# Decision-focused learning: theory, applications, challenges

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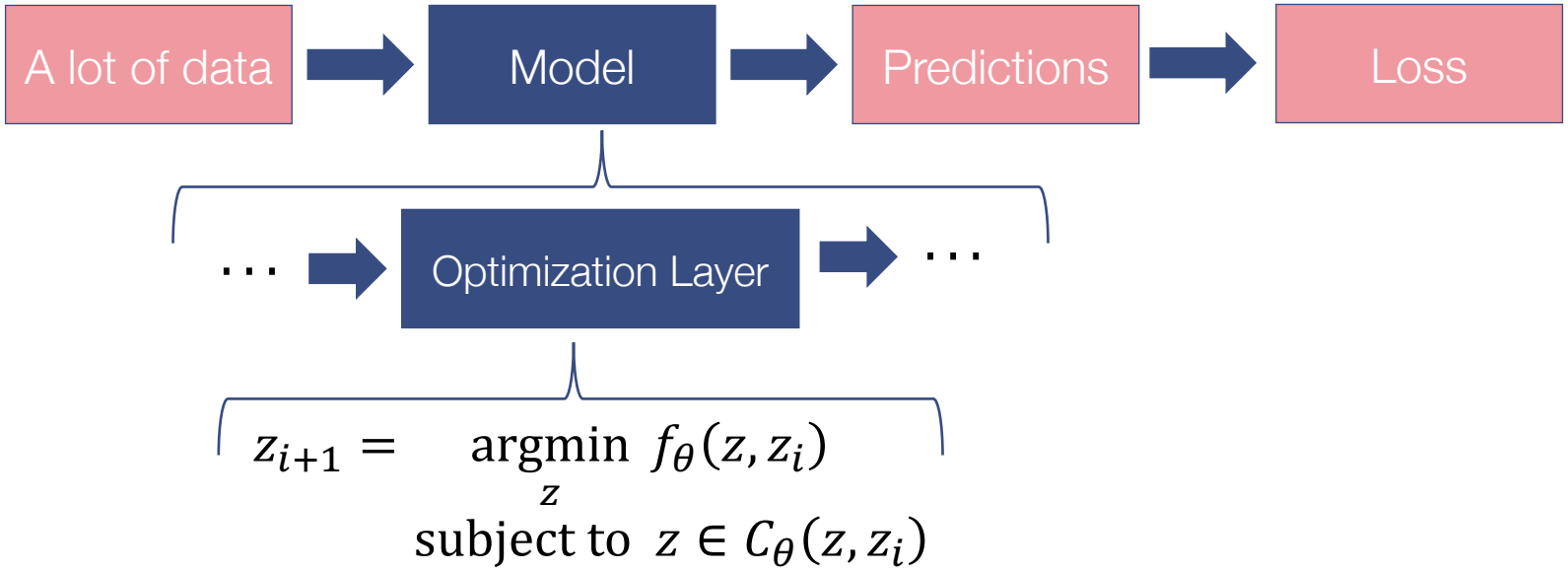
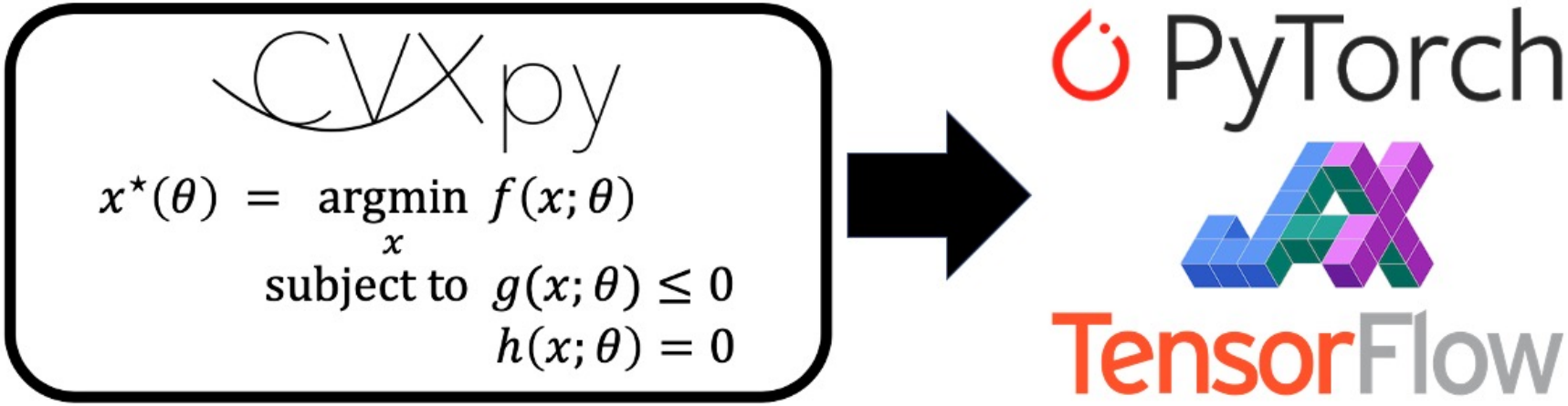
THE OHIO STATE UNIVERSITY

# Brandon's talk recap



# Agenda

What is decision-focused learning? Why should you care?

Decision-focused learning for sequential decision problems (NeurIPS 2021)

Learning convex & smooth loss functions for decision-focused learning (arXiv)

# Notation: predict-then-optimize

Observable feature/context vector $x \in X$

Unobserved ground truth environment parameter $\theta^* \in \Theta$

$x$ and $\theta^*$ drawn jointly from fixed distribution $\mathcal{D}$

Decision/control variable $z \in Z$

Objective function $f(z, \theta^*)$

Goal: $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

Wilder et al. (AAAI 2019)

# Notation: predict-then-optimize

Observable feature/context vector $x \in X$

Unobserved ground truth environment parameter $\theta^* \in \Theta$

$x$ and $\theta^*$ drawn jointly from fixed distribution $\mathcal{D}$

Observed at training time, but not test time

Decision/control variable $z \in Z$

Objective function $f(z, \theta^*)$

Goal: $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

# Notation: predict-then-optimize

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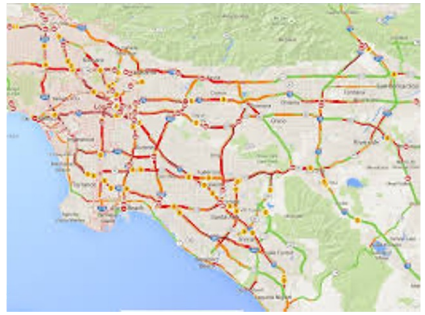
**Predict-then-optimize routing**

**Context $x$**

**Decision: route $z$**

**Objective $f(x, z)$: minimize travel time under traffic**



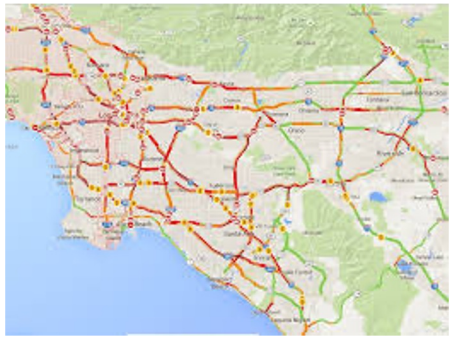
Wilder et al. (AAAI 2019)

# Motivation of predict-then-optimize

**Data =**

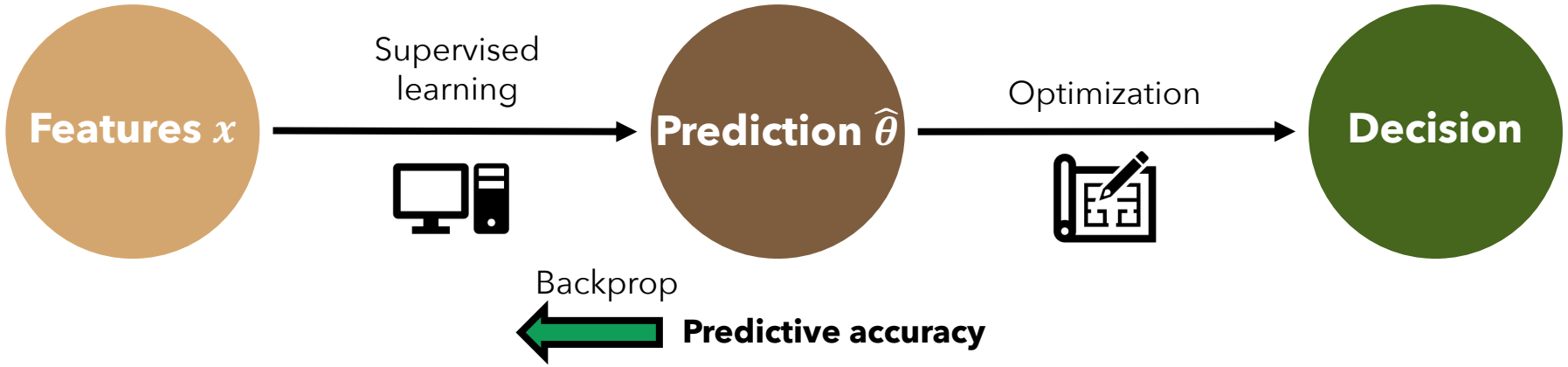
$$\{( \quad , \quad )\}$$

$i$



$i$

# Two-stage pipeline for predict-then-optimize



# What do we lose by simplifying?

$\min_{z \in Z} f(z, \mathbb{E}(\theta|x))$ instead of $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

Two-stage

What we want

# What do we lose by simplifying?

$\min_{z \in Z} f(z, \mathbb{E}(\theta|x))$ instead of $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

Consider $f(z, \theta) = \sum_i \theta_i z_i$. Then,

$$\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta) = \min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} \sum_i \theta_i z_i$$

$$= \min_{z \in Z} \sum_i \mathbb{E}[\theta_i|x] z_i = \min_{z \in Z} f(z, \mathbb{E}(\theta|x))$$

# Product of predictions

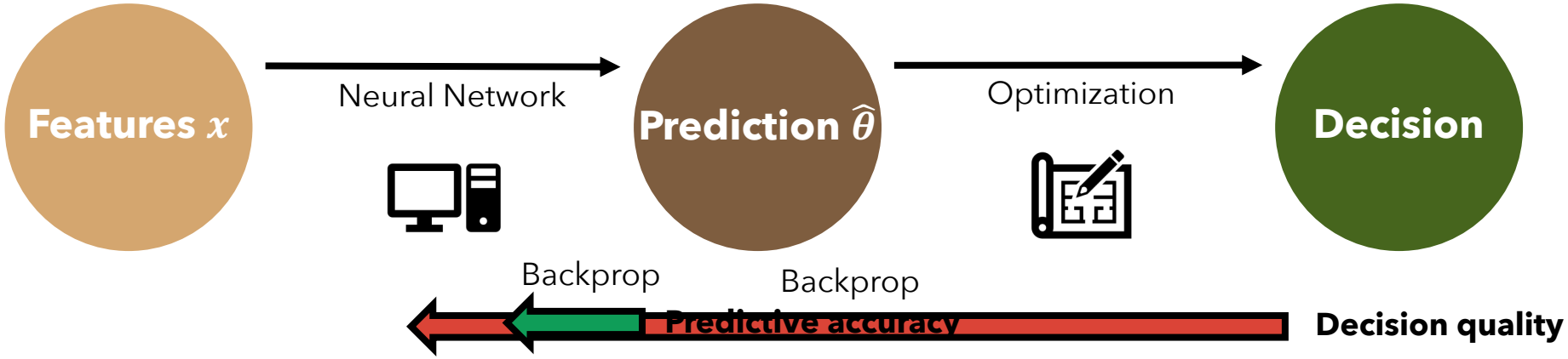
$\min_{z \in Z} f(z, \mathbb{E}(\theta|x))$ instead of $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

Consider $f(z, \theta) = \sum_i \theta_{2i}\theta_{2i+1}z_{2i}$. Then,

$$\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta) = \min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} \sum_i \theta_{2i}\theta_{2i+1}z_{2i}$$

$$\neq \min_{z \in Z} \sum_i \mathbb{E}[\theta_{2i}|x]\mathbb{E}[\theta_{2i+1}|x]z_{2i}$$

# Does differentiable optimization help?




Wilder et al. (AAAI 2019)

Theorem (Cameron et al., 2022): There exists a class of problems (two-stage minimum cost flow from Agrawal et al., 2012) such that:

- $\mathbf{DFL} = \mathbf{OPT}$
- $\frac{\mathbf{2S}}{\mathbf{DFL}}$ is at least $\Omega(2^d)$, where $d = \dim(\mathrm{Z}) = \dim(\Theta)$

# Optimizing policies in unknown MDPs

Environment (MDP)

RL solver

RL policy

# Planning for Community Health Workers

Key tasks:
Maternal health checkups
Behavioral health interventions
Medication adherence support

Photo credit: Pippa Ranger

# Adherence monitoring for TB

Tuberculosis (TB): 500,000 deaths/year, 3 million infected in India

Curing TB requires 6 months of daily medication

Symptoms disappear quickly

Mate, Killian, Xu, P, Tambe (NeurIPS 2020)

# TB medication adherence

today | February | 2016

enrollment/end | received | shared phone numbers | manual | not on 99DOTS | missed (hover for reason)

**ART Programs**

Showing: NKL

| ID # | Attention Required | Patient |
|---|---|---|
| 6204 | MEDIUM | |
| 6214 | MEDIUM | |
| 6218 | MEDIUM | |
| 6231 | MEDIUM | |
| 6232 | MEDIUM | |
| 6235 | MEDIUM | |
| 6260 | MEDIUM | |
| 6264 | MEDIUM | |
| 6272 | MEDIUM | |
| 6287 | MEDIUM | |
| 6312 | MEDIUM | |
| 6334 | HIGH | |

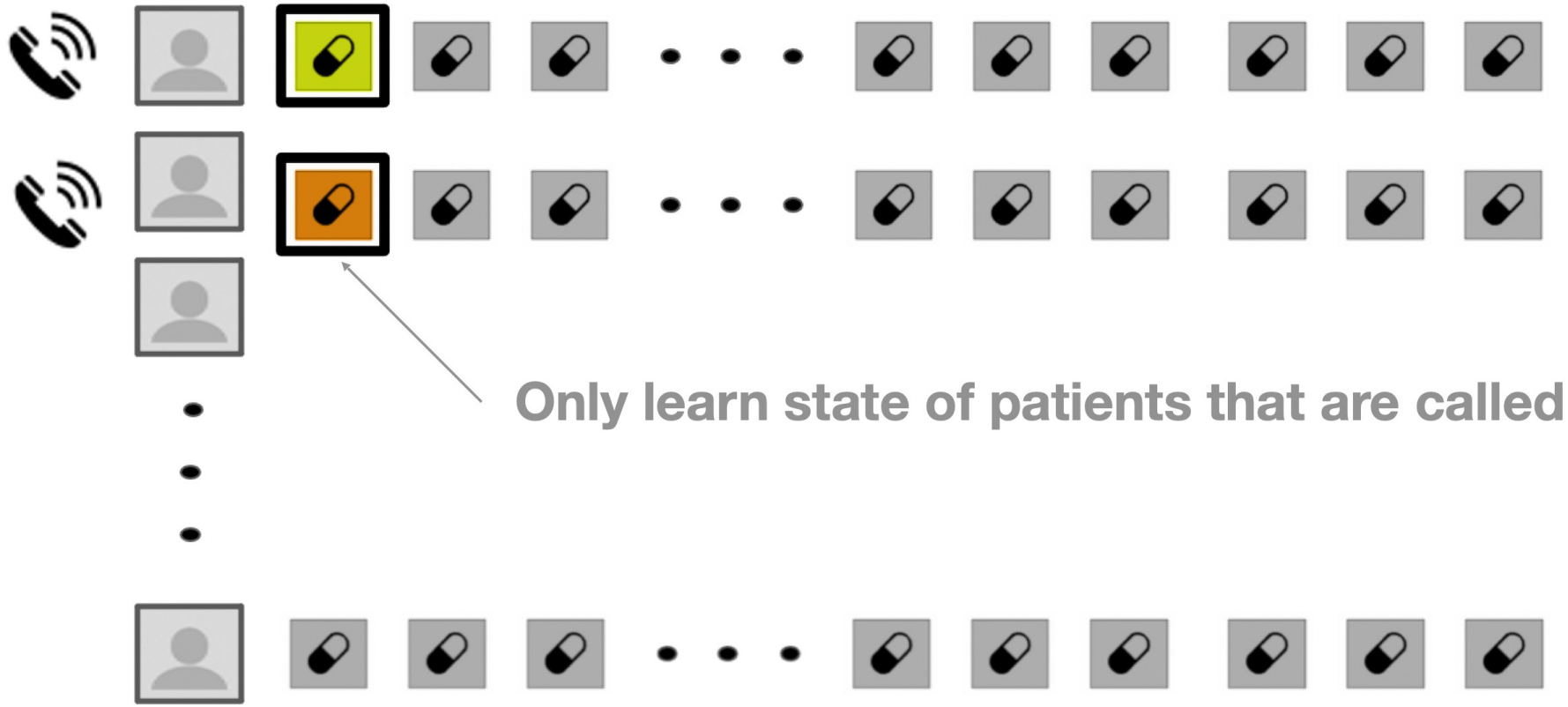
Everwell

Mate, Killian, Xu, P, Tambe (NeurIPS 2020)

# Adherence example

6 months

# Adherence example

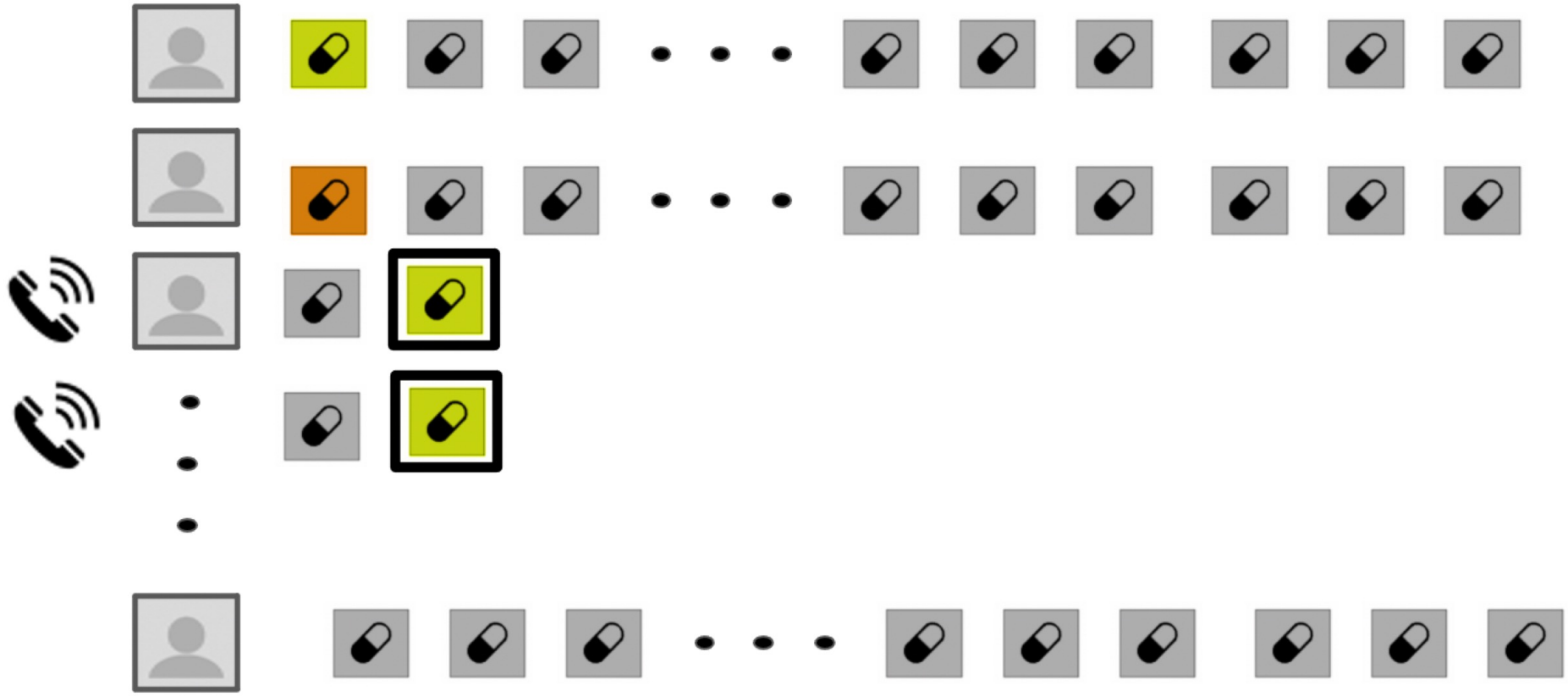



Adhering

Not adhering

Unknown

# Adherence example



Adhering

Not adhering

Unknown

# POMDP formulation

Each patient is represented by a partially observable Markov decision process (POMDP)

Shared action budget across all processes

States 

Actions 

Observations 

Transitions $P_n^{\text{call}}$ $P_n^{\text{no call}}$

Rewards  = 1  = 0

Goal: find optimal policy $\pi^*$—a mapping from the action-observation history to actions that maximizes reward

# POMDP formulation

Each patient is represented by a partially observable Markov decision process (POMDP)

Shared action budget across all processes

States 

Actions 

Observations 

Transitions $P_n$ $P_n$

Rewards  = 1  = 0

Unknown and different per patient!

Goal: find optimal policy $\pi^*$—a mapping from the action-observation history to actions that maximizes reward

# Patient data

Patient context $x$

Trajectory $\{(s_t, a_t, r_t, s_{t+1})\}$

# Predict-then-optimize?

Observable feature/context vector $x \in X$

Unobserved ground truth environment parameter $\theta^* \in \Theta$

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Decision/control variable $z \in Z$

Objective function $f(z, \theta^*)$

Goal: $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

# Predict-then-optimize?

Observable feature/context vector
$x \in X$

Unobserved ground truth environment parameter $\theta^* \in \Theta$

$x$ and $\theta^*$ drawn jointly from fixed distribution $\mathcal{D}$

Not available at training time–only have trajectories

Decision/control variable $z \in Z$

Objective function $f(z, \theta^*)$

Goal: $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

# Contributions

How to differentiate through the optimal policy in sequential decision problems

(and how to speed it up)

Do DFL with only trajectories (i.e., without $\theta^*$ labels)

# Problem setting

Let $(\mathcal{S}, s_0, A, T, R)$ be an *incomplete* MDP specification with:

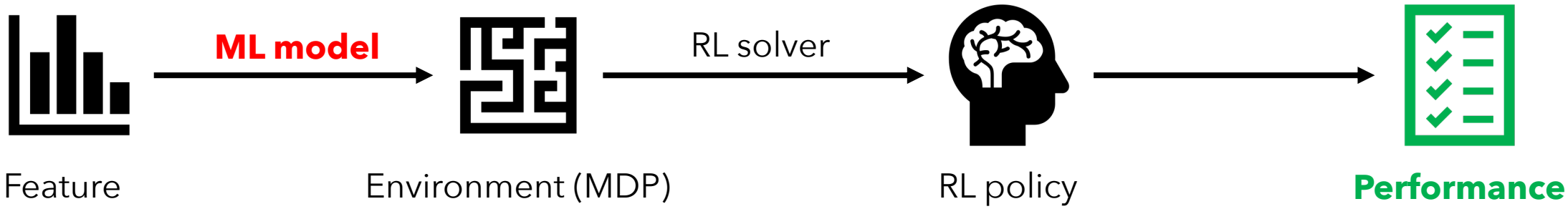
- Initial state $s_0$
- Set of states $\mathcal{S}$
- Set of actions $A$
- Possibly incomplete transition function: $T: \mathcal{S} \times A \to \Delta\mathcal{S}$
- Possible incomplete reward function: $\mathrm{R}: \mathcal{S} \times A \to \mathbb{R}$

Each MDP has a context vector $\boldsymbol{x}$

Each training MDP has a set of trajectories $\mathcal{T}$

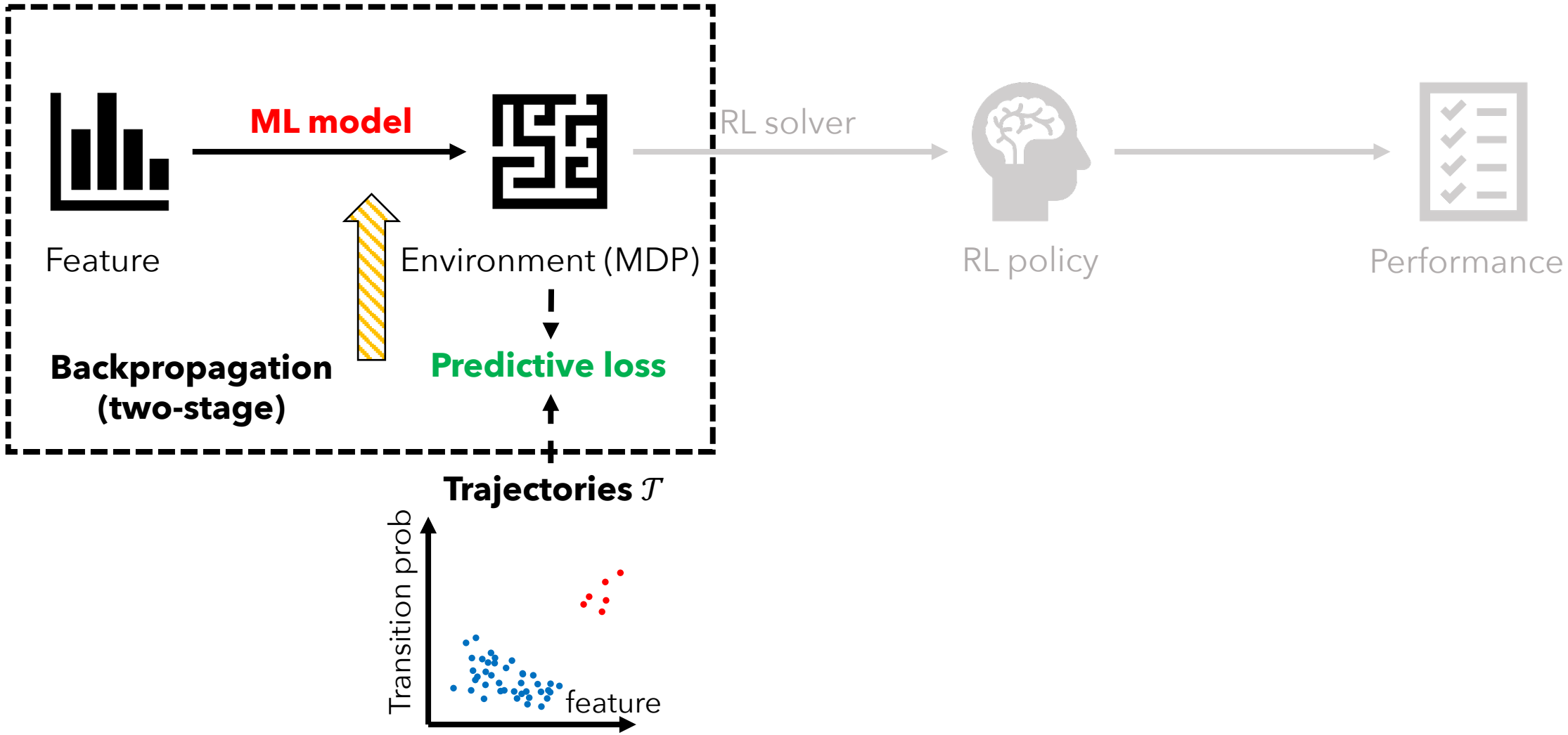
Goal: learn a predictive model $m_w$ that "completes" the MDP from $\boldsymbol{x}$ and maximizes reward on $\mathcal{T}$

# Pipeline visualized

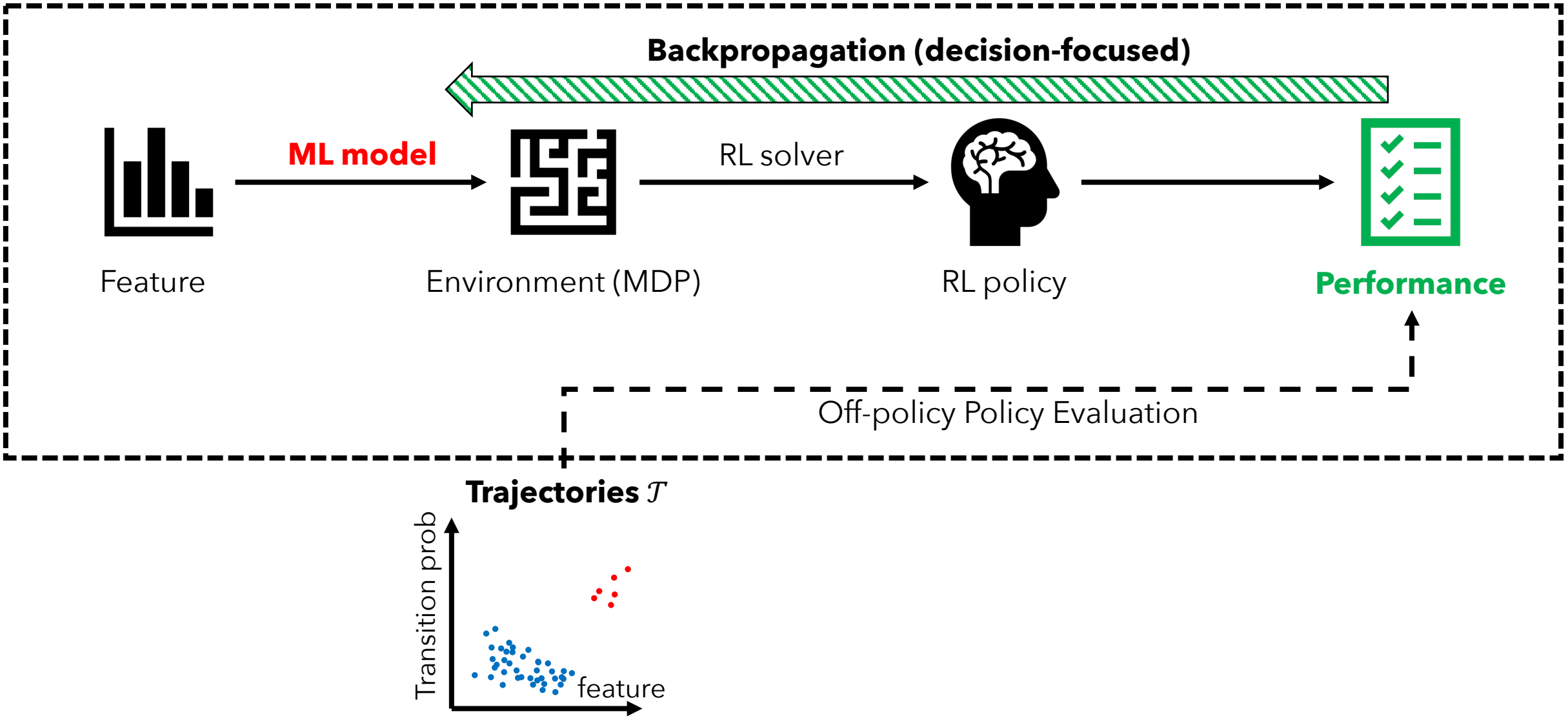



Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

# Two-stage approach

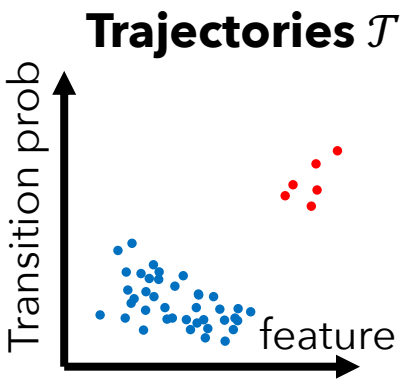


# Decision-focused approach




Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

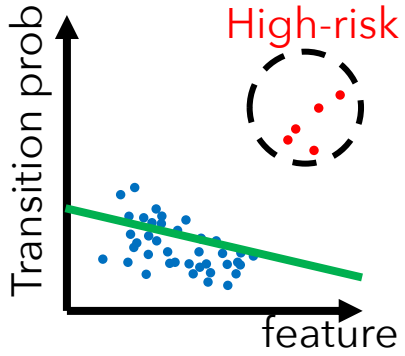
# Two-stage vs. DFL



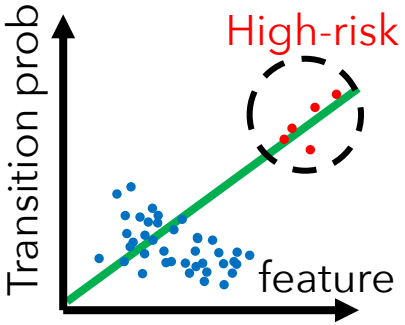

**Trajectories** $\mathcal{T}$

**Two-stage**
Focus on predictive accuracy

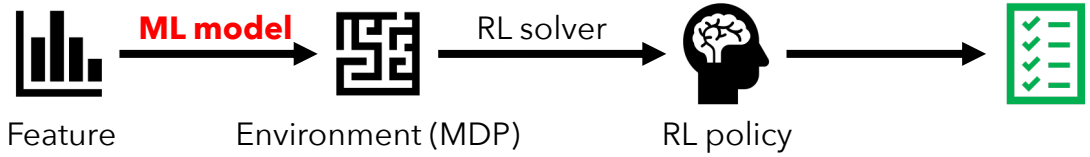
**Decision-focused**
Focus on decision quality




High predictive accuracy
Low decision quality




Low predictive accuracy
High decision quality




Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

# How DFL works

To run gradient descent, we need to compute

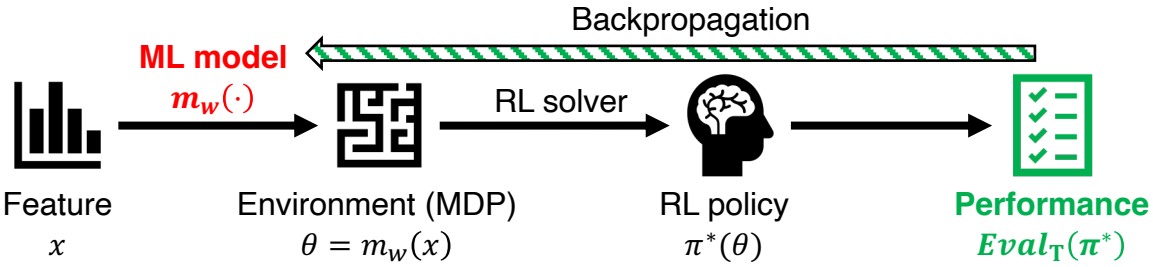
$$\frac{dEval_{\mathrm{T}}(\pi^*)}{dw} = \frac{d\theta}{dw}\frac{\boldsymbol{d\pi^*}}{\boldsymbol{d\theta}}\frac{dEval_{\mathrm{T}}(\pi^*)}{d\pi^*}$$

**Weights $w$ of predictive model**

**We use a metric from Futoma et al.**

$$\mathrm{Eval}_{\mathcal{T}}(\pi) := V^{\mathrm{CWPDIS}}(\pi) - \lambda_{\mathrm{ESS}}/\sqrt{\mathrm{ESS}(\pi)} \quad (1)$$

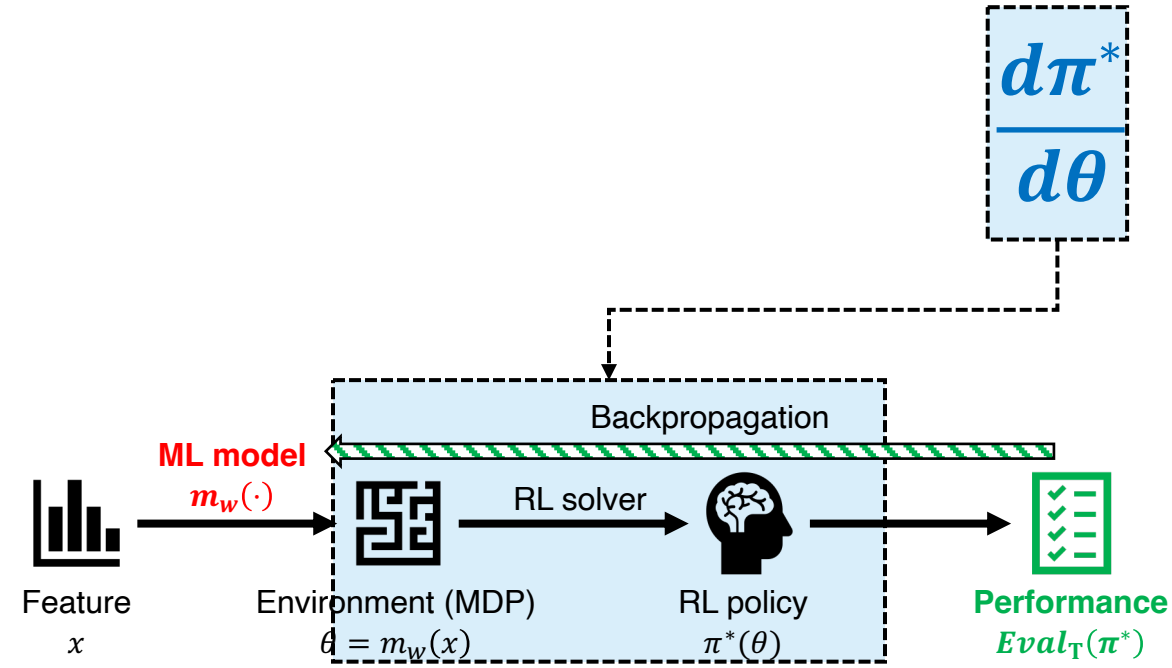
where $V^{\mathrm{CWPDIS}}(\pi) := \sum_{t=1}^{h} \gamma^t \frac{\sum_i r_{it}\rho_{it}(\pi)}{\sum_i \rho_{it}(\pi)}$ and $\mathrm{ESS}(\pi) := \sum_{t=1}^{h} \frac{(\sum_i \rho_{it})^2}{\sum_i \rho_{it}^2}$, and $\rho_{it}(\pi)$ is the ratio of the proposed policy and the behavior policy likelihoods up to time t: $\rho_{it}(\pi) := \prod_{t'=1}^{t} \frac{\pi(a_{it'}|s_{it'})}{\pi_{\mathrm{beh}}(a_{it'}|s_{it'})}$.




Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

# Leveraging optimality conditions

Differentiate through one-shot optimization problem by optimality condition (Amos et al., 2017)



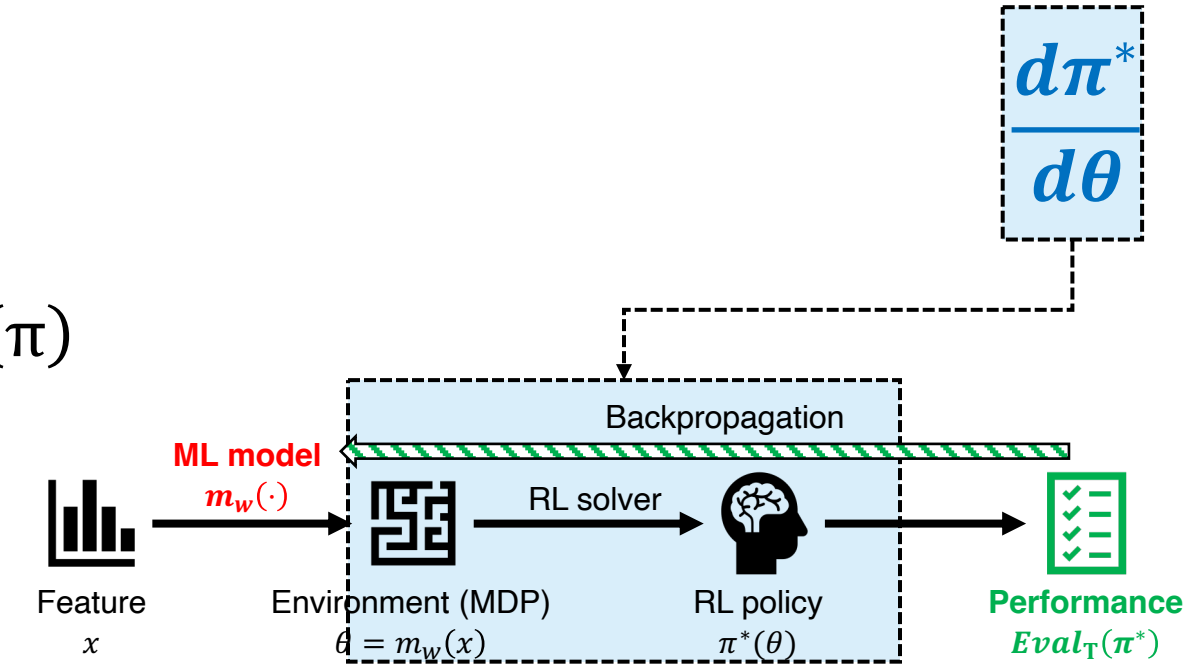
# Leveraging optimality conditions

Expected cumulative return

Policy optimality: $\pi^* = \text{argmax}_\pi \, J_\theta(\pi)$

Bellman optimality: $\pi^* = \text{argmin}_\pi \, B_\theta(\pi)$

Differentiate through one-shot optimization problem by optimality condition (Amos et al., 2017)



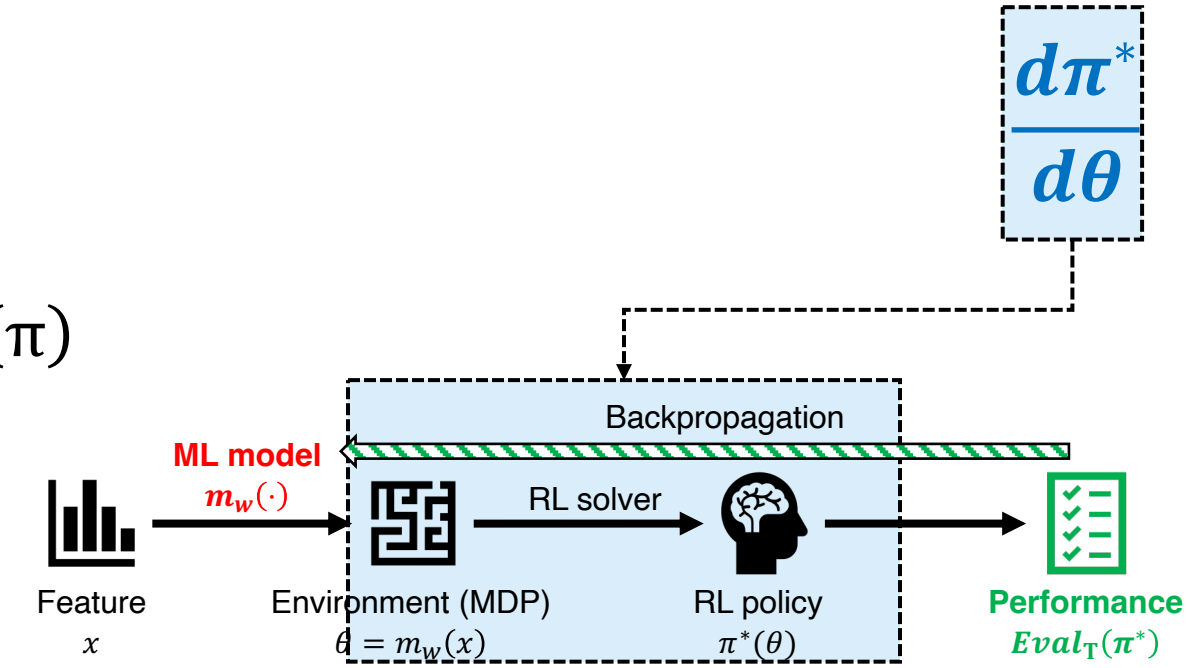
# Leveraging optimality conditions

Expected cumulative return

Policy optimality: $\pi^* = \text{argmax}_\pi \, J_\theta(\pi)$

KKT conditions: $\nabla_\pi J_\theta(\pi^*) = 0$

Bellman optimality: $\pi^* = \text{argmin}_\pi \, B_\theta(\pi)$

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# Leveraging optimality conditions

Expected cumulative return

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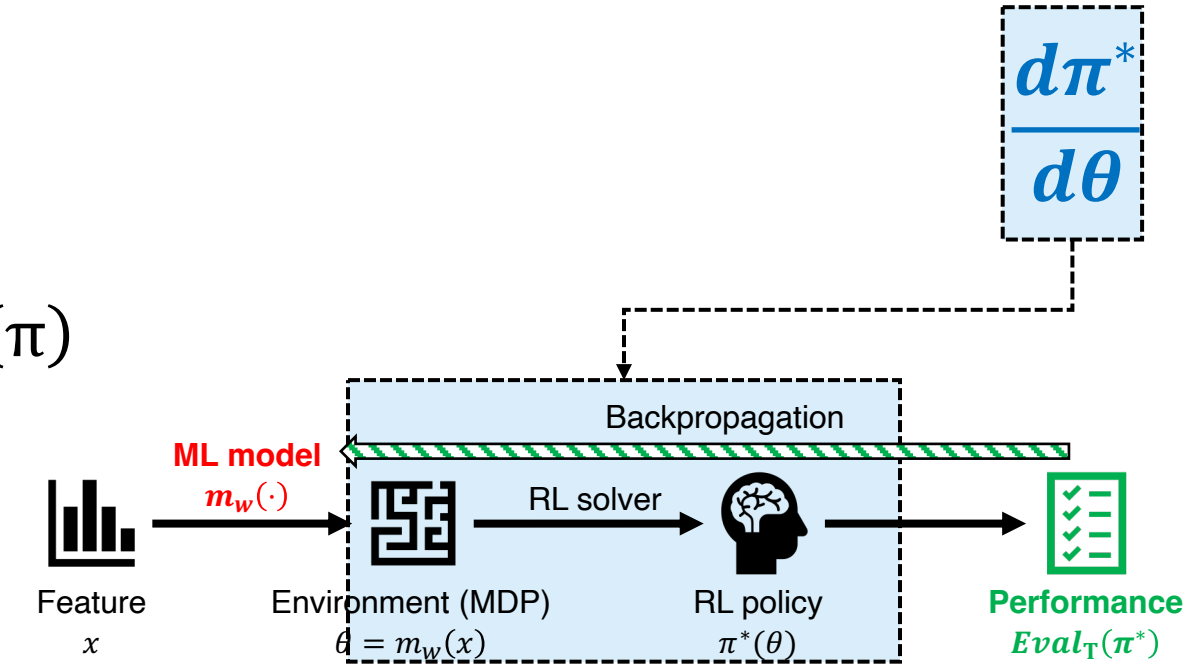



Differentiate through one-shot optimization problem by optimality condition (Amos et al., 2017)

# Leveraging optimality conditions

Expected cumulative return

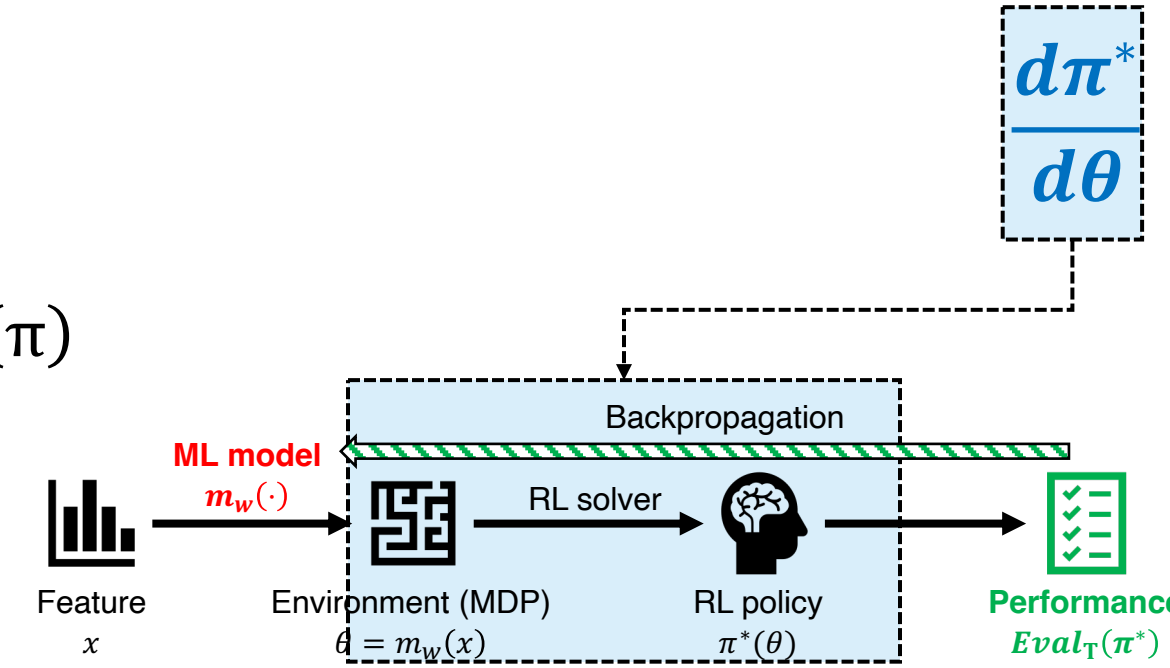
Policy optimality: $\pi^* = \text{argmax}_\pi \, J_\theta(\pi)$

KKT conditions: $\frac{d}{d\theta} \nabla_\pi J_\theta(\pi^*) = 0$

$$\nabla^2_\pi J_\theta(\pi^*) \frac{\mathbf{d}\boldsymbol{\pi}^*}{\mathbf{d}\boldsymbol{\theta}} + \nabla^2_{\theta\pi} J_\theta(\pi^*) = 0$$

Bellman optimality: $\pi^* = \text{argmin}_\pi \, B_\theta(\pi)$

Differentiate through <u>one-shot optimization problem</u> by optimality condition (Amos et al., 2017)



# Leveraging optimality conditions

Expected cumulative return (implicitly defined)

Policy optimality: $\pi^* = \text{argmax}_\pi \, J_\theta(\pi)$

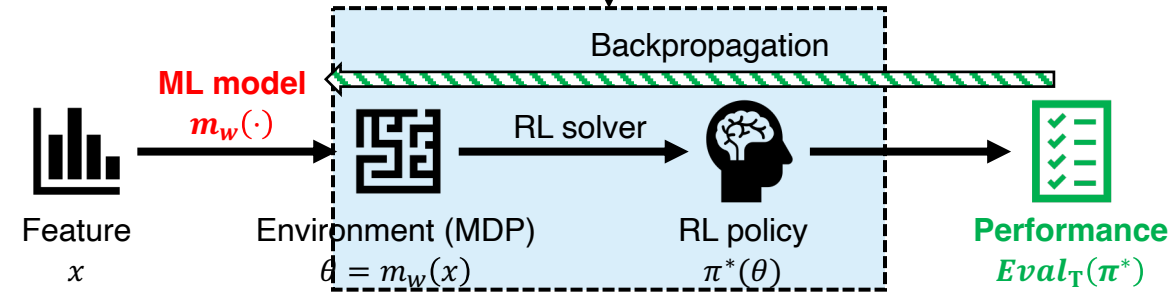
KKT conditions: $\frac{d}{d\theta} \nabla_\pi J_\theta(\pi^*) = 0$

$$\nabla^2_\pi J_\theta(\pi^*) \frac{\mathbf{d}\boldsymbol{\pi}^*}{\mathbf{d}\boldsymbol{\theta}} + \nabla^2_{\theta\pi} J_\theta(\pi^*) = 0$$

$$\frac{\boldsymbol{d\pi}^*}{\boldsymbol{d\theta}} = \left(\nabla^2_\pi J_\theta(\pi^*)\right)^{-1} \nabla^2_{\theta\pi} J_\theta(\pi^*)$$

Bellman optimality: $\pi^* = \text{argmin}_\pi \, B_\theta(\pi)$

Differentiate through one-shot optimization problem by optimality condition (Amos et al., 2017)



# Computational challenges

Policy optimality: $\pi^* = \text{argmax}_\pi J_\theta(\pi)$

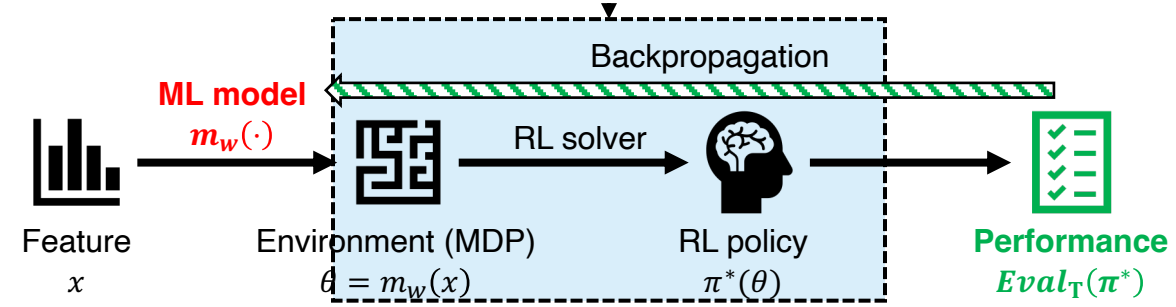
Bellman optimality: $\pi^* = \text{argmin}_\pi B_\theta(\pi)$

Different approximations of $\nabla^2_\pi J_\theta(\pi^*)$

| Method | Computation | Accuracy |
|---|---|---|
| Full Hessian | $n^2k + n^\omega$ ✗ | High |

$n$: size of $\pi$
$k$: number of trajectories to compute the policy gradient

$$\frac{d\pi^*}{d\theta} = \left(\nabla^2_\pi J_\theta(\pi^*)\right)^{-1} \nabla^2_{\theta\pi} J_\theta(\pi^*)$$




Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

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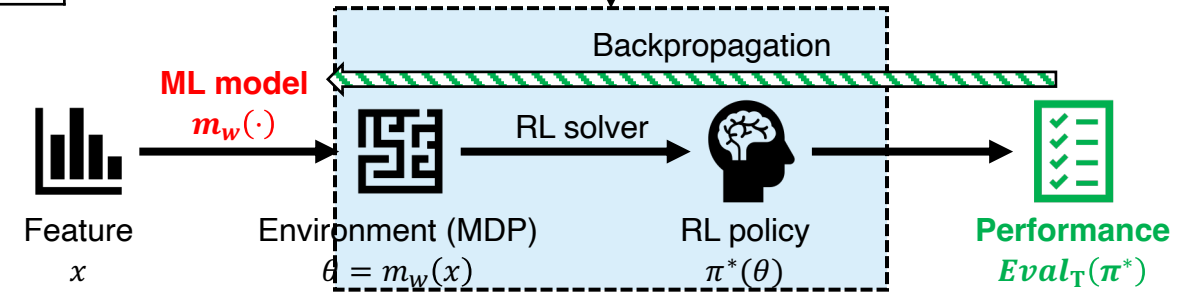
Different approximations of $\nabla^2_\pi J_\theta(\pi^*)$

| Method | Computation | Accuracy |
|---|---|---|
| Full Hessian | $n^2k + n^\omega$ ✗ | High |
| Identity matrix | $nk$ ✓ | Low |

$n$: size of $\pi$
$k$: number of trajectories to compute the policy gradient

$$\frac{d\pi^*}{d\theta} = \left(\nabla^2_\pi J_\theta(\pi^*)\right)^{-1} \nabla^2_{\theta\pi} J_\theta(\pi^*)$$

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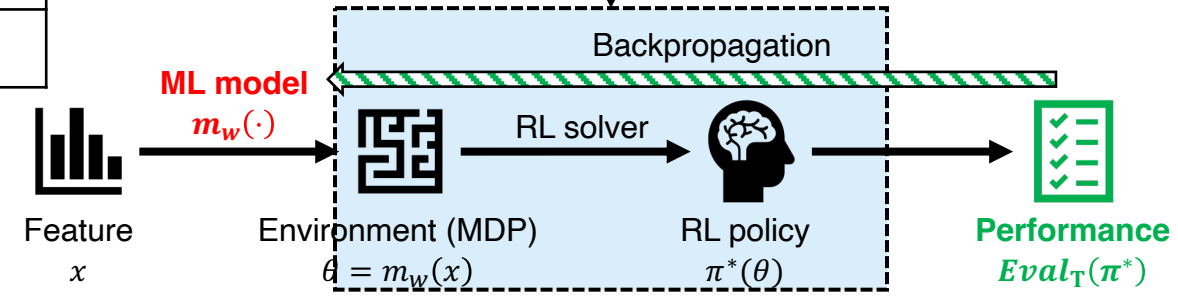
Different approximations of $\nabla^2_\pi J_\theta(\pi^*)$

| Method | Computation | Accuracy |
|---|---|---|
| Full Hessian | $n^2k + n^\omega$ ✗ | High |
| Identity matrix | $nk$ ✓ | Low |
| Woodbury (low-rank $k$) | $nk + k^\omega$ ✓ | Medium |

$n$: size of $\pi$
$k$: number of trajectories to compute the policy gradient

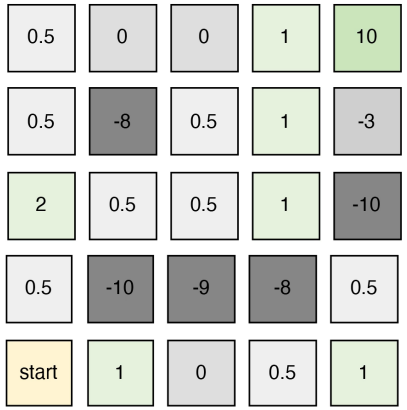
$$\frac{d\pi^*}{d\theta} = \left(\nabla^2_\pi J_\theta(\pi^*)\right)^{-1} \nabla^2_{\theta\pi} J_\theta(\pi^*)$$



# Experiments

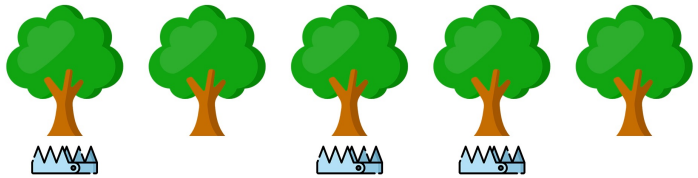
## Predict-then-optimize problems with missing MDP parameters

Reward




**Gridworld problem**
**Feature**: grid cell features
**Prediction**: grid cell reward
**Action**: movement

Transition probability



**Snare-finding problem**
**Feature**: location features
**Prediction**: snaring risk
**Action**: visit a location to remove snares

Transition probability

**Tuberculosis problem**
**Feature**: patient features
**Prediction**: patient transition probabilities
**Action**: visit a patient to intervene

# Methods

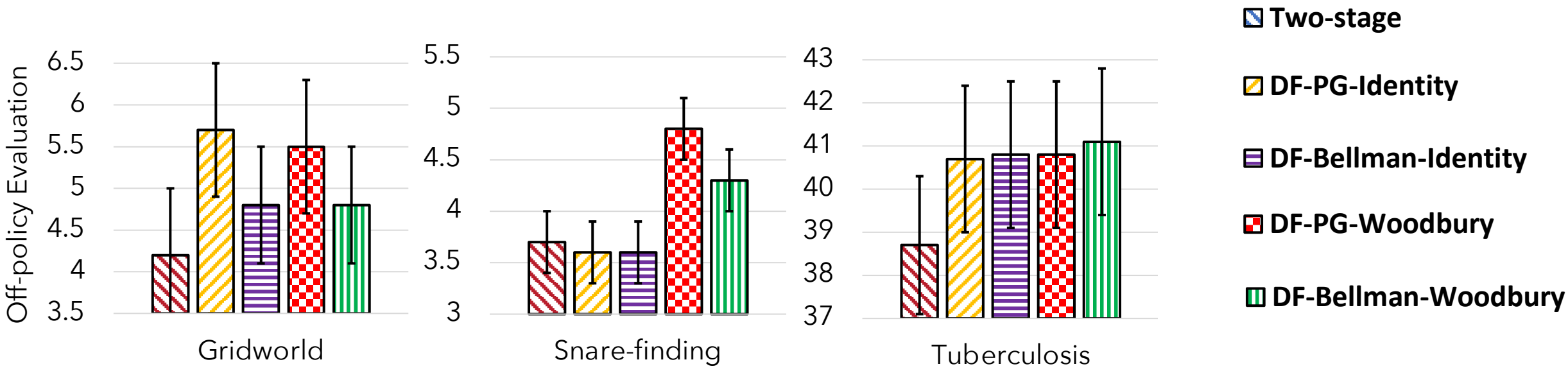
**Standard two-stage approach**

**Two-stage**

**Optimality condition**

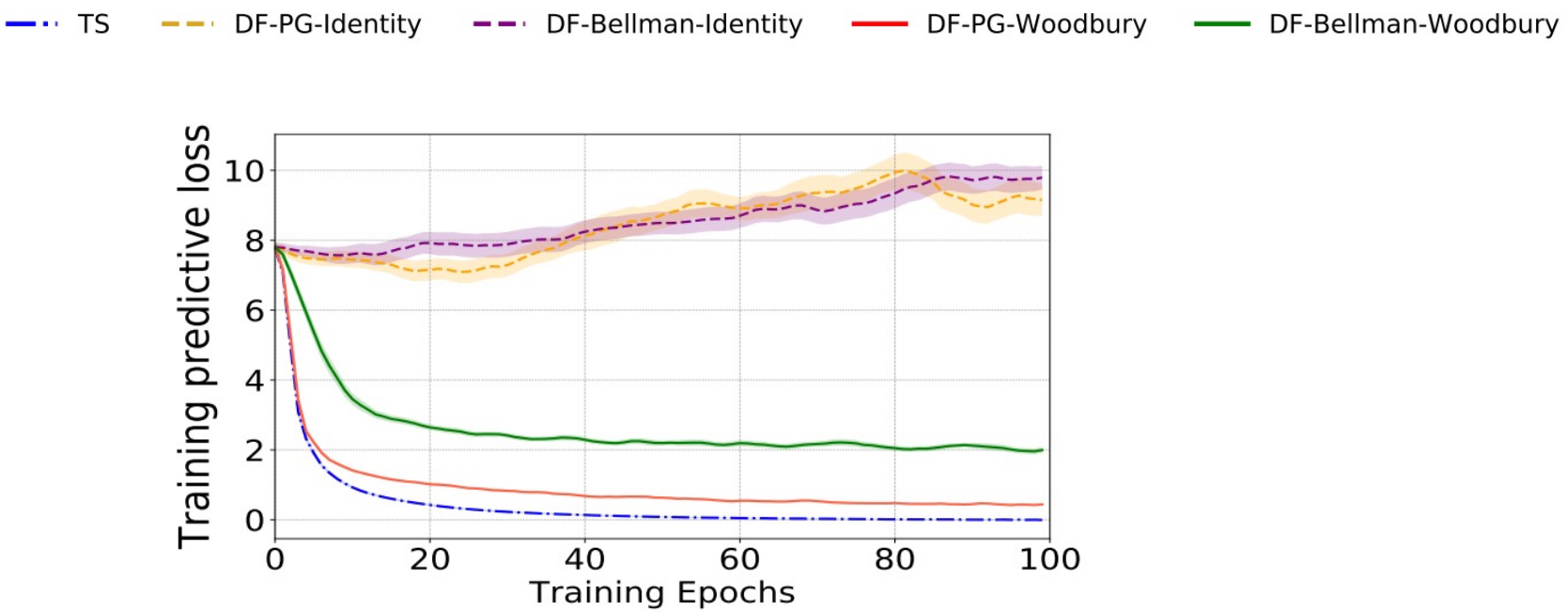
| **Approximation** | Policy gradient | Bellman error |
| --- | --- | --- |
| Identity | **DF-PG-Identity** | **DF-Bellman-Identity**<br>Futoma et al. (AISTATS 2020) |
| Woodbury (low-rank) | **DF-PG-Woodbury** | **DF-Bellman-Woodbury** |

# Results



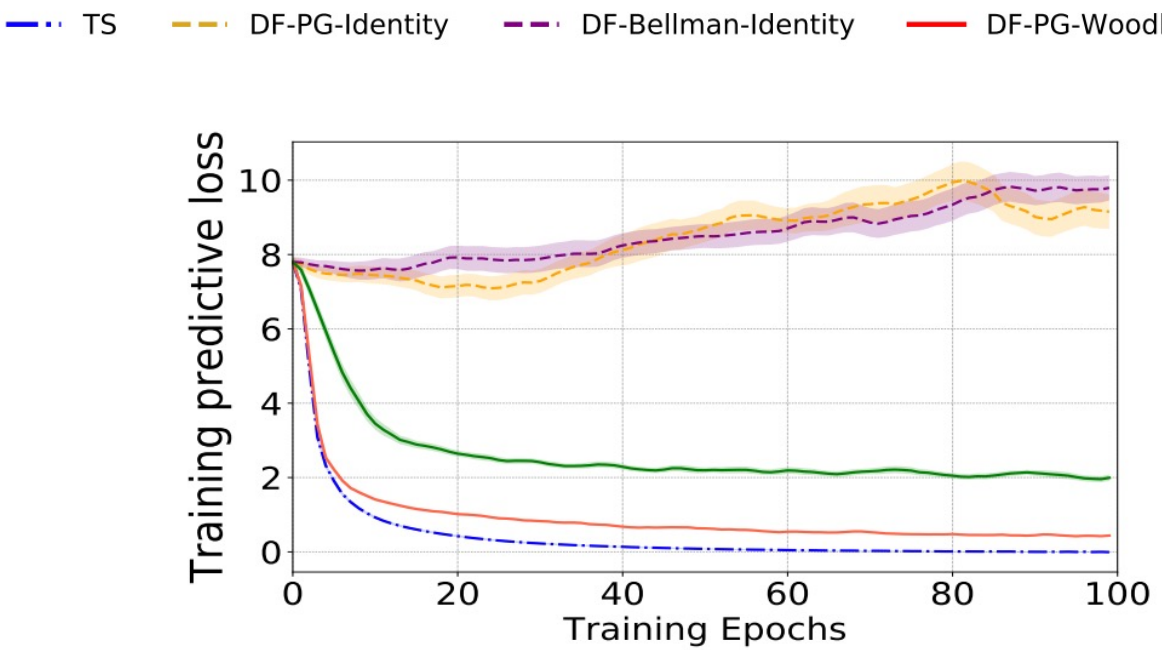

DFL outperforms two-stage
Woodbury-based are more consistent than identity-based

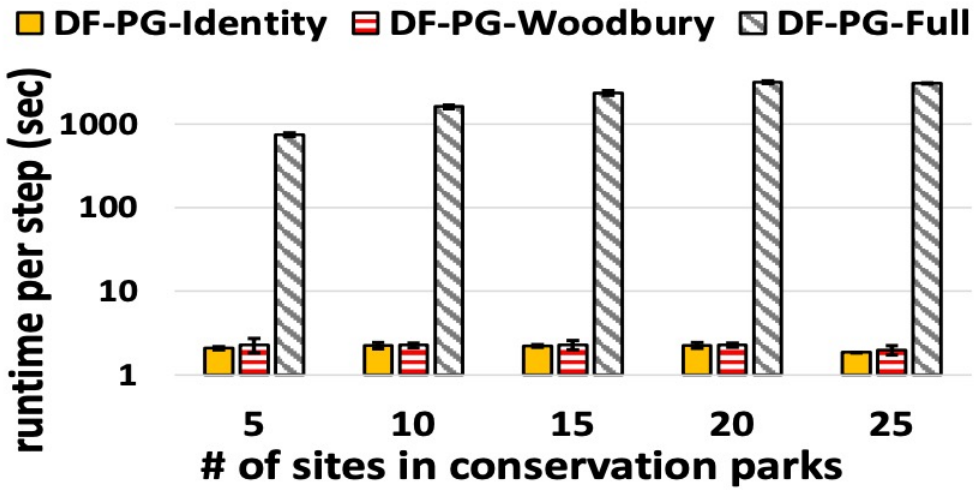
# Analysis (snare-finding)




DFL models learn less accurate models than two-stage
Hessian approximation saves ~3 orders of magnitude

# Analysis (snare-finding)




DFL models learn less accurate models than two-stage
Hessian approximation saves ~3 orders of magnitude

Wang, Shah, Chen, P, Doshi-Velez, Tambe (NeurIPS 2021)

# Why is DFL helpful?

Consider $f(z, \theta) = \sum_i \theta_i z_i$. Then,

$$\max_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} \sum_i \theta_i z_i = \max_{z \in Z} \sum_i \mathbb{E}[\theta_i | x] z_i$$

# Why is DFL helpful?

Consider $f(z, \theta) = \sum_i \theta_i z_i$.

$\max_{z \in Z} \sum_i m_{w^*}(x) z_i$ instead of $\max_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} \sum_i \theta_i z_i$

s.t. $w^* = \text{argmin}_w \mathcal{L}(w, \text{training data})$

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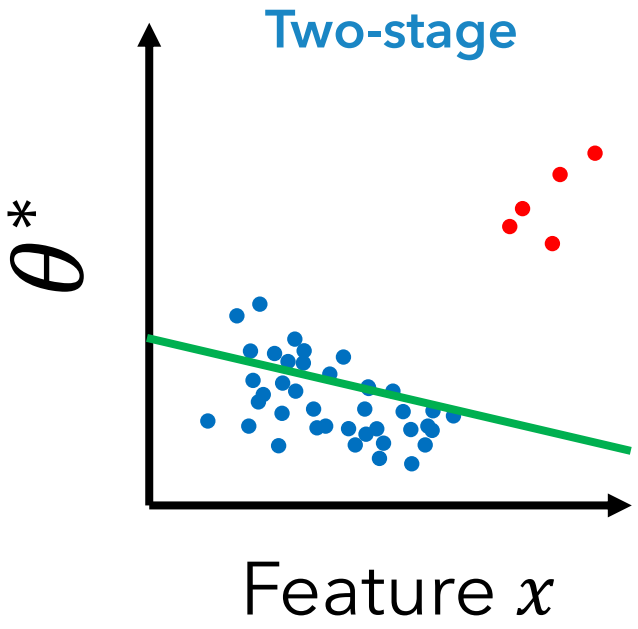

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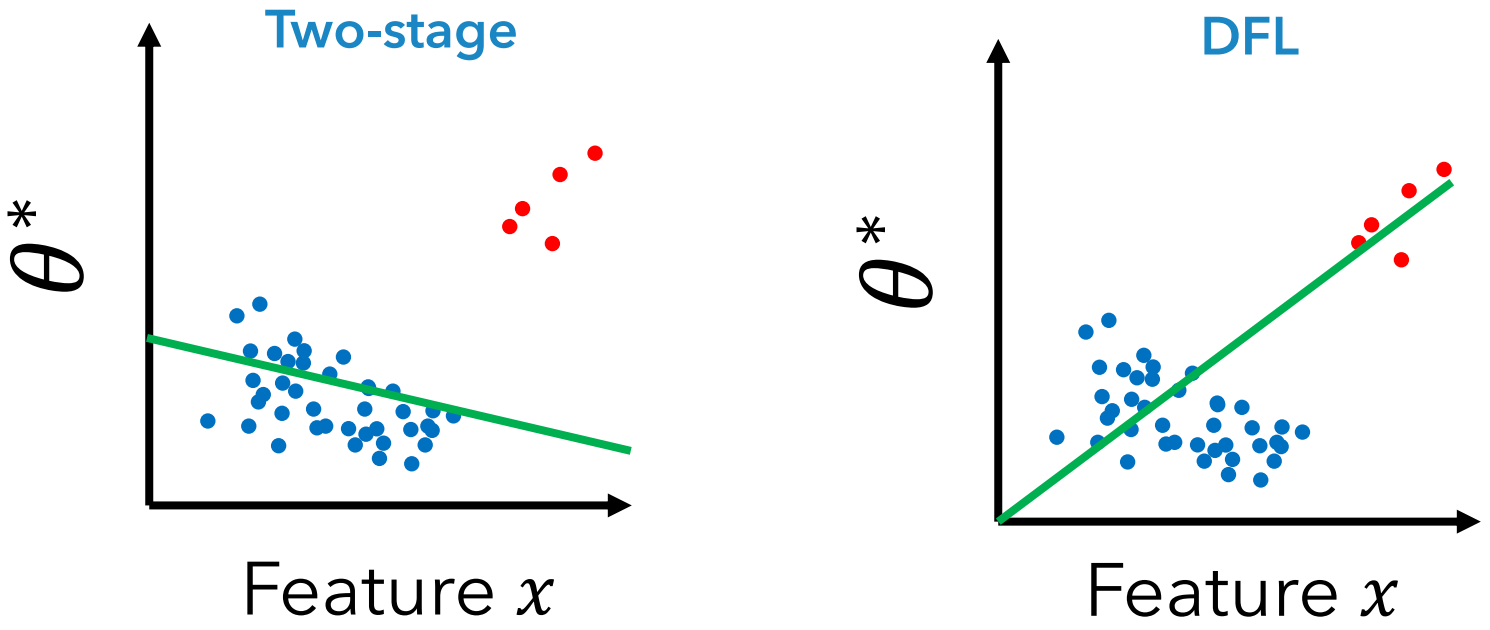
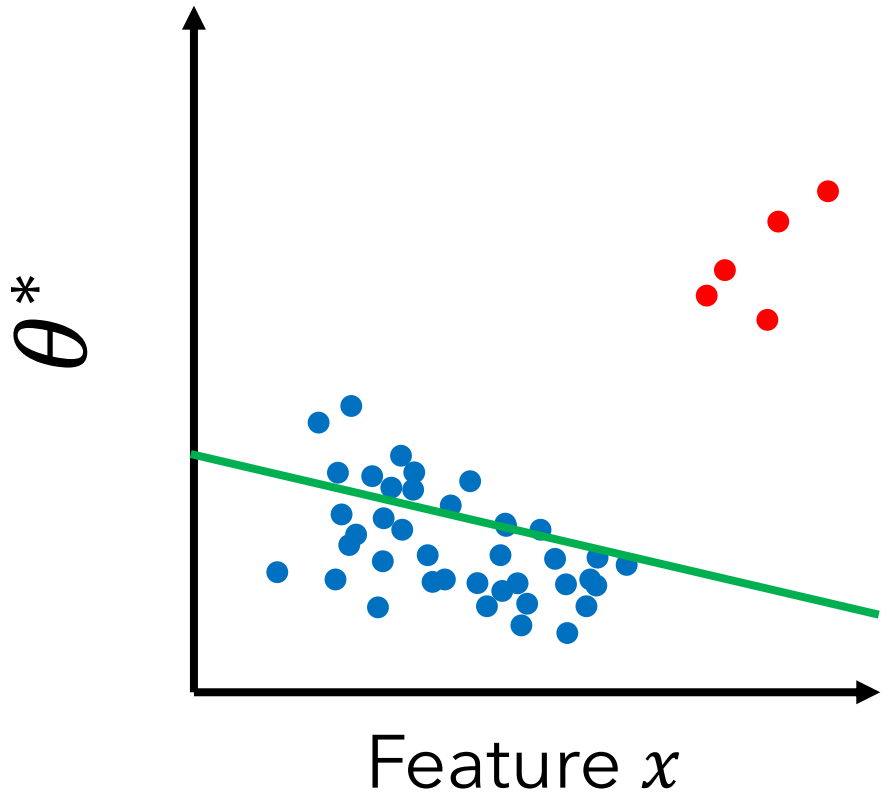


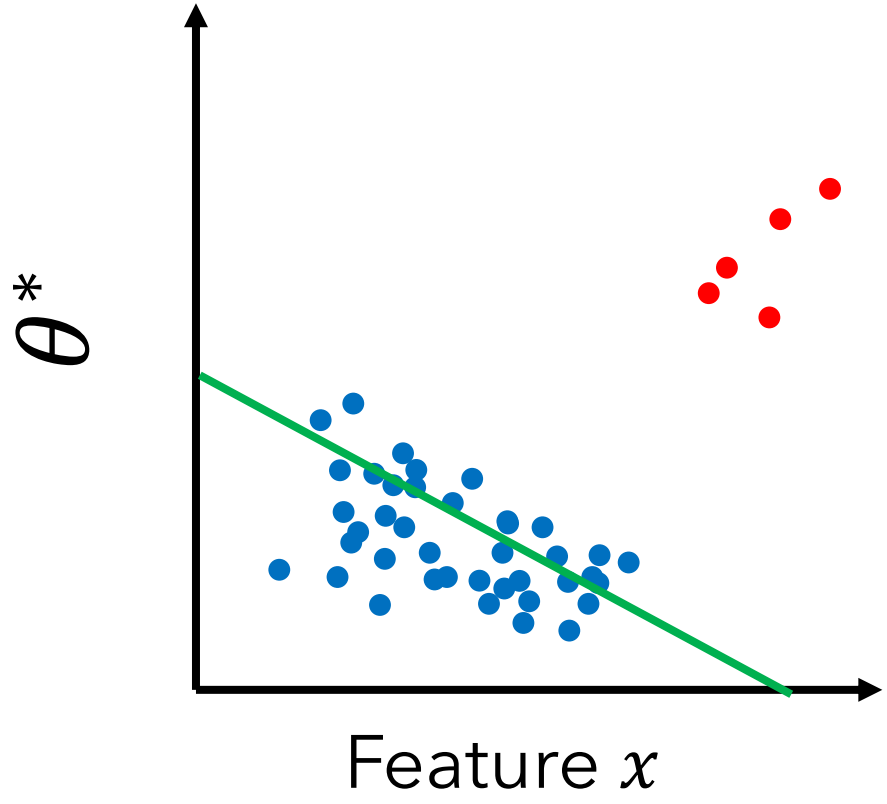
# The problem of zero gradient

$$\max_{z} \sum_{i} m_{\omega^*}(x) z_i$$

s.t. $w^* = \text{argmin}_w \mathcal{L}(w, \text{training data})$

$z_i \geq 0, \sum_i z_i \leq 1$



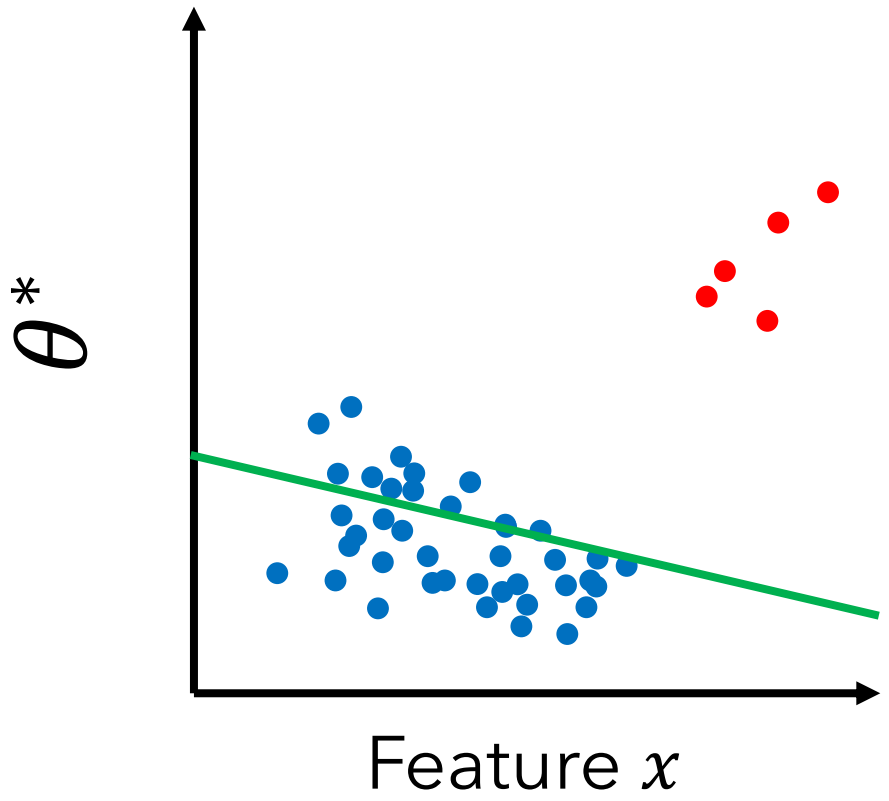



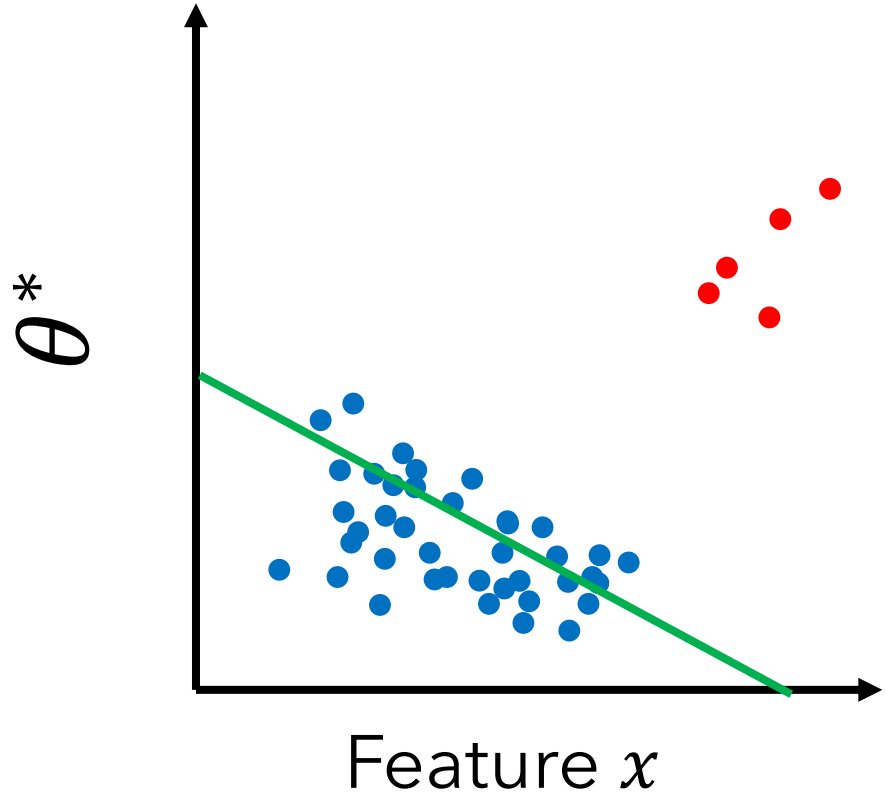
# The problem of zero gradient

$$\max_{z} \sum_{i} m_{\omega^*}(x) z_i + \lambda z_i^2$$

s.t. $w^* = \text{argmin}_w \mathcal{L}(w, \text{training data})$

$z_i \geq 0, \sum_i z_i \leq 1$



# The problem of non-convexity

$$\max_{z} \sum_{i} m_{\omega^*}(x) z_i + \lambda z_i^2$$

s.t. $w^* = \text{argmin}_w \mathcal{L}(w, \text{training data})$

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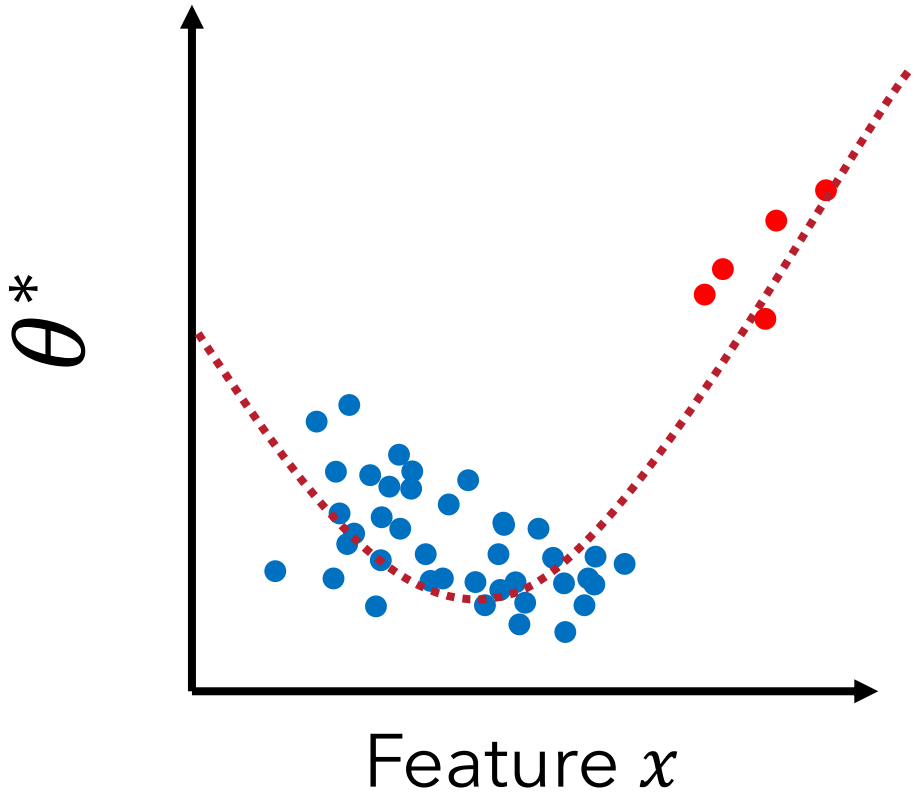

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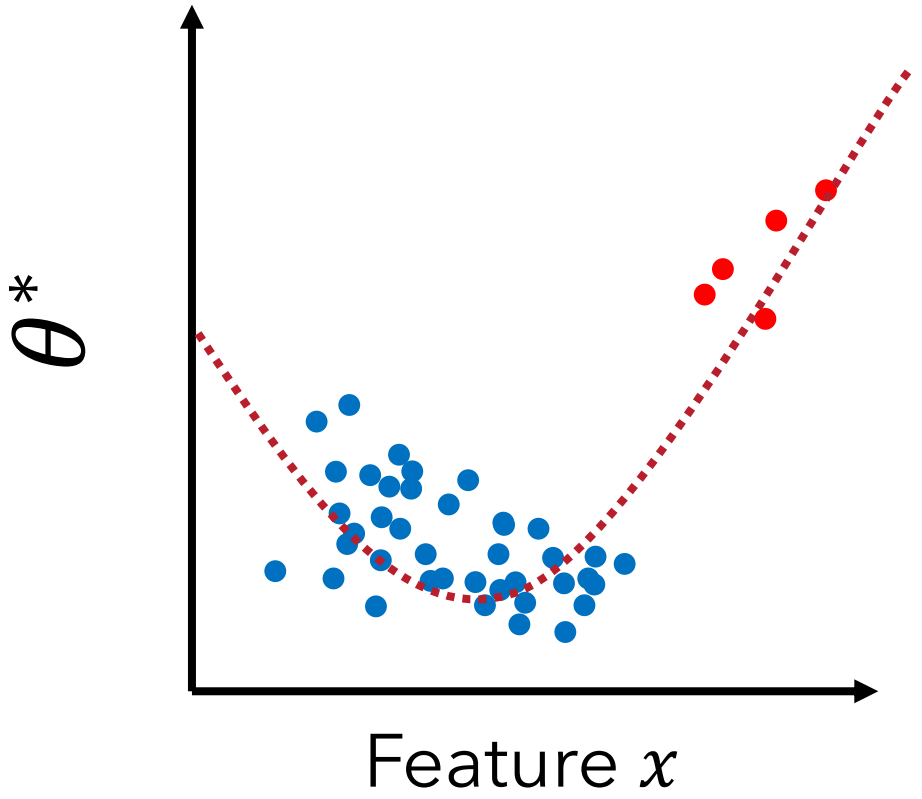
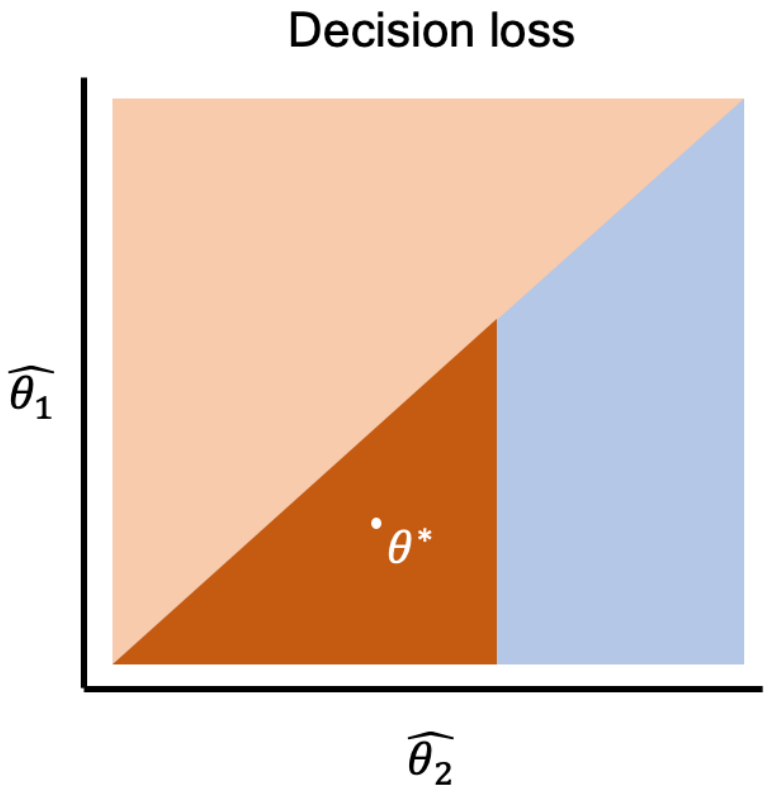


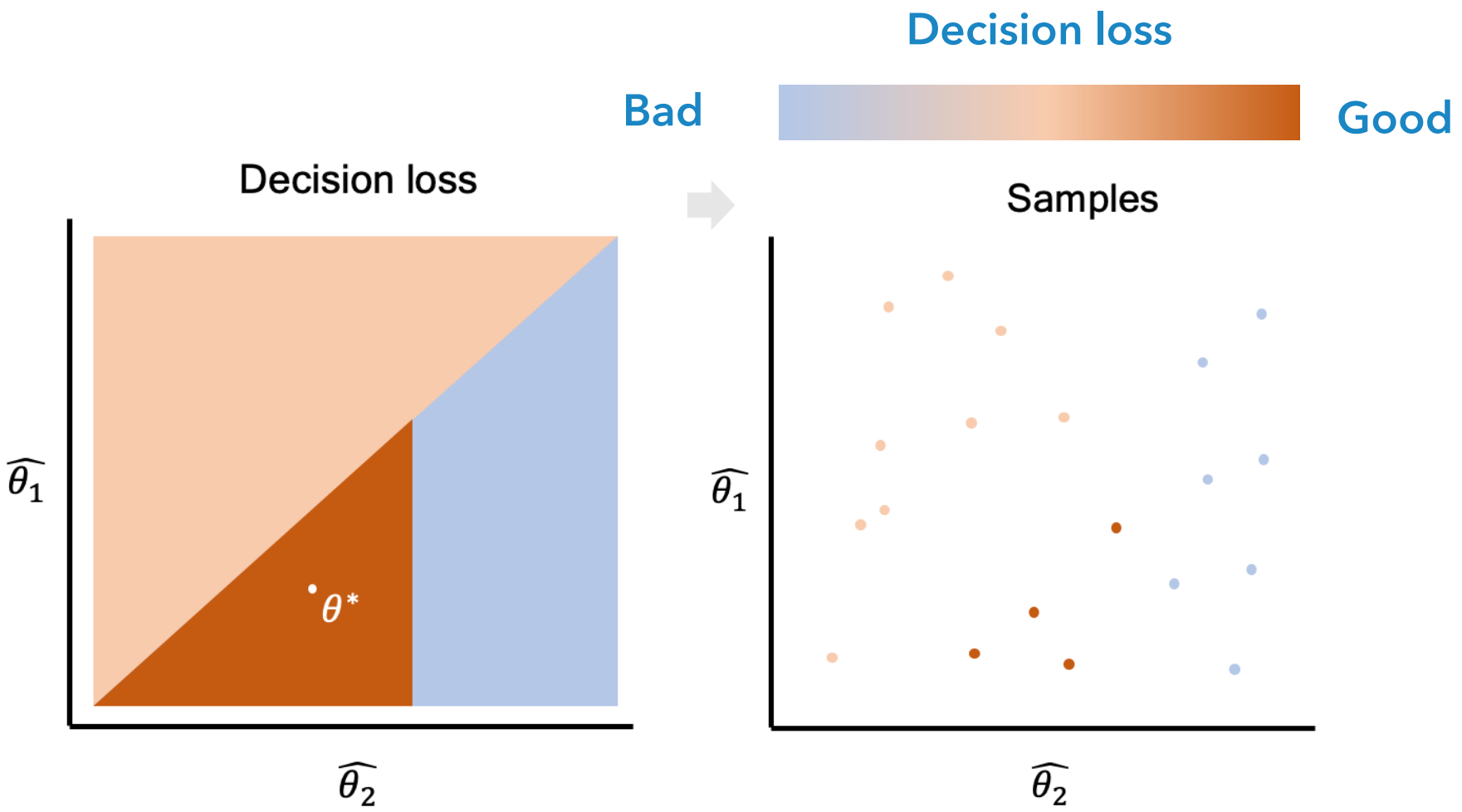

**Cool theory for linear objectives: Elmachtoub and Grigas (2022)**

Decision loss

Bad Good




Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

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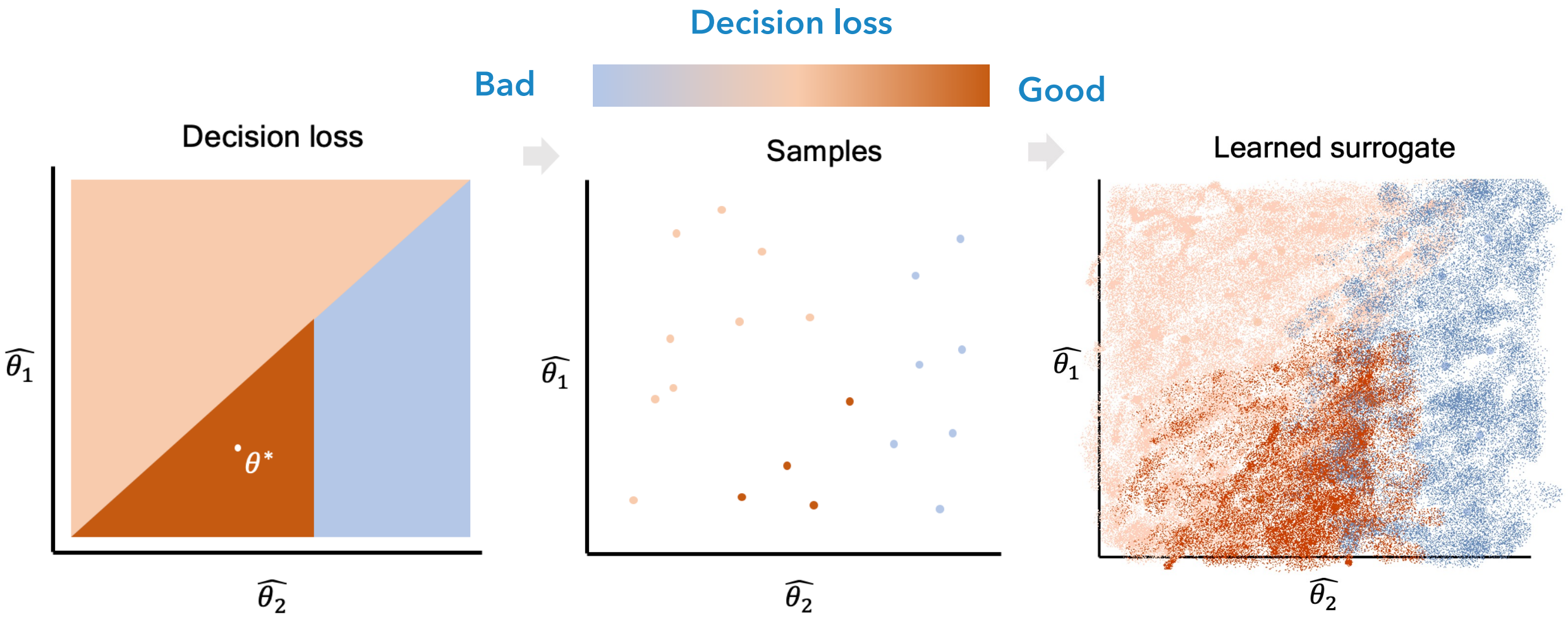



Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Questions

1. Where to sample from the decision loss function?

2. Where is the local minimum?

3. What function to fit?

# Notation

Predicted environment parameter $\hat{\theta}$

Decision induced by $\hat{\theta}$:
$z^*(\hat{\theta}) = \mathbf{argmin}_{z \in Z} f(z, \hat{\theta})$

Decision loss of $\hat{\theta}$:
$\ell(\hat{\theta}) = f(z^*(\hat{\theta}), \theta^*)$

**Standard DFL notation**

Observable feature/context vector $x \in X$

Unobserved ground truth environment parameter $\theta^* \in \Theta$

$x$ and $\theta^*$ drawn jointly from fixed distribution $\mathcal{D}$

Decision/control variable $z \in Z$

Objective function $f(z, \theta^*)$

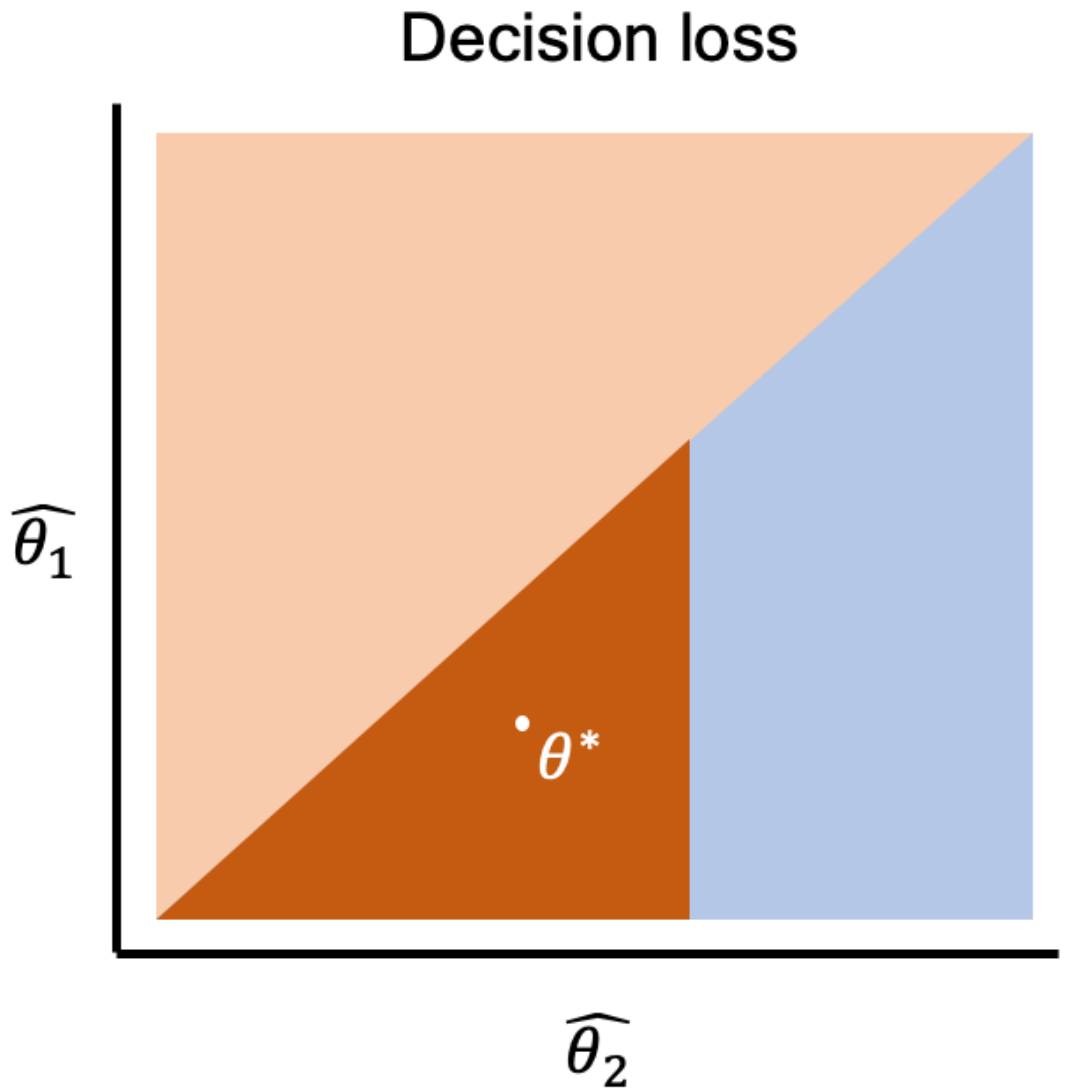
Goal: $\min_{z \in Z} \mathbb{E}_{\theta \sim P(\Theta|x)} f(z, \theta)$

1. Sample a dataset of pairs $\mathcal{D} = \{\left(\theta_j, \ell\left(\theta_j\right)\right)\}$

2. Fit a parametric loss $\hat{\ell}_\omega(\theta)$ to minimize MSE on training data

3. Train predictive model $m: X \to \Theta$ using $\hat{\ell}_\omega(\theta)$

Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

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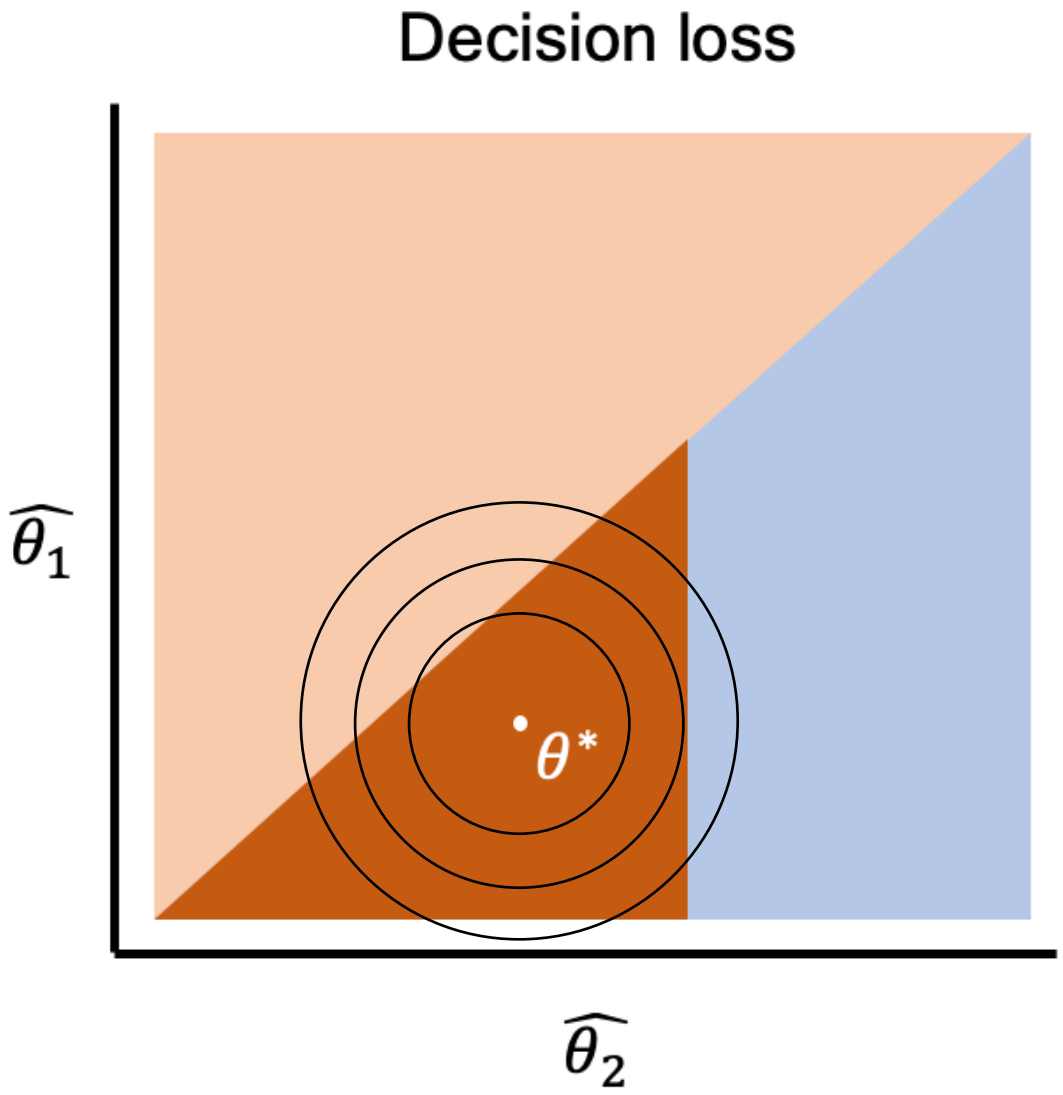
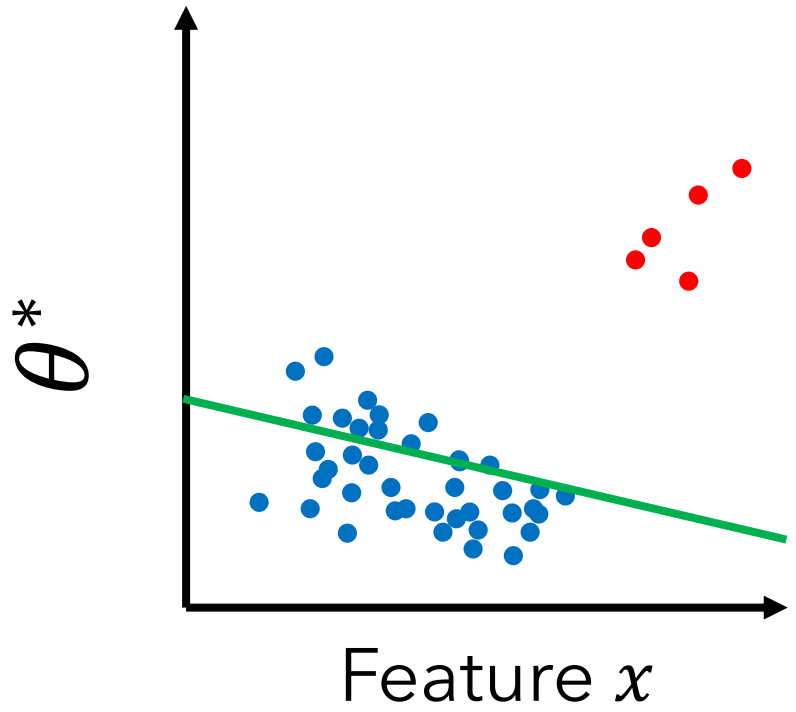



Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Choosing a parametric family

1. Capture differing importance of dimensions of $\theta$

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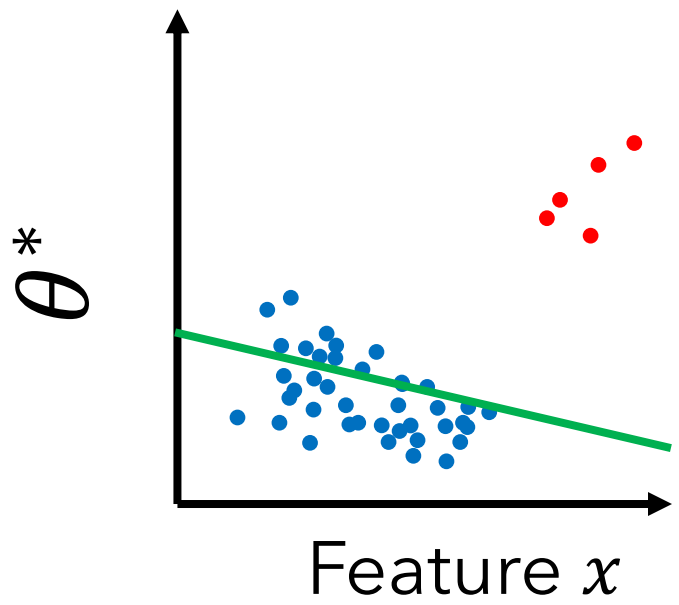
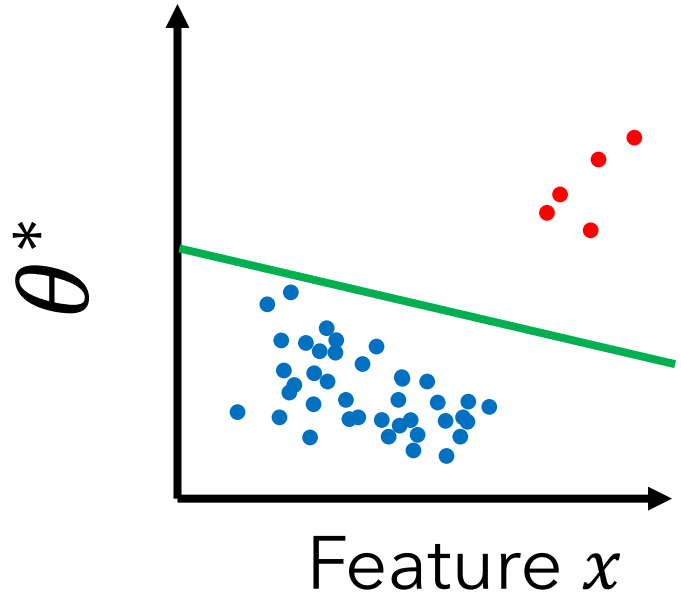
# Choosing a parametric family

1. Capture differing importance of dimensions of $\theta$
2. Capture pairwise interactions between dimensions of $\theta$

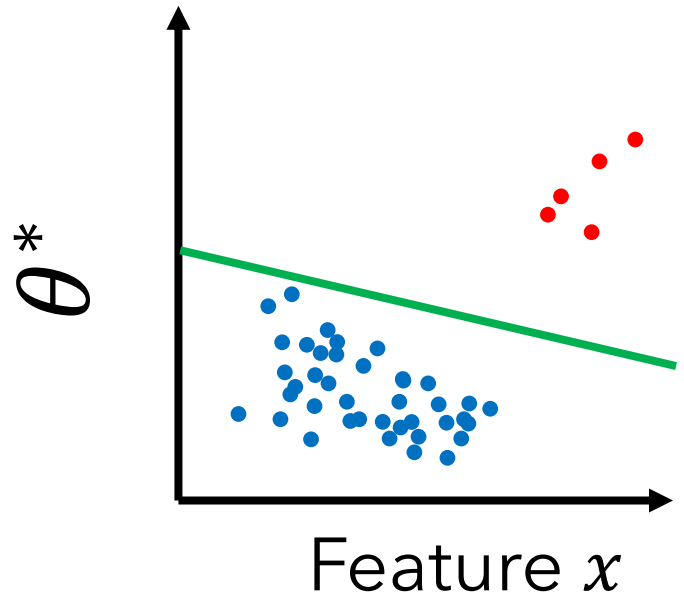



Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Choosing a parametric family

1. Capture differing importance of dimensions of $\theta$
2. Capture pairwise interactions between dimensions of $\theta$
3. Capture asymmetry in over- vs. under-predicting




Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Choosing a parametric family

Starting point: quadratic loss

$$\left(\hat{\theta} - \theta^*\right)^T H \left(\hat{\theta} - \theta^*\right)$$

where $H$ is the learned parameter.

Low-rank, PSD decomposition: $H = LL^T$

Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Choosing a parametric family

Starting point: quadratic loss

$$(\hat{\theta} - \theta^*)^T H (\hat{\theta} - \theta^*)$$

where $H$ is the learned parameter.

Low-rank, PSD decomposition: $H = LL^T$

✔ Capture differing importance of dimensions of $\theta$

✔ Capture *pairwise interactions* between entries of $\theta$

✘ Capture *asymmetry* in over vs under predicting

Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Choosing a parametric family

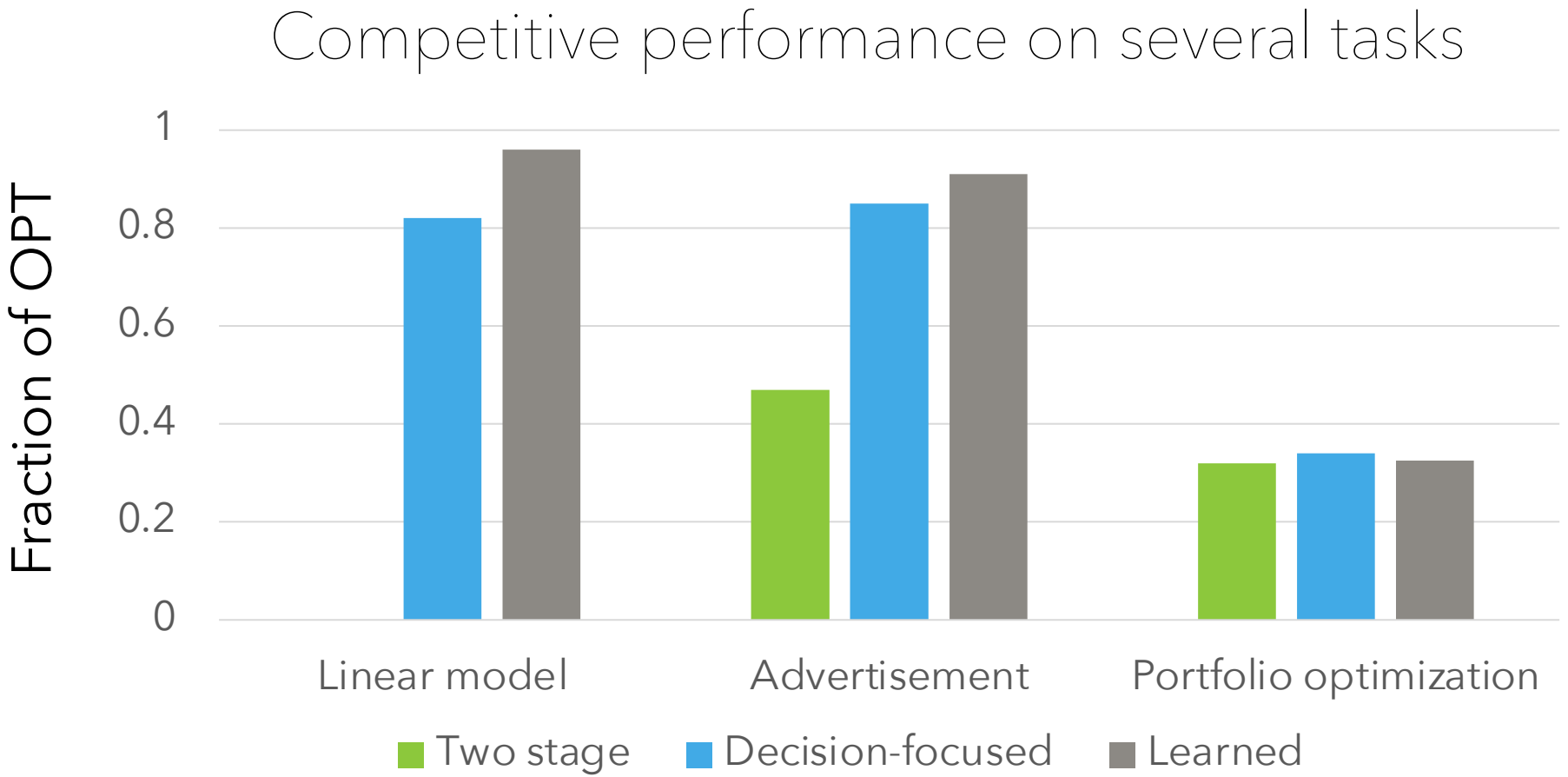
Refinement: *directed* quadratic loss.

Each $\boldsymbol{i, j}$ pair of coordinates gets a loss which depends on direction of errors for the prediction of each

Instantiate via four copies of the parameter $L$ ($H = LL^T$)

$$
\begin{aligned}
&L_{ij}^{++}, && \text{if } \hat{y}_i - y_i \geq 0 \text{ and } \hat{y}_j - y_j \geq 0 \\
&L_{ij}^{+-}, && \text{if } \hat{y}_i - y_i \geq 0 \text{ and } \hat{y}_j - y_j < 0 \\
&L_{ij}^{-+}, && \text{if } \hat{y}_i - y_i < 0 \text{ and } \hat{y}_j - y_j \geq 0 \\
&L_{ij}^{--}, && \text{otherwise}
\end{aligned}
$$

# Experiments




Shah, Wang, Wilder, P, Tambe (arXiv, 2022)

# Conclusion/future directions

1. Cost of training
2. Exploiting correlation structure
3. Accessibility of code/methods
4. Benchmarks

# References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Futoma et al. POPCORN: Partially Observed Prediction COnstrained ReiNforcement learning. AISTATS 2020.

Elmachtoub and Grigas. Smart "Predict, then Optimize". Management Science, 2022.

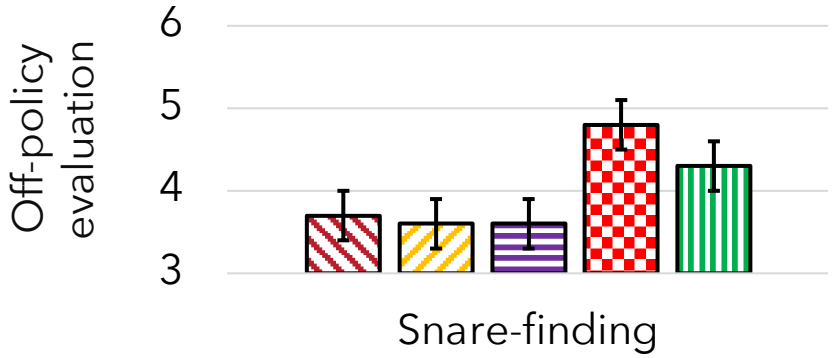
Shah et al. Decision-Focused Learning without Decision-Making: Learning Locally Optimized Decision Losses. arXiv, 2022.

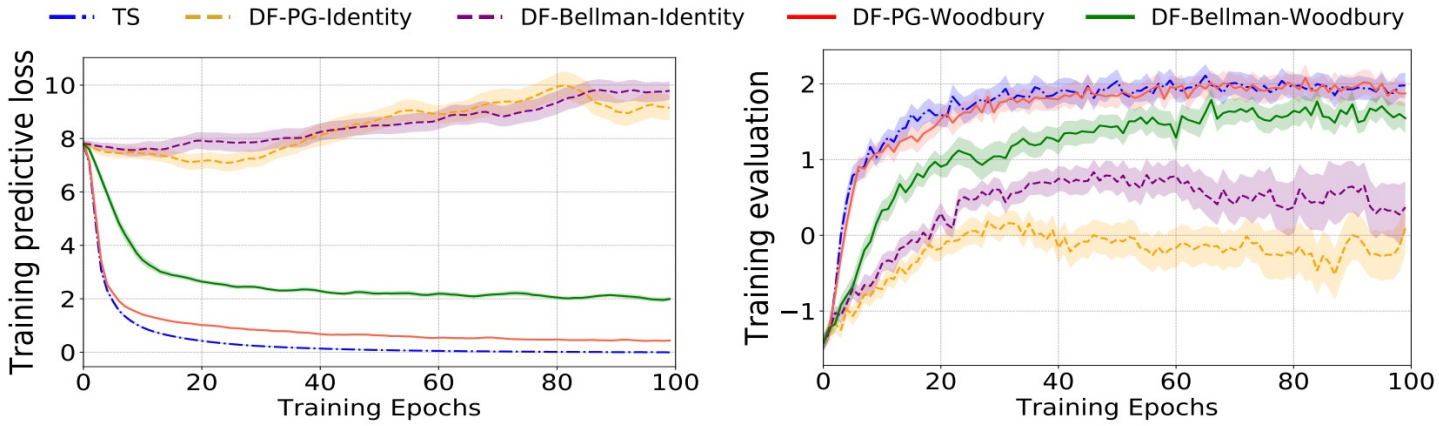
# References (tutorials)

Deep implicit layers (NeurIPS 2020): http://implicit-layers-tutorial.org/

Deep declarative networks (ECCV 2020): https://anucvml.github.io/ddn-eccvt2020/

# Analysis (snare-finding)





(a) Predictive loss in training MDPs (b) Performance in training MDPs

DFL models learn less accurate models than two-stage
Two-stage scores better on train but worse on test

# Price of correlation

Definition (price of correlation): for an objective function $f$, the price of correlation is ratio $\frac{f(x',y)}{f(x^*,y)}$, where

- $x^* = \min_{x \in X} \mathbb{E}_{y \sim P(y|\theta)} f(x,y)$
- $x' = \min_{x \in X} \mathbb{E}_{y \sim P(y|\theta)} f(x,y)$ assuming $y_i$ mutually independent