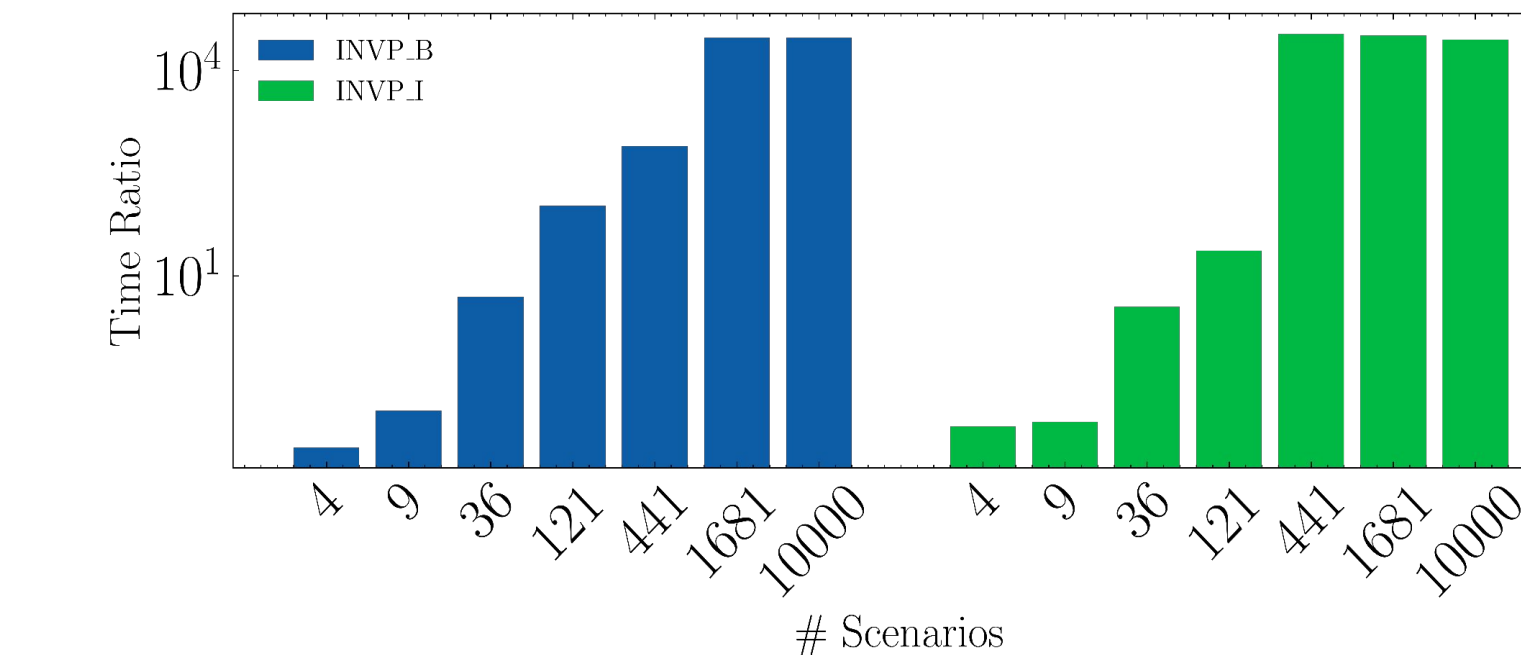
Stochastic Server Location Problem (Gap: -14.91%)



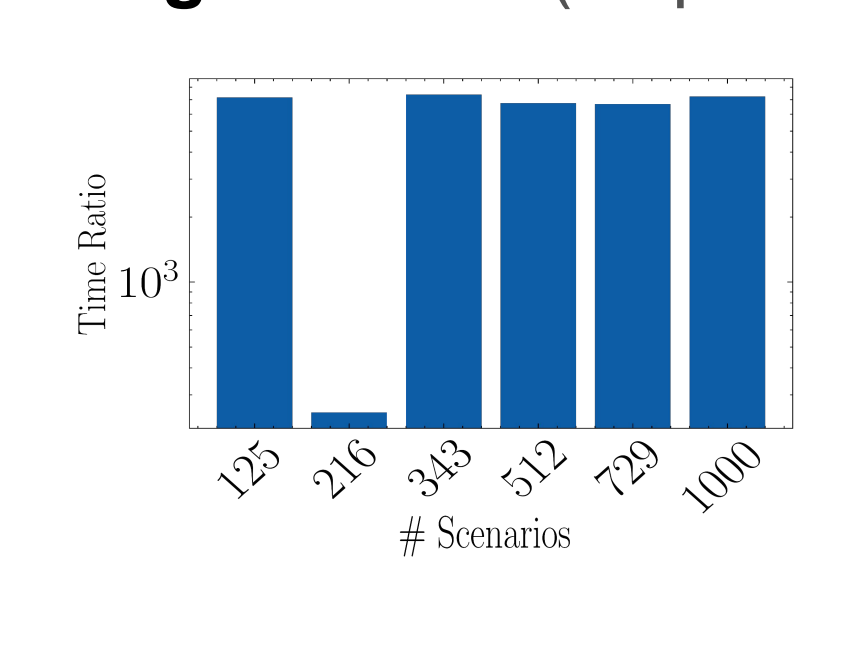
Capacitated Facility Location Problem (Gap: -2.93%)



Investment Problem (Gap: 3.82%)

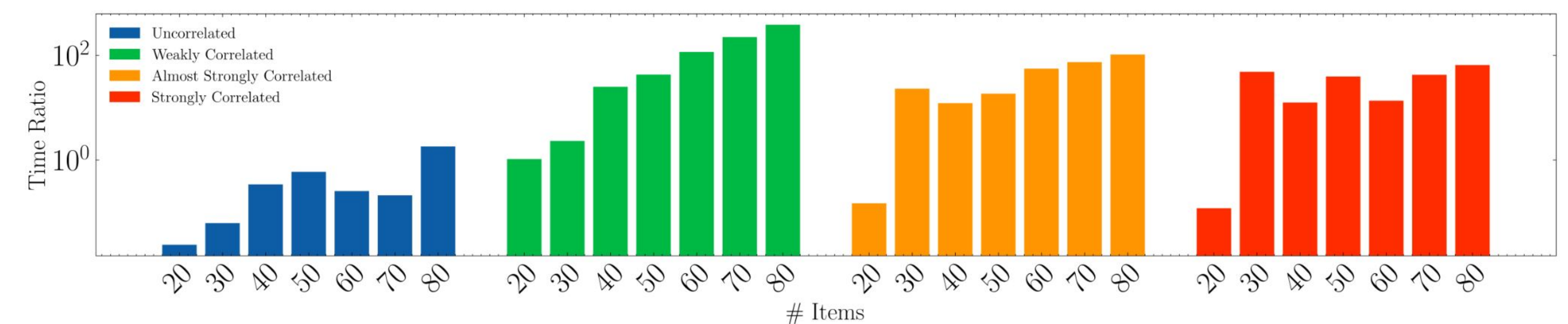


Pooling Problem (Gap: 4.82%)



Reduction factor in computing time over baseline (WHICH) (higher is better).

Robust Optimization



Average Optimality Gaps:

Uncorrelated: 3.96%

Weakly Correlated: 7.25%

Almost Strongly Correlated: 5.63%

Strongly Correlated: 4.69%



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