Introduction to Contextual (Stochastic) Optimization

Erick Delage
GERAD & Department of Decision Sciences
HEC MONTRÉAL

(Joint work with Utsav Sadana, Abhilash Chenreddy, Alexandre Forel, Emma Frejinger, Thibaut Vidal)

ICSP Tutorial on End-to-end Learning
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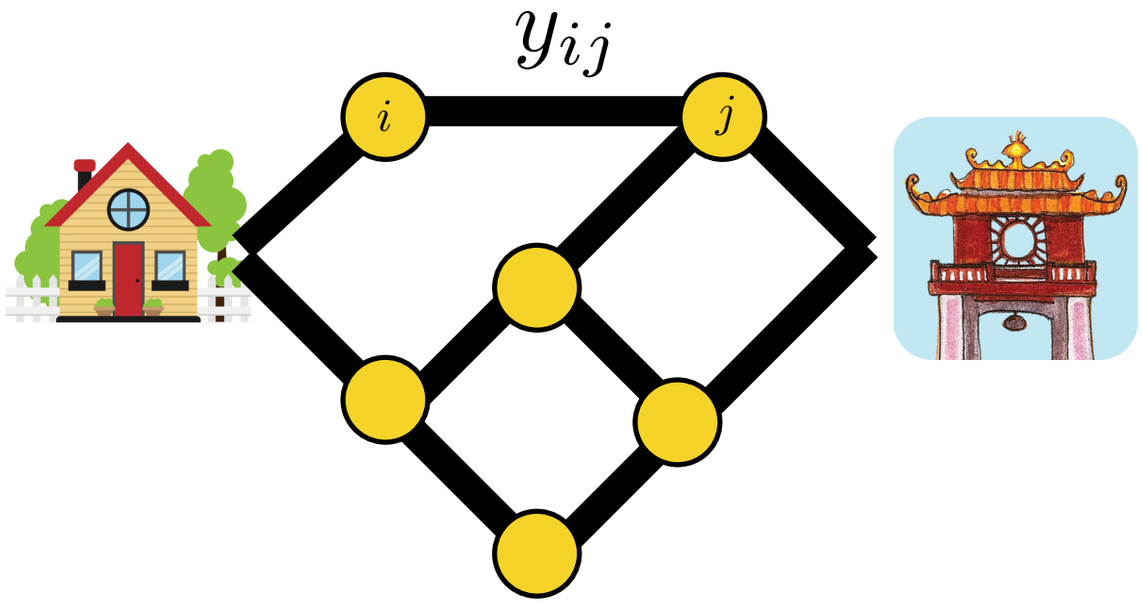
Why contextual stochastic optimization?

Decision Making with Contextual Information

- Revealed contextual information x
- Hidden random variables y



Decision Making with Contextual Information

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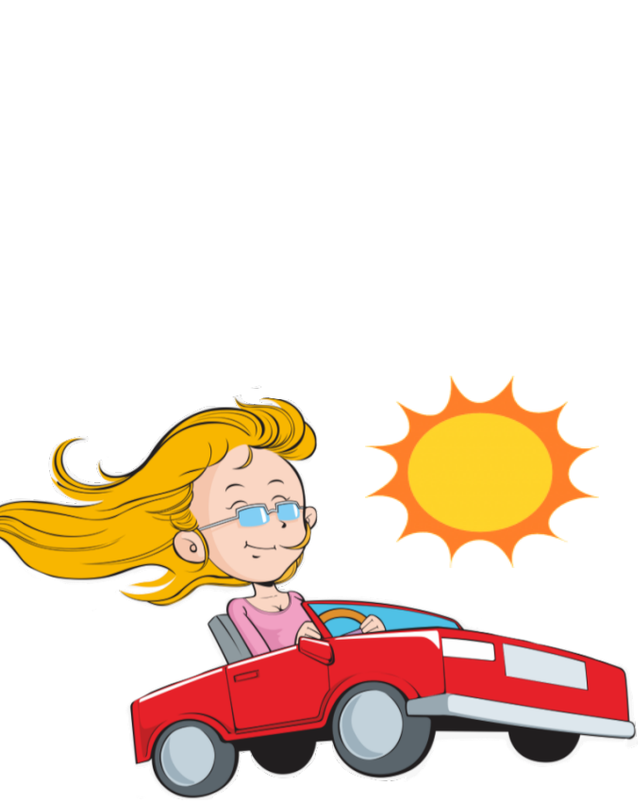
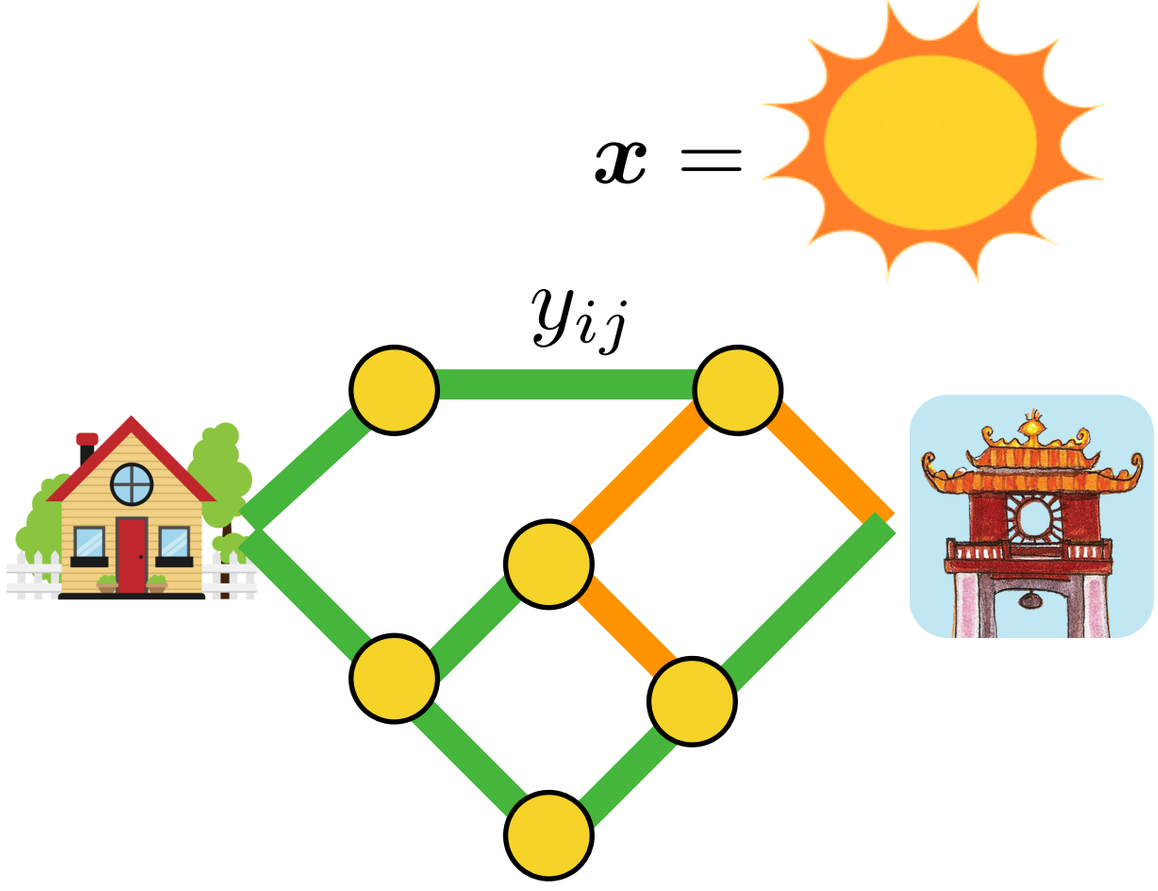
- Hidden random variables y

$$\boldsymbol{x} =$$



y_{ij}



Decision Making with Contextual Information

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$x =$

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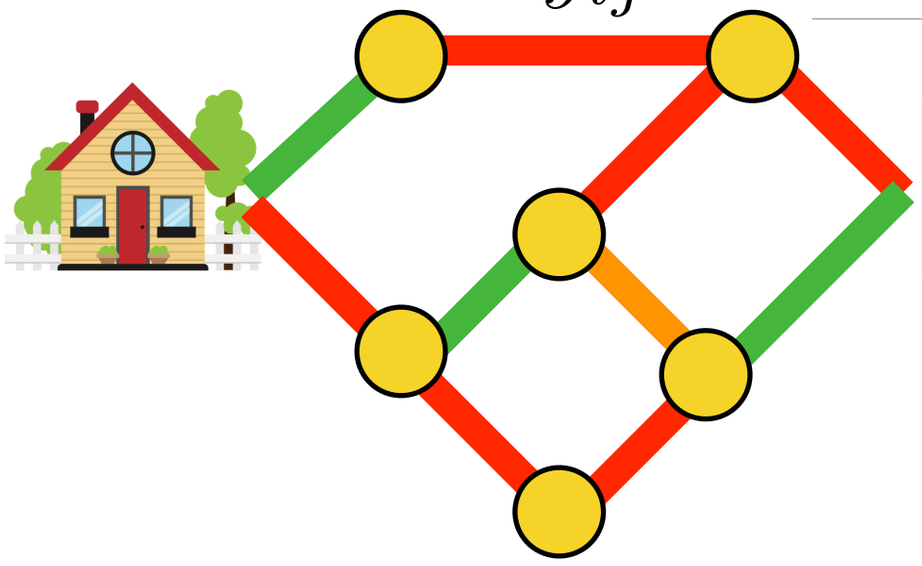

Decision Making with Contextual Information

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$\mathbb{E}^{\mathbb{P}}[y|x =$  $]$

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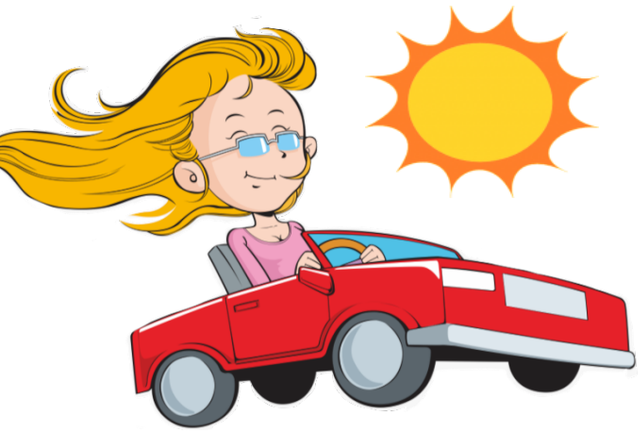
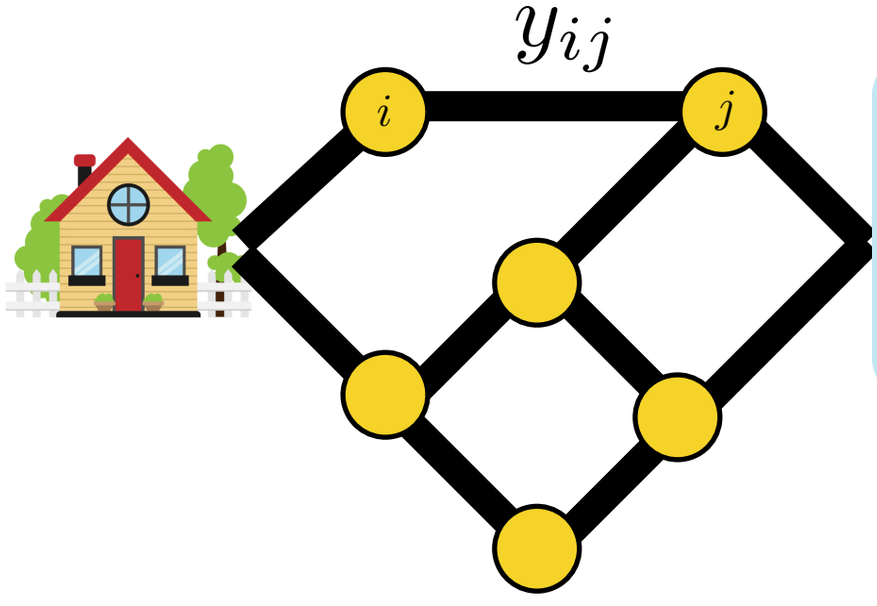


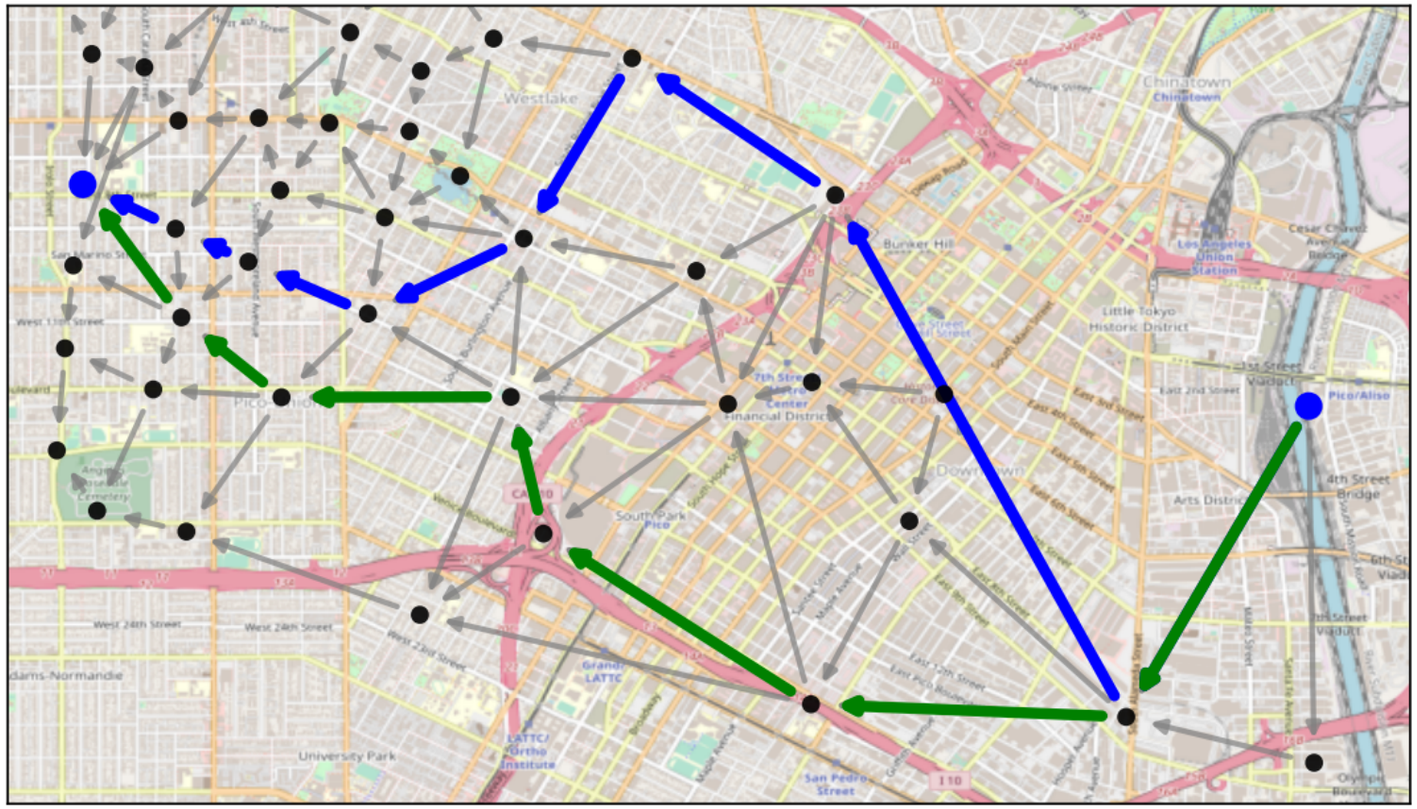


Practical motivation

Example 1:
Shortest path over Los Angeles downtown (Kallus & Mao, 2022)

Problem: find shortest path traversing Los Angeles downtown area from East to West

Travel times over all arcs are uncertain. We have relevant contextual information.



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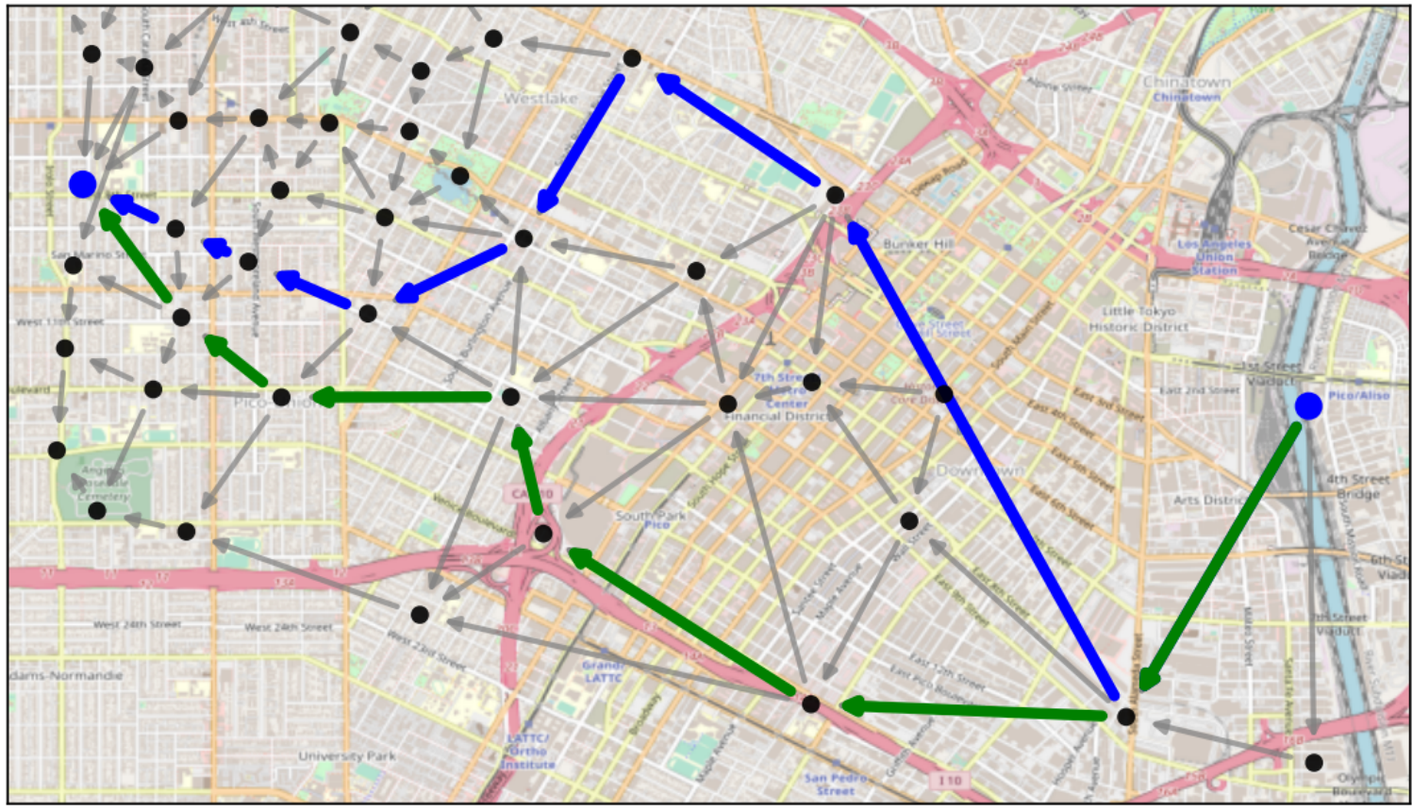


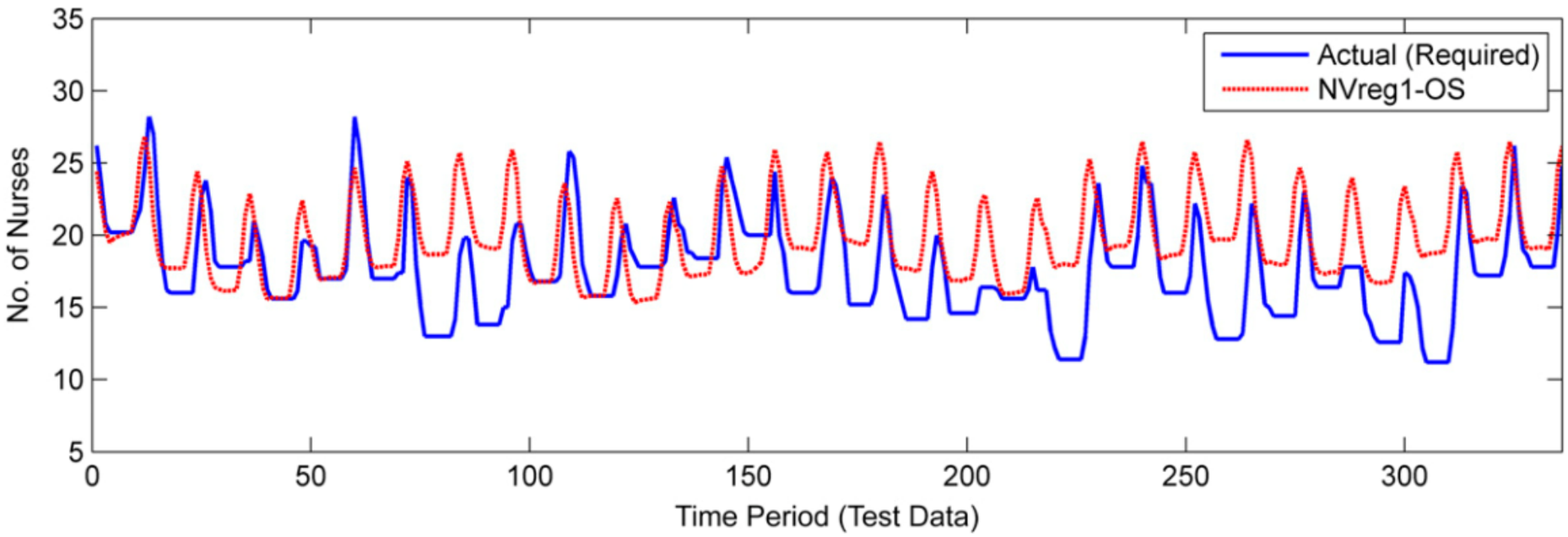
	Period	Temp.	Wind speed	Rain	Visibility	Day	Month
Green path is optimal →	**Midday**	57.17	4	0	6.99	2	11
Blue path is optimal →	**AM**	57.17	4	0	6.99	2	11

Practical motivation

Example 2:
Nurse Staffing in a Hospital (Ban & Rudin, 2019)

Decide how many nurse to schedule on a given day:
large penalty for under-/over-staffing
➢ **A newsvendor model** with uncertain demand

Historical data:
Demand and context



Features
Day of the week
Time of the day
Past demand observations

Practical motivation

In uncertain environments: we should use available contextual information to improve decisions

Manage inventory

Build portfolio

Deliver packages

What is contextual optimization?

Problem Definition

Stochastic optimization

$$\boldsymbol{z}^* \in \arg\min_{\boldsymbol{z}\in\mathcal{Z}} \mathbb{E}_{\mathbb{P}(\boldsymbol{y})}[c(\boldsymbol{z},\boldsymbol{y})]$$

Problem Definition

Stochastic optimization

$$z^* \in \arg\min_{z \in \mathcal{Z}} \mathbb{E}_{\mathbb{P}(y)}[c(z, y)]$$

Context

Conditional stochastic optimization (CSO)

$$z^*(x) \in \arg\min_{z \in \mathcal{Z}} \mathbb{E}_{\mathbb{P}(y|x)}[c(z, y)]$$

Contextual information / covariate / features

Problem Definition

Stochastic optimization

$$\boldsymbol{z}^* \in \underset{\boldsymbol{z}\in\mathcal{Z}}{\arg\min}\, \mathbb{E}_{\mathbb{P}(\boldsymbol{y})}[c(\boldsymbol{z},\boldsymbol{y})]$$

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$$\boldsymbol{z}^*(\boldsymbol{x}) \in \underset{\boldsymbol{z}\in\mathcal{Z}}{\arg\min}\, \mathbb{E}_{\mathbb{P}(\boldsymbol{y}|\boldsymbol{x})}[c(\boldsymbol{z},\boldsymbol{y})]$$

Contextual information / covariate / features

Connection between CSO and policy optimization:

$$\pi^* \in \underset{\pi:\mathcal{X}\to\mathcal{Z}}{\arg\min}\, \mathbb{E}_{\mathbb{P}}[c(\pi(\boldsymbol{x}),\boldsymbol{y})] \quad \Leftrightarrow \quad \pi^*(\boldsymbol{x}) \in \underset{\boldsymbol{z}\in\mathcal{Z}}{\arg\min}\, \mathbb{E}_{\mathbb{P}(\boldsymbol{y}|\boldsymbol{x})}[c(\boldsymbol{z},\boldsymbol{y})] \text{ a.s.}$$

Problem Definition

Stochastic optimization

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Conditional stochastic optimization (CSO)

$$\boldsymbol{z}^*(\boldsymbol{x}) \in \arg\min_{\boldsymbol{z}\in\mathcal{Z}} \mathbb{E}_{\mathbb{P}(\boldsymbol{y}|\boldsymbol{x})}[c(\boldsymbol{z},\boldsymbol{y})]$$

$$h(\boldsymbol{z},\mathbb{P}(\boldsymbol{y}|\boldsymbol{x}))$$

Conditional expected cost

Contextual information / covariate / features

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$$\boldsymbol{z}^* \in \arg\min_{\boldsymbol{z}\in\mathcal{Z}} \mathbb{E}_{\mathbb{P}(\boldsymbol{y})}[c(\boldsymbol{z},\boldsymbol{y})]$$

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Conditional stochastic optimization (CSO)

$$\boldsymbol{z}^*(\boldsymbol{x}) \in \arg\min_{\boldsymbol{z}\in\mathcal{Z}} \underbrace{\mathbb{E}_{\mathbb{P}(\boldsymbol{y}|\boldsymbol{x})}[c(\boldsymbol{z},\boldsymbol{y})]}_{h(\boldsymbol{z},\mathbb{P}(\boldsymbol{y}|\boldsymbol{x}))}$$

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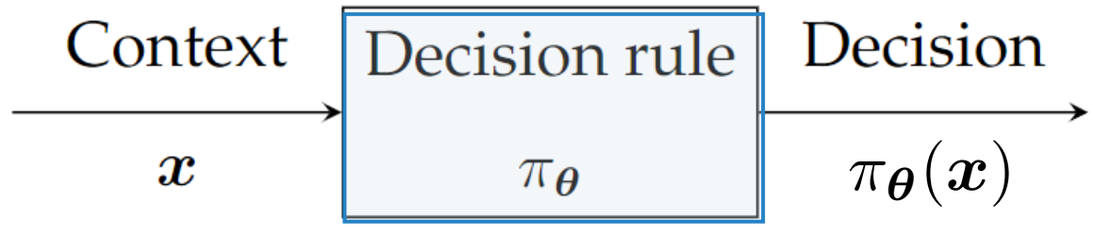
(Unconditional) expected cost

Overview of the three frameworks

Decision rule/Policy optimization



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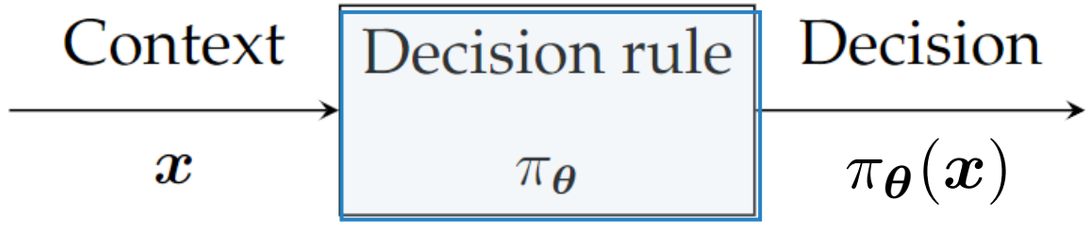
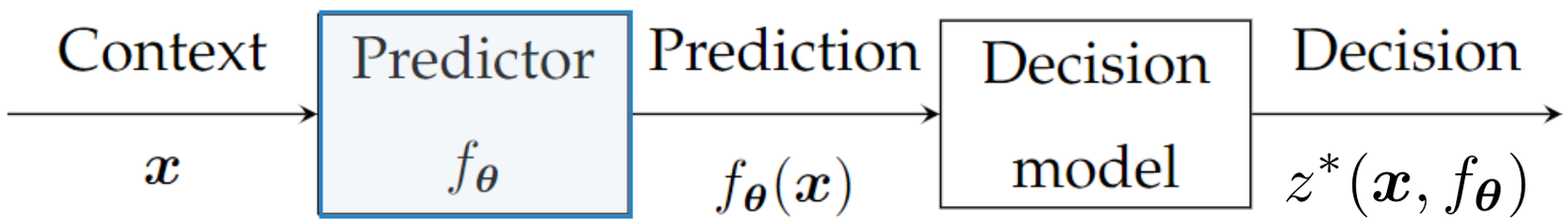


Sequential learning and optimization



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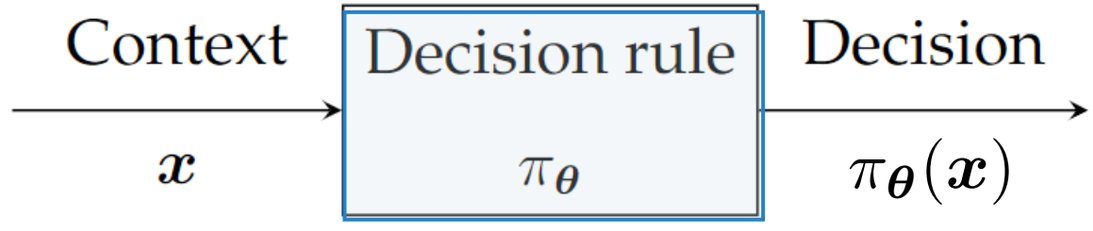
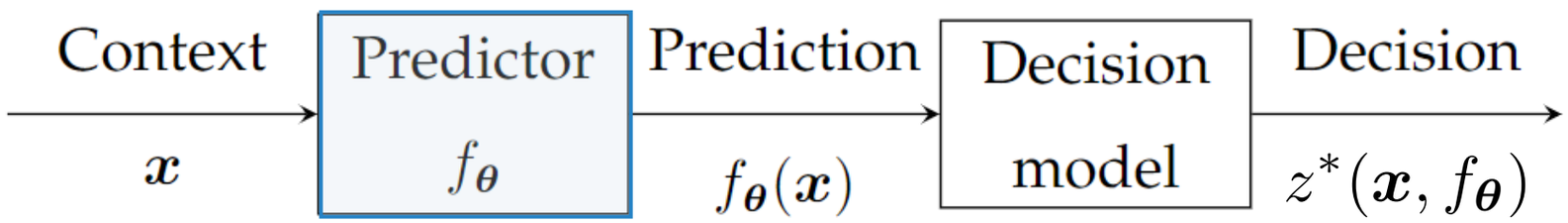
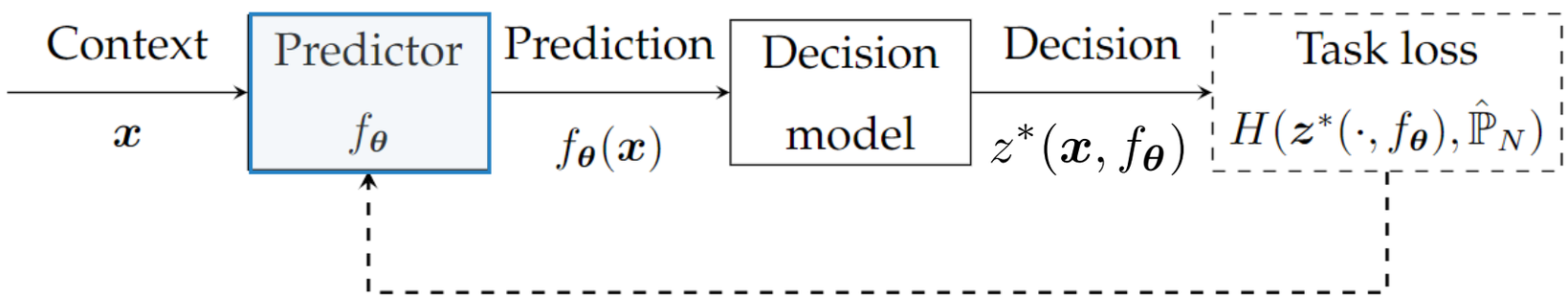


Sequential learning and optimization



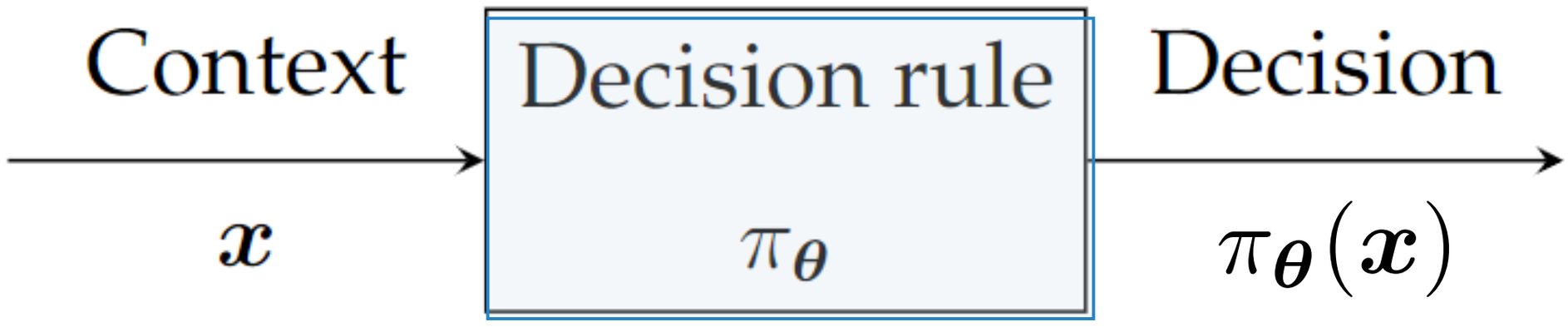
Integrated learning and optimization



Outline of the Tutorial

- Decision rule optimization
- Sequential learning and optimization
- Integrated learning and optimization
- Take-away messages

Decision rule optimization



Learning decision rules (LDRs)

- Find policy to minimize the expected cost
  - Infinite dimensional problem

- Linear DRs to solve newsvendor problem [Ban & Rudin, 2019]

$$\min_{\pi:\pi(\boldsymbol{x})=\boldsymbol{q}^\top \boldsymbol{x}} H(\pi, \hat{\mathbb{P}}_N) + \lambda\Omega(\boldsymbol{\pi}) := \min_{\boldsymbol{q}} \frac{1}{N}\sum_{i=1}^{N} c(\boldsymbol{q}^\top \boldsymbol{x}^i, \boldsymbol{y}^i) + \lambda\|\boldsymbol{q}\|_k$$

  - Linear DR have finite sample guarantees
  - Linear DRs are asymptotically suboptimal in general

Decision rules on lifted space

- Linear in transformation of features: [Ban & Rudin, 2019]
- Policies in the reproducing kernel Hilbert space (RKHS) [Bertsimas & Koduri, 2023]
- Piecewise affine decision rules [Zhang et al., 2023]
  - Outperforms models with policy in the RKHS
- Policy Net [Oroojlooyjadid et al., 2020]
  - Lack interpretability
- Challenge: Ensure constraints are satisfied

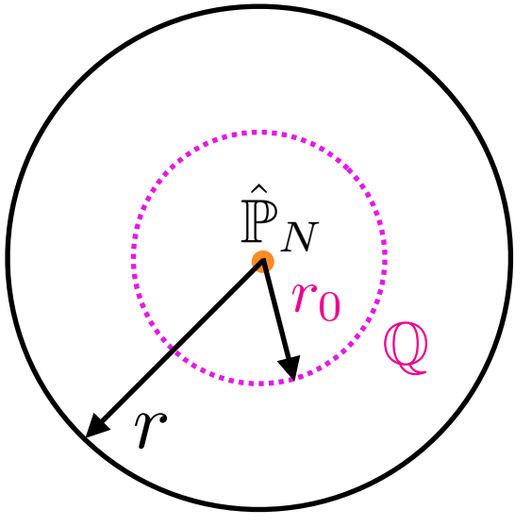
Distributionally robust optimization

- Estimation error: Empirical distribution biased in low data regime
- One can robustify against all distributions in an ambiguity set:

$$\min_{\pi \in \Pi} \sup_{\mathbb{Q} \in \mathcal{D}} H(\pi, \mathbb{Q})$$

- E.g.: Wasserstein ambiguity set [Mohajerin and Kuhn 2018]

$$\mathcal{D} := \{\mathbb{Q} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}) : \mathcal{W}(\mathbb{Q}, \hat{\mathbb{P}}_N) \leq r\}$$



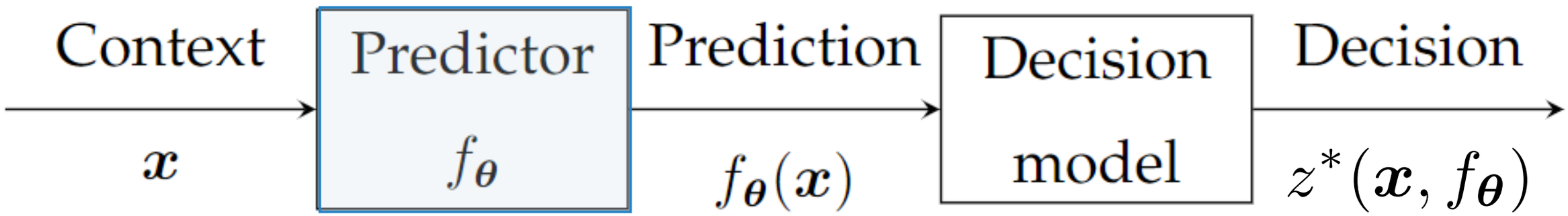
DR-Newsvendor

- Two-step procedure [Zhang et al., 2023]
  - Solve DRO problem with policy defined on historical observations of features
  - Use Shapley extension to interpolate to all unobserved realizations of features
- Outperforms linear decision rules, kNN, random forest, StochOptForest

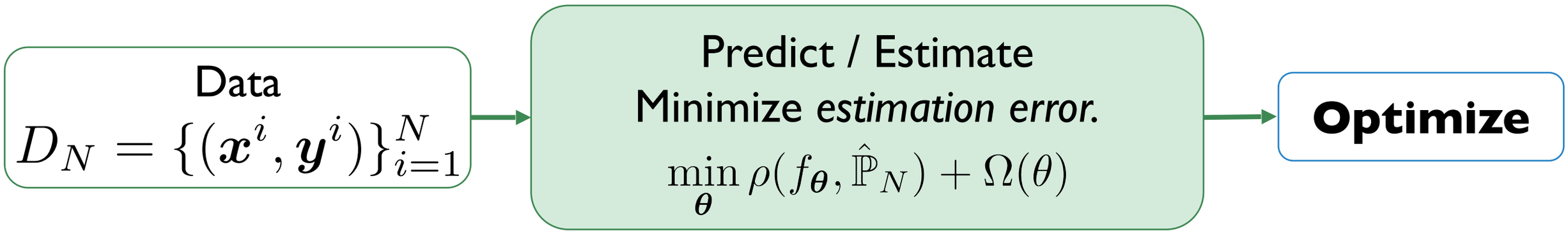
DRO with causal transport

- [Yang et al. 2023] raises issue that Wasserstein distance distorts the conditional information structure
- They suggest using a Causal transport metric, which protects causal effects found in the data
- Tractable reformulations obtained when:
  - Linear decision rules
  - Cost function is affine

Sequential learning and optimization



Learning predictors



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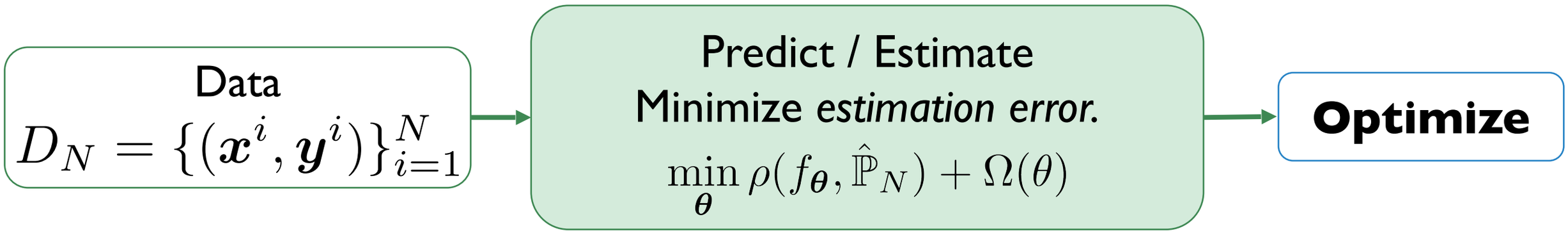


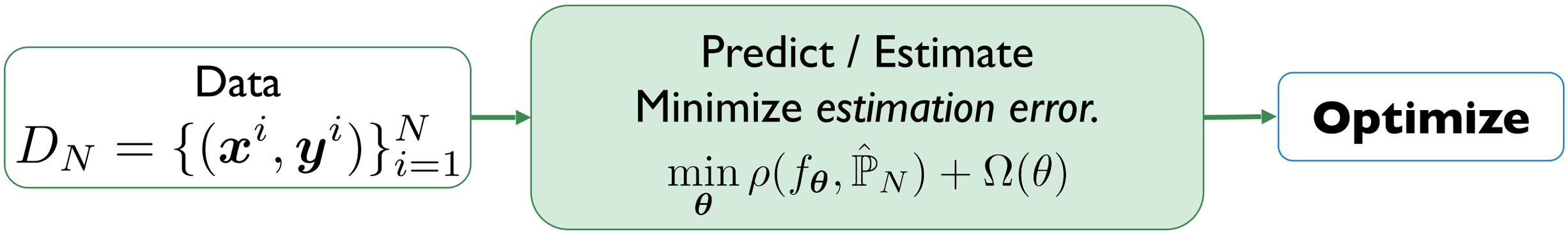
Non-linear cost function

f_θ is a **conditional density estimator**

Maximum Log-Likelihood

$$\hat{\theta} = \arg\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} -\log(\mathbb{P}_{f_\theta(\boldsymbol{x}^i)}(\boldsymbol{y}^i)) + \Omega(\theta)$$

Learning predictors



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Linear cost function

f_θ replaced with **point predictor**

(denoted g_θ)

Mean Square Error

$$\hat{\theta} = \arg\min_\theta \frac{1}{N} \sum_{i=1}^{N} \|g_\theta(\boldsymbol{x}^i) - \boldsymbol{y}^i\|^2 + \Omega(\theta)$$

$$h(z, f_\theta) = \mathbb{E}_{f_\theta(\boldsymbol{x})}[\boldsymbol{y}^\top \boldsymbol{z}] = \mathbb{E}_{f_\theta(\boldsymbol{x})}[\boldsymbol{y}]^\top \boldsymbol{z} = g_\theta(\boldsymbol{x})^\top \boldsymbol{z} = h(z, g_\theta)$$

Weighted SAA

Minimizing expected costs w.r.t. a distribution is often done through SAA:

$$\min_{\boldsymbol{z}\in\mathcal{Z}} \mathbb{E}_{f_\theta(\boldsymbol{x})}[c(\boldsymbol{z},\boldsymbol{y})] \text{ with } f_\theta(\boldsymbol{x}) := \frac{1}{N}\sum_{i=1}^{N} \delta_{\boldsymbol{y}^i(\boldsymbol{x})}$$

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Residual based

Measure the **error of a trained regression model** on the historical data

$$f_\theta(\boldsymbol{x}) := \frac{1}{N}\sum_{i=1}^{N} \delta_{g_\theta(\boldsymbol{x})+\epsilon_i}$$

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Residual based

Measure the **error of a trained regression model** on the historical data

$$f_\theta(\boldsymbol{x}) := \frac{1}{N}\sum_{i=1}^{N} \delta_{g_\theta(\boldsymbol{x})+\epsilon^i}$$

Weight based

Measure **proximity in feature space** between x and historical covariates x^i

Weighted SAA

Proximity in feature space

- k-nearest neighbor: $w_i^{\mathrm{kNN}}(\boldsymbol{x}) := (1/k)\mathbb{1}[\boldsymbol{x}^i \in \mathcal{N}_k(\boldsymbol{x})]$
- Kernel density estimation: $w_i^{\mathrm{KDE}}(\boldsymbol{x}) := \dfrac{\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}^i)}{\sum_{j=1}^{N} \mathcal{K}(\boldsymbol{x}, \boldsymbol{x}^j)}$

Weighted SAA

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Supervised learning

- Decision tree: $w_i^{\mathrm{DT}}(\boldsymbol{x}) := \dfrac{\mathbb{1}[\mathcal{R}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x}^i)]}{\sum_{j=1}^N \mathbb{1}[\mathcal{R}(\boldsymbol{x}) = \mathcal{R}(\boldsymbol{x}^j)]}$
- Random forest: average over set of decision trees.

Why do sequential learning and optimization?

It's fast!

➢Train once on historical data:
no need to solve optimization models during training

It works

➢Can perform better than non-contextual approach
➢Can be trained using less data when model is well specified

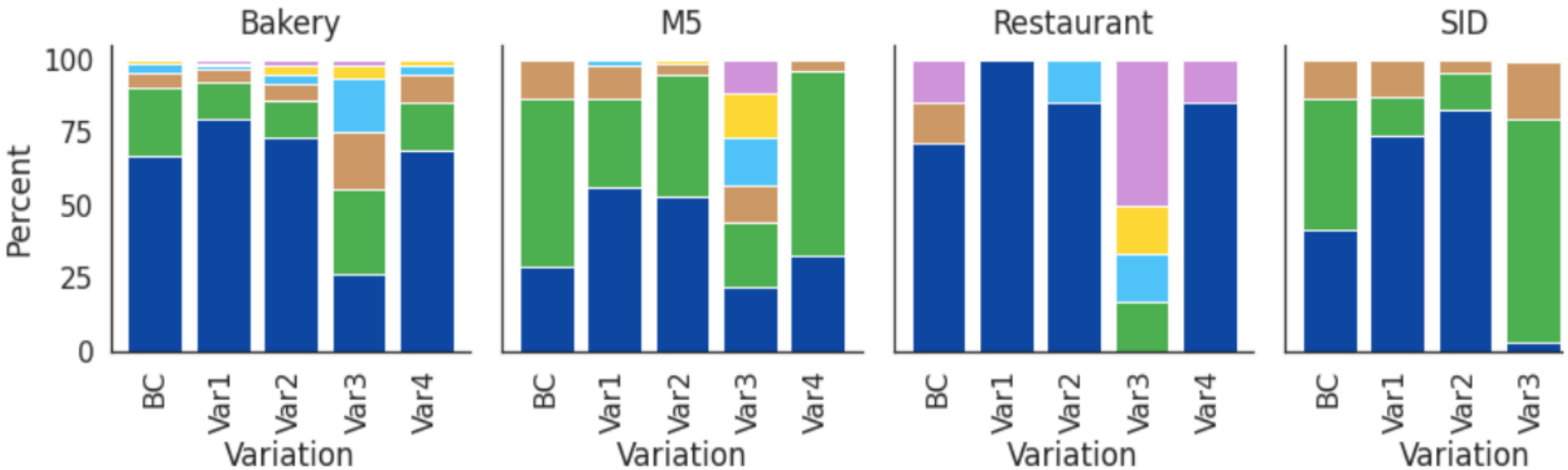
Theoretical guarantees

➢Converges to optimal contextual policy as the size of the training set increases **when model is well specified**.

Some benchmark results (Buttler et al., 2023)

Newsvendor Problem	Compare **sequential** L&O and **decision rules** on 4 data sets.

Proportion of instances where methods achieved best performance



Models:

- Linear rule
- Deep learning
- Kernel weights
- K-nearest neighbour weights
- Decision tree weights
- Random forest weights

Sequential Learning & Optimization References

	Method			Regularization		Learning model					
	rCSO	**wSAA**	**EVB**	Reg. CSO	DRO	General	Linear	Kernel	kNN	DT	RF
Hannah et al. (2010)	✗	✔	✗	✗	✗	✗	✗	✔	✗	✗	✗
Ferreira et al. (2016)	✗	✗	✔	✗	✗	✗	✗	✗	✗	✔	✗
Ban et al. (2019)	✔	✗	✗	✗	✗	✗	✔	✗	✗	✗	✗
Chen and Paschalidis (2019)	✗	✔	✗	✗	✔	✗	✗	✗	✔	✗	✗
Bertsimas and Kallus (2020)	✗	✔	✗	✗	✗	✗	✔	✗	✔	✔	✔
Kannan et al. (2020)	✔	✗	✗	✗	✗	✔	✔	✔	✔	✔	✔
Kannan et al. (2021)	✔	✗	✗	✗	✔	✔	✔	✔	✔	✔	✔
Liu et al. (2021)	✗	✗	✔	✗	✗	✗	✔	✗	✗	✔	✗
Srivastava et al. (2021)	✗	✔	✗	✔	✗	✗	✗	✔	✗	✗	✗
Wang et al. (2021)	✗	✔	✗	✗	✔	✗	✗	✔	✗	✗	✗
Bertsimas and Van Parys (2022)	✗	✔	✗	✗	✔	✗	✗	✔	✔	✗	✗
Deng and Sen (2022)	✔	✗	✗	✗	✗	✔	✔	✔	✔	✔	✔
Esteban-Pérez and Morales (2022)	✗	✔	✗	✗	✔	✗	✗	✔	✔	✗	✗
Kannan et al. (2022)	✔	✗	✗	✗	✔	✔	✔	✔	✔	✔	✔
Lin et al. (2022)	✗	✔	✗	✔	✗	✗	✗	✗	✔	✔	✔
Nguyen et al. (2021)	✗	✔	✗	✗	✔	✗	✗	✗	✔	✗	✗
Notz and Pibernik (2022)	✗	✔	✗	✗	✗	✗	✗	✔	✗	✔	✗
Zhu et al. (2022)	✗	✗	✔	✗	✔	✔	✔	✔	✔	✔	✔
Perakis et al. (2023)	✔	✗	✗	✗	✔	✗	✔	✗	✗	✗	✗

Going beyond SLO:
Integrated learning and optimization

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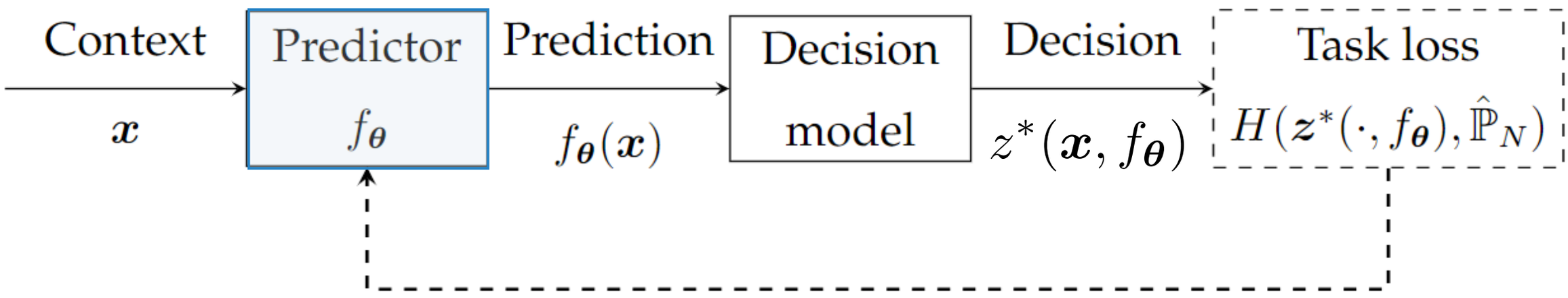
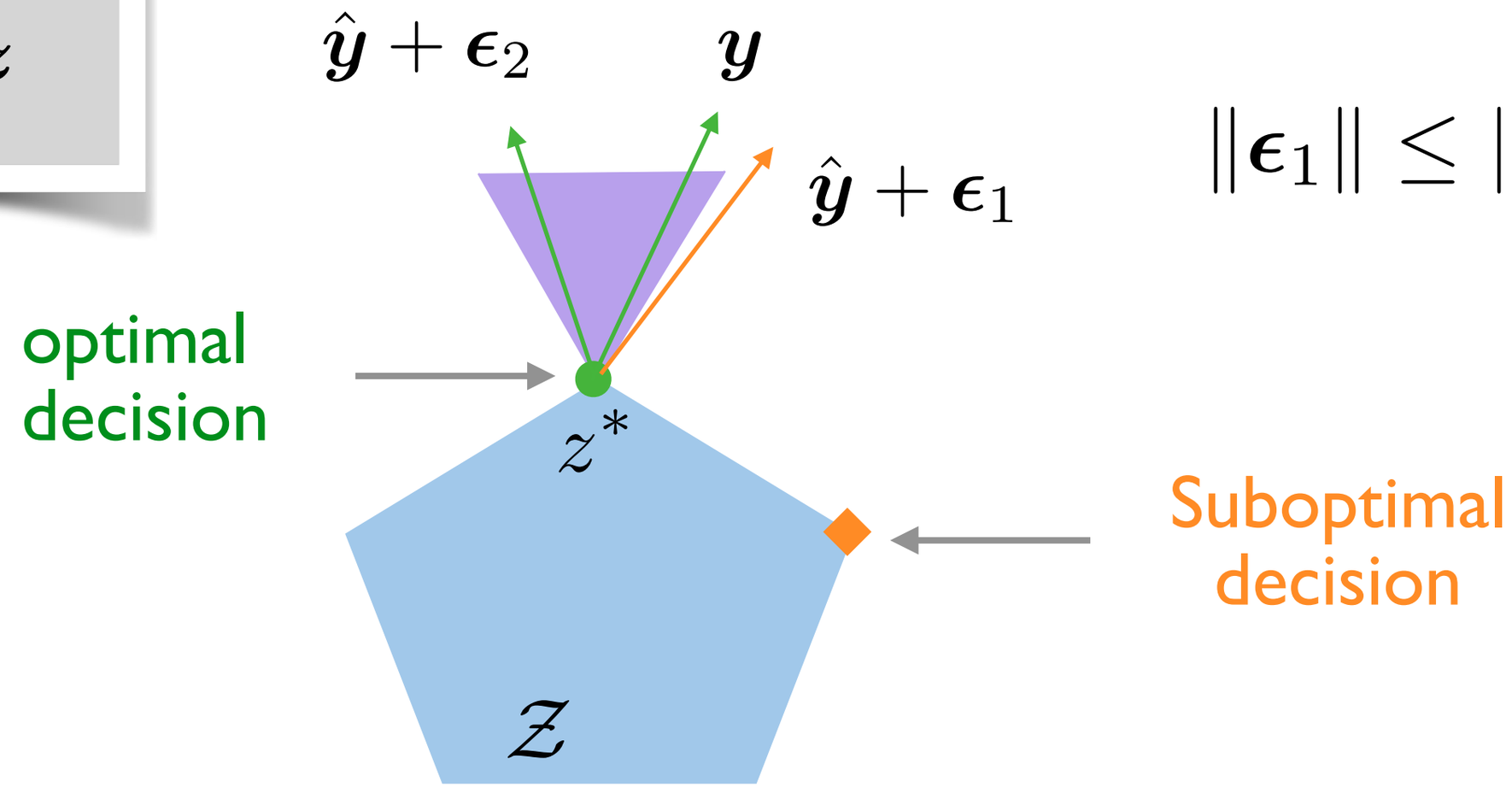


Wrong predictions lead to suboptimal decisions

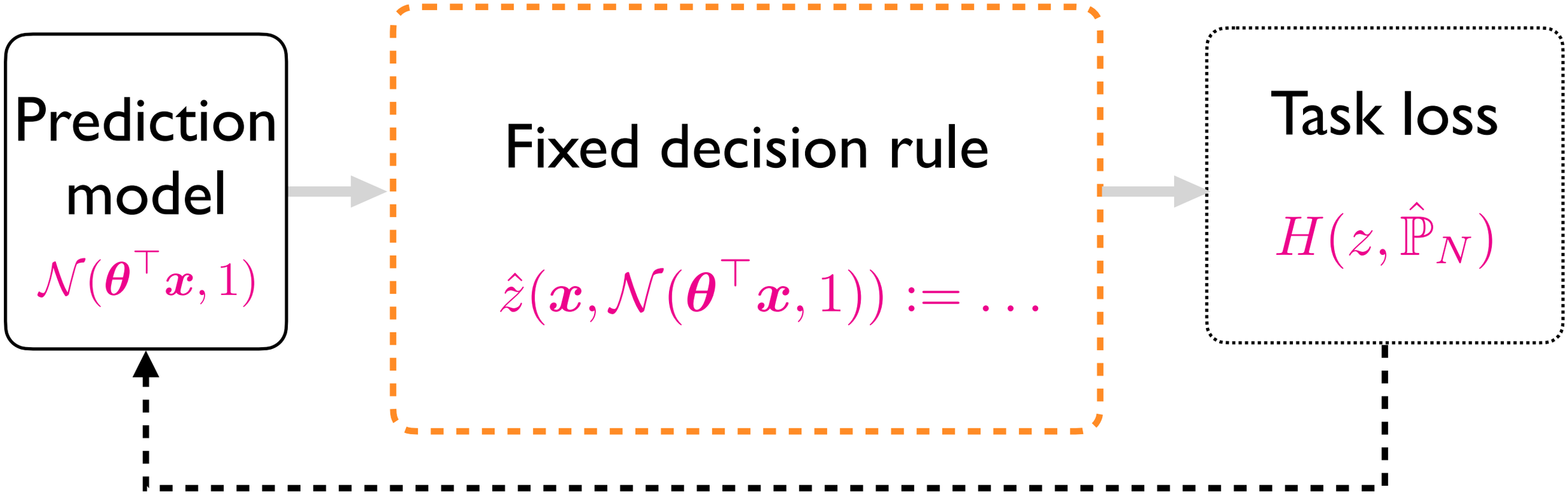
$$\max_{\boldsymbol{z} \in \mathcal{Z}} \boldsymbol{y}^\top \boldsymbol{z}$$



$$\|\boldsymbol{\epsilon}_1\| \leq \|\boldsymbol{\epsilon}_2\|$$

Figure adapted from [Elmachtoub and Grigas 2022]

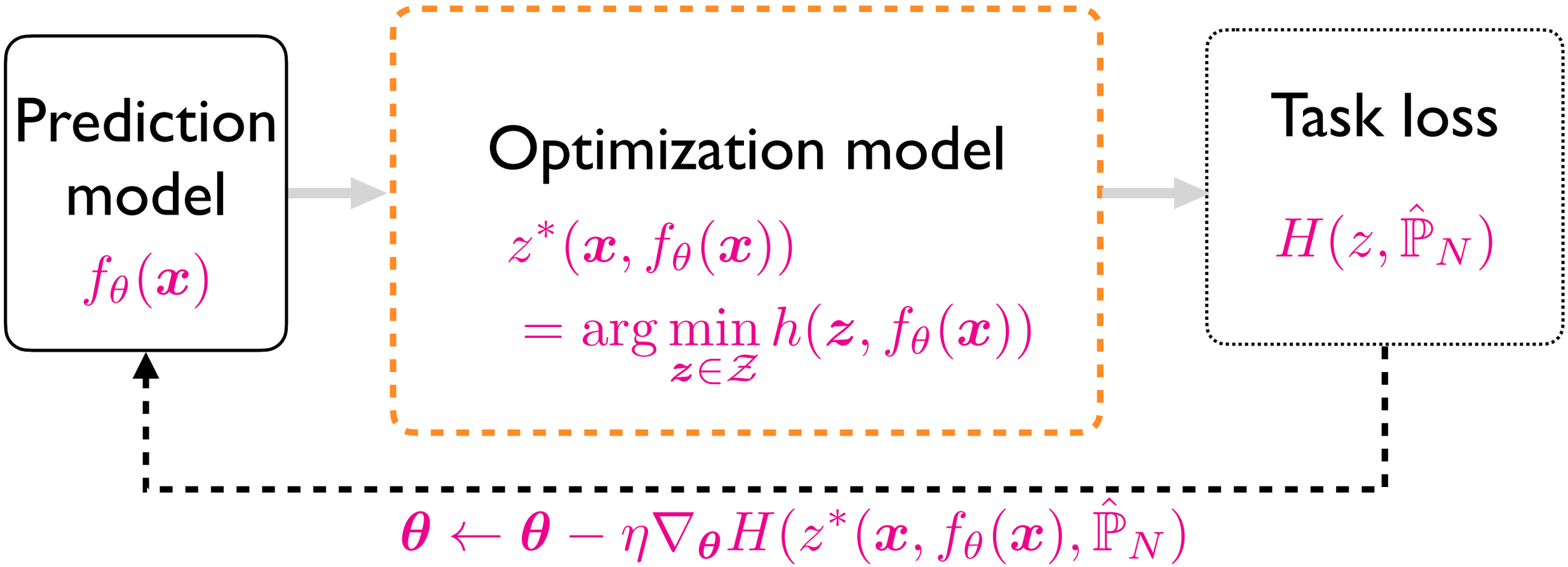
ILO training pipeline



$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} H(\hat{z}(\boldsymbol{x}, \mathcal{N}(\boldsymbol{\theta}^\top \boldsymbol{x}, 1)), \hat{\mathbb{P}}_N)$$

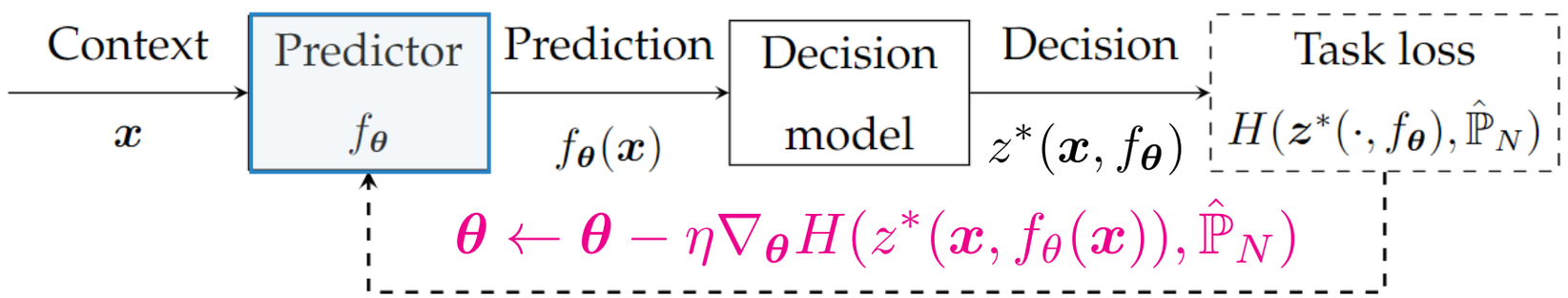
- [Bengio 1997] : Task-aware point prediction under a **fixed decision rule**

ILO training pipeline



- [Bengio 1997] : Task-aware point prediction under a **fixed decision rule**
- [Donti et al. 2017] : Task-aware conditional density prediction under **CSO model**

How to differentiate through argmin operation?



- Implicit differentiation through KKT conditions for convex problems
- Unroll the operations made by the optimization process:
  - Differentiate through its computational graph
  - Implicit differentiation of the fixed point equations at local optimum [Butler and Kwon, 2023] and [Kotary et al. 2023]
- Replace optimizer with a differentiable deep neural network [Grigas et al. 2021]
- Libraries: TorchOpt [Bilevel], CvxpyLayer [Convex], PyEPO [Linear]

Smart "Predict, then optimize"

- Regret minimization [Elmachtoub & Grigas, 2022]:

$$H(z^*(\boldsymbol{x}, f_\theta), \mathbb{P}) \ := \mathbb{E}_{\mathbb{P}}[c(z^*(\boldsymbol{x}, f_\theta), \boldsymbol{y})]$$

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  - Non-convex and discontinuous in θ
  - Replace with SPO+:

$$\min_{\theta} \mathbb{E}_{\mathbb{P}} \left[\ell_{\text{SPO+}}(g_\theta(\boldsymbol{x}), \boldsymbol{y}) \right]$$

where

$$\ell_{\text{SPO+}}(\hat{\boldsymbol{y}}, \boldsymbol{y}) := \sup_{\boldsymbol{z} \in \mathcal{Z}} (\boldsymbol{y} - 2\hat{\boldsymbol{y}})^T \boldsymbol{z} + 2\hat{\boldsymbol{y}}^T \boldsymbol{z}^*(\boldsymbol{x}, \boldsymbol{y}) - \boldsymbol{y}^T \boldsymbol{z}^*(\boldsymbol{x}, \boldsymbol{y}),$$

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  - Solve an optimization problem at each iteration
  - SPO+ has slower convergence rate than SLO approach
  - If model misspecified, SPO+ can outperform SLO

Optimal action imitation

- Imitation performance metric:

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Optimal action imitation

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Optimal action imitation

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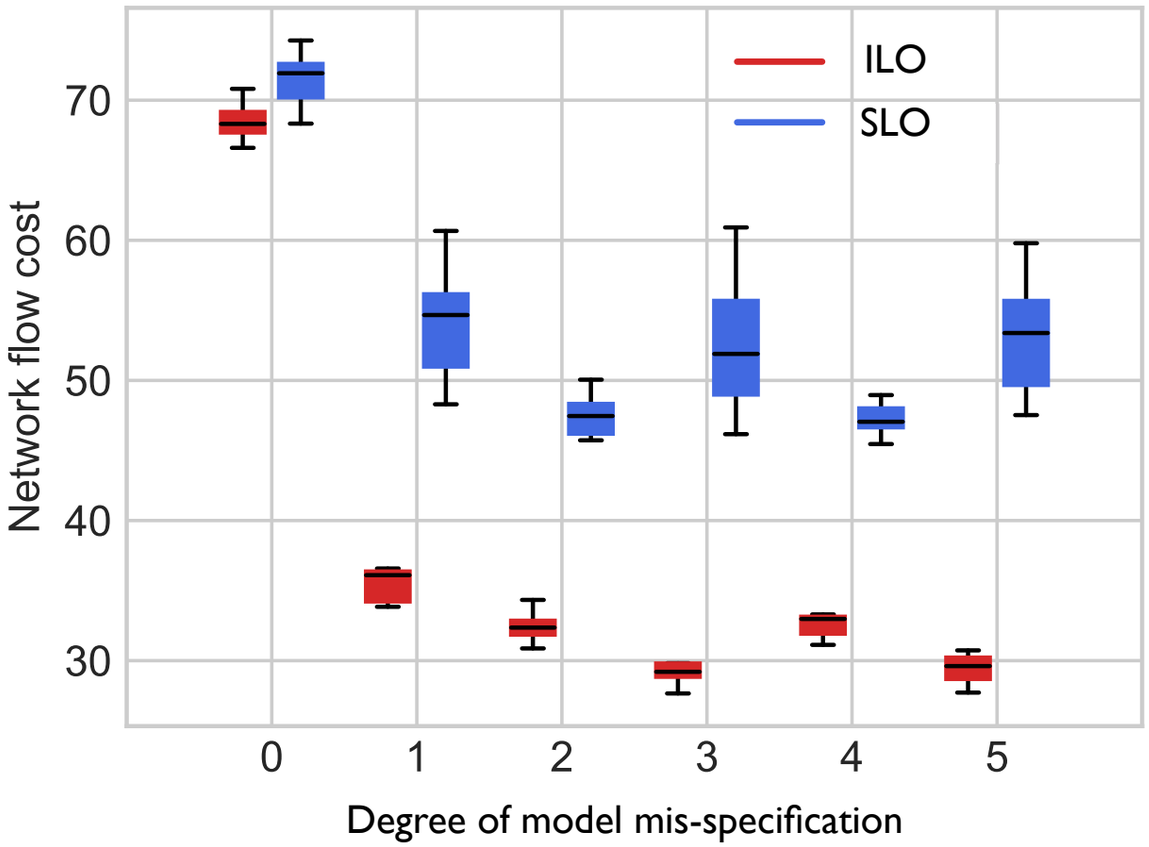
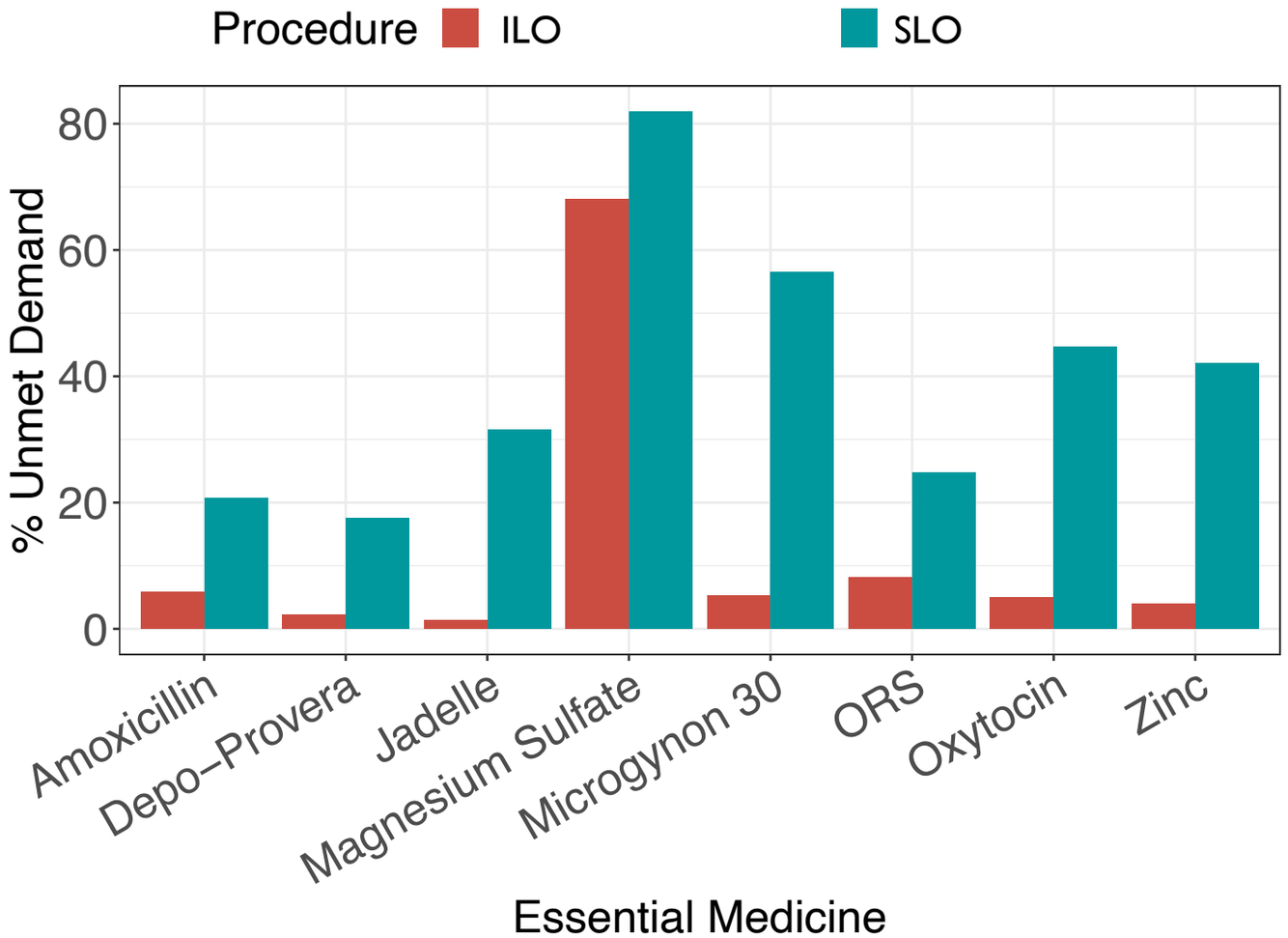
- Training based on perturbed optimizers:
  - [Berthet et al., 2020] uses additive perturbation of point prediction
  - [Dalle et al. , 2022] uses multiplicative perturbations
  - [Mulamba et al., 2021] and [Kong et al., 2022] uses energy-based optimizer

$$\tilde{z}(\boldsymbol{x}, f_\theta) \sim \frac{\exp(-\alpha h(\boldsymbol{z}, f_\theta(\boldsymbol{x}))}{\int \exp(-\alpha h(\boldsymbol{z}, f_\theta(\boldsymbol{x}))d\boldsymbol{z}}$$

ILO outperforms SLO



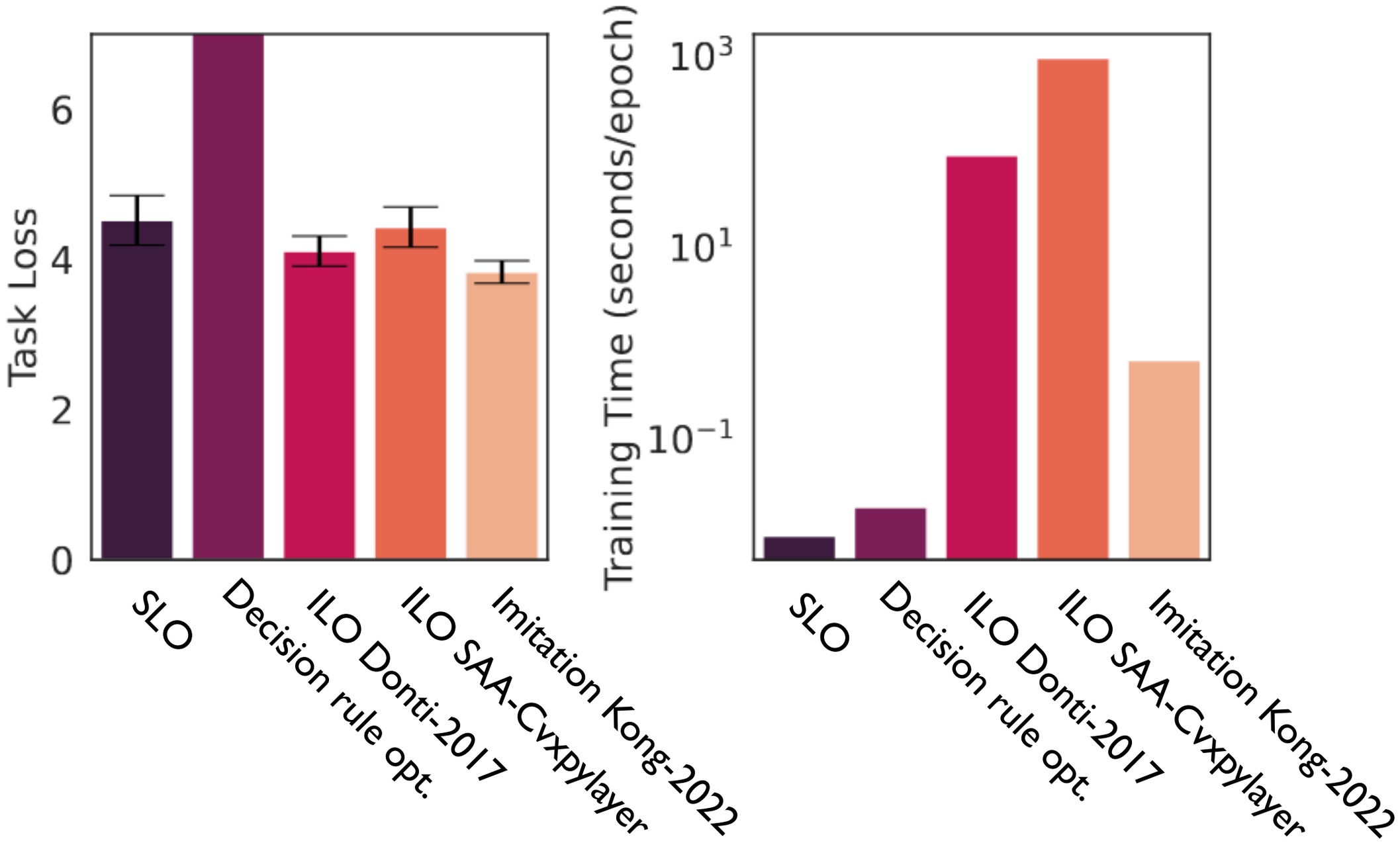
Source: [Grigas et al. 2021]



Source: [Chung et al. 2022]

Comparison of different approaches

Load forecasting and generator scheduling problem



Source: [Kong et al. 2022]

Take-away messages

- Contextual stochastic optimization is a rapidly evolving field that provides methods for identifying data-driven decision that exploit most recently available information.
- Three types of approaches:
  - Decision rule/policy optimization
  - Sequential learning and optimization
  - Integrated learning and optimization
- Four types of performance measures:
  - Statistical accuracy of prediction model
  - Task-based expected cost of induced policy
  - Task-based expected regret of induced policy
  - Quality of imitation
- Many potential applications ?

(Link to survey paper)

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