Toward Robust and Reliable Post-hoc Explanations to Machine Learning Models

Ngoc Bui - Graph and Geometric Deep Learning Group - Sep 2023

Why’s Explainable AI?

Input

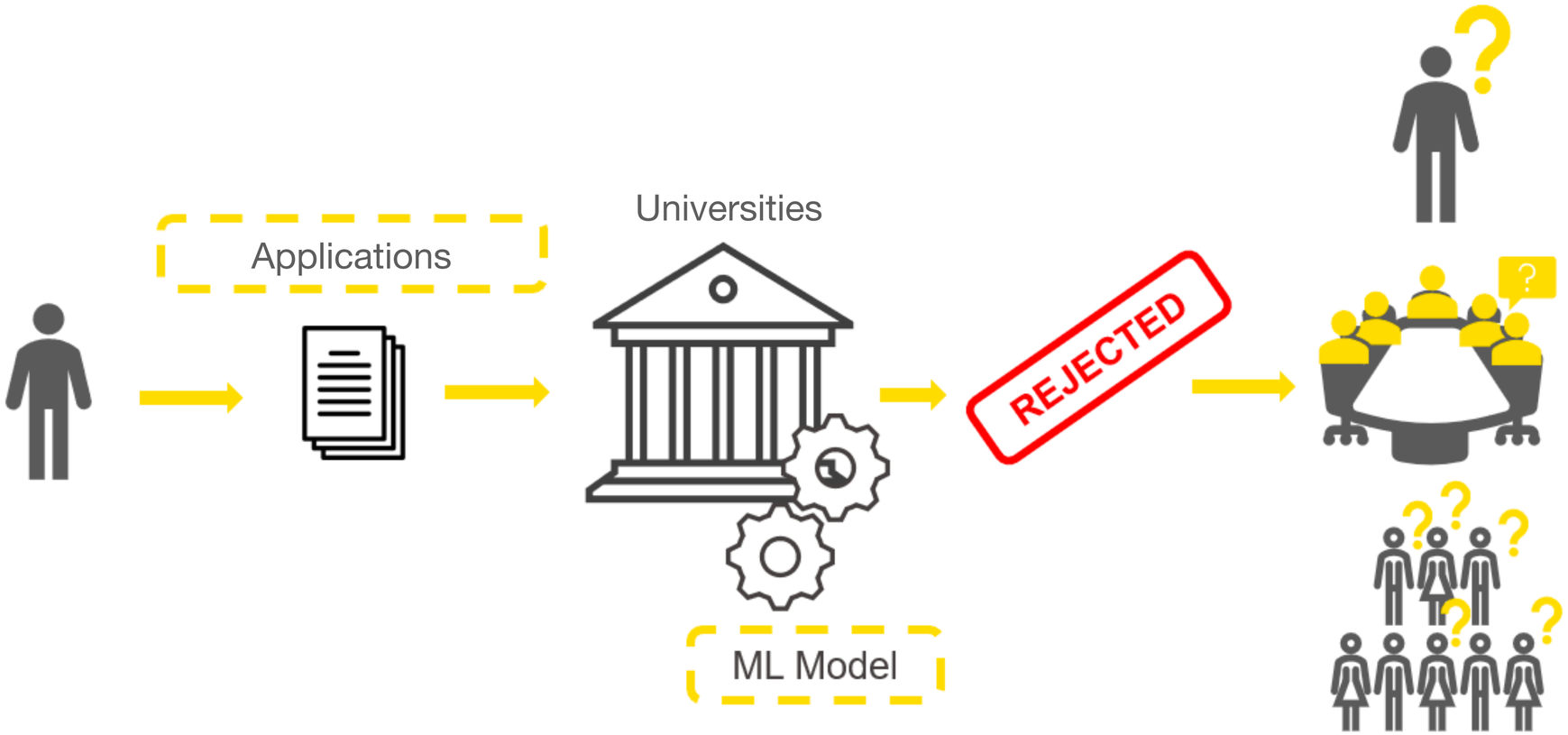
Output

Input is converted into output

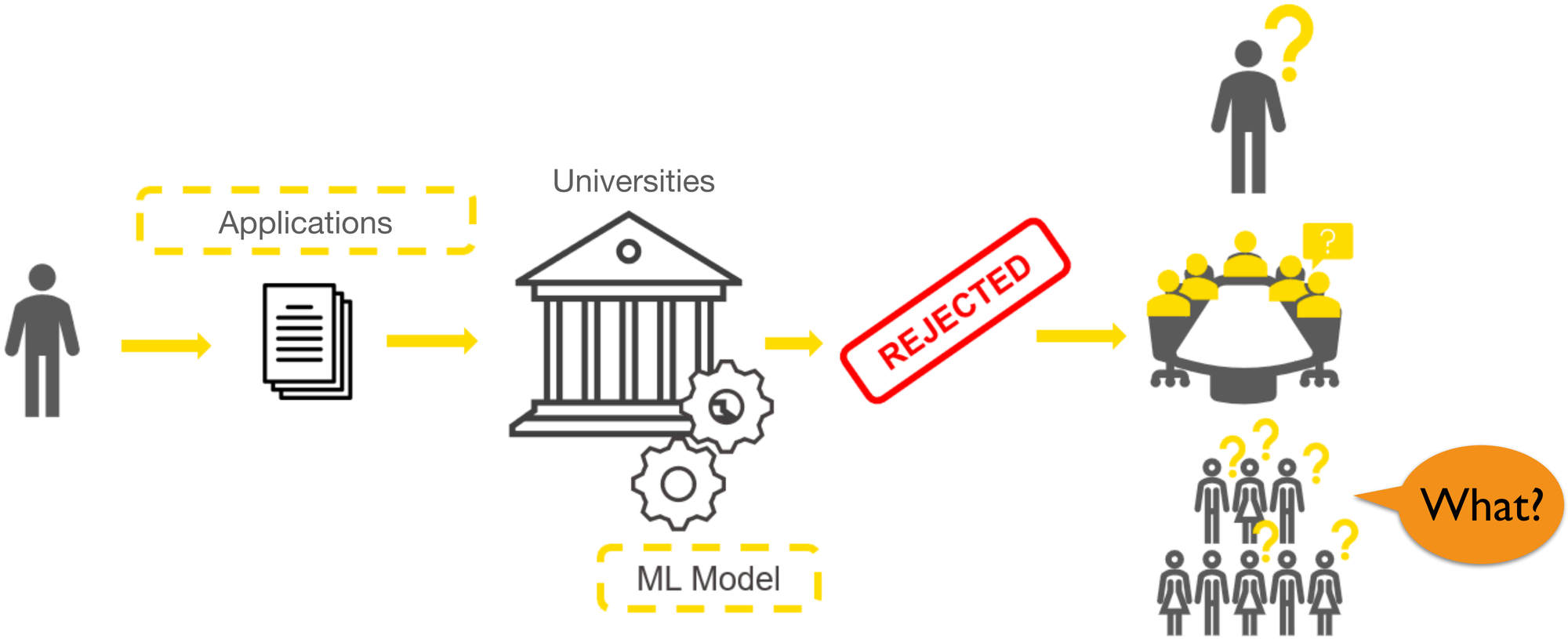
Why’s Explainable AI?

Input is converted into output

Why’s Explainable AI?



Why's Explainable AI?



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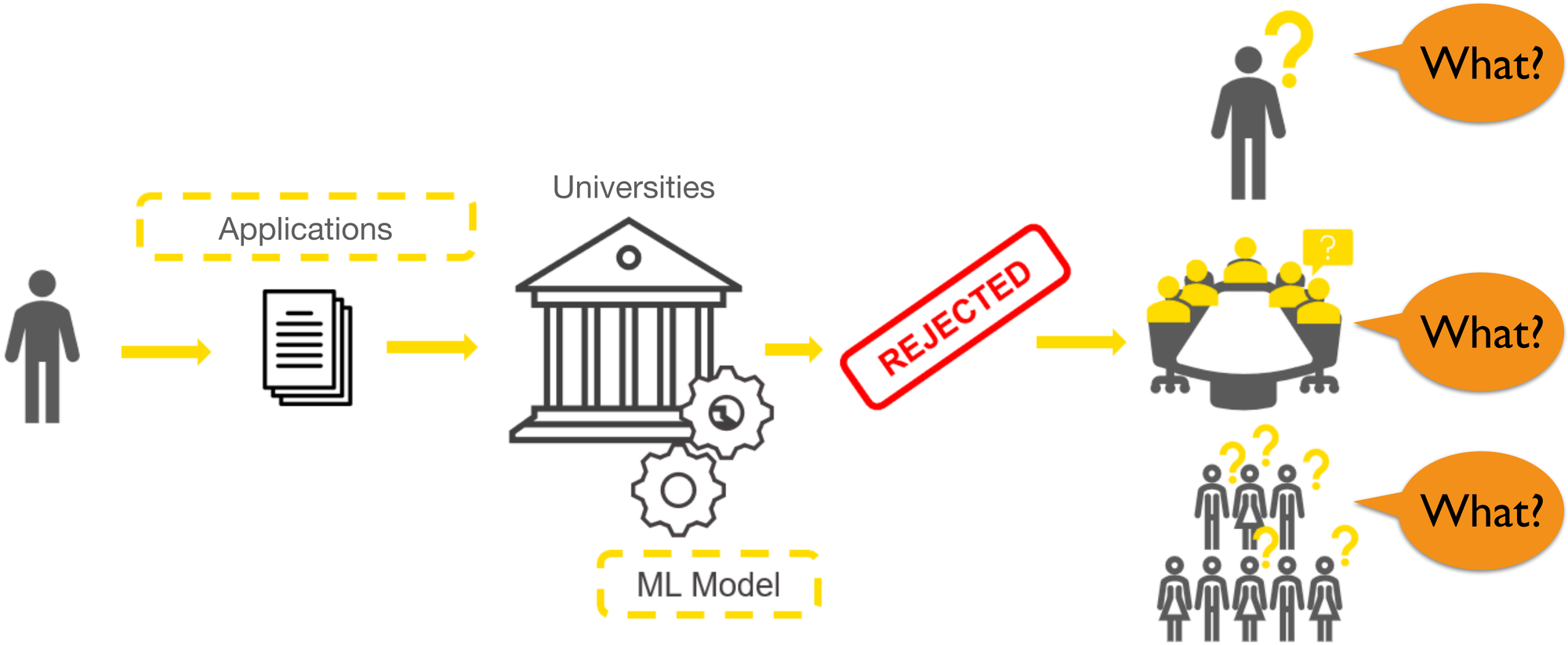

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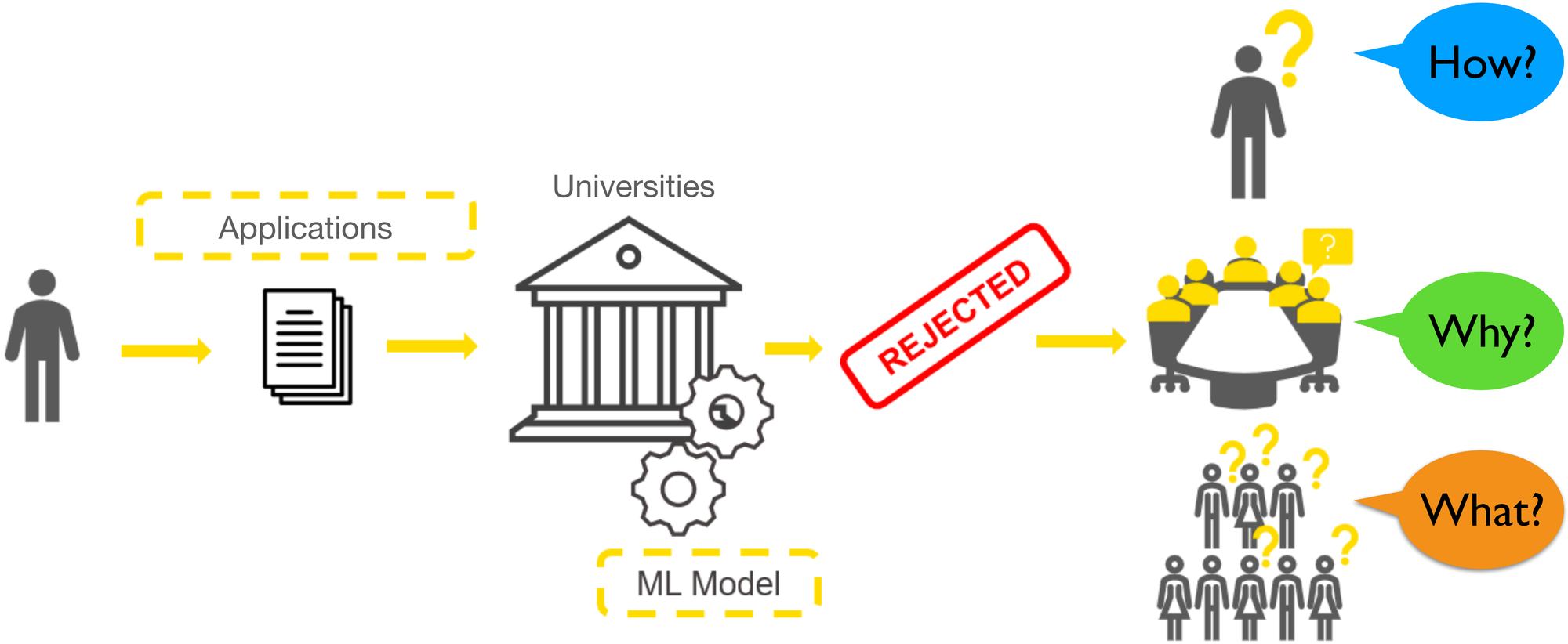
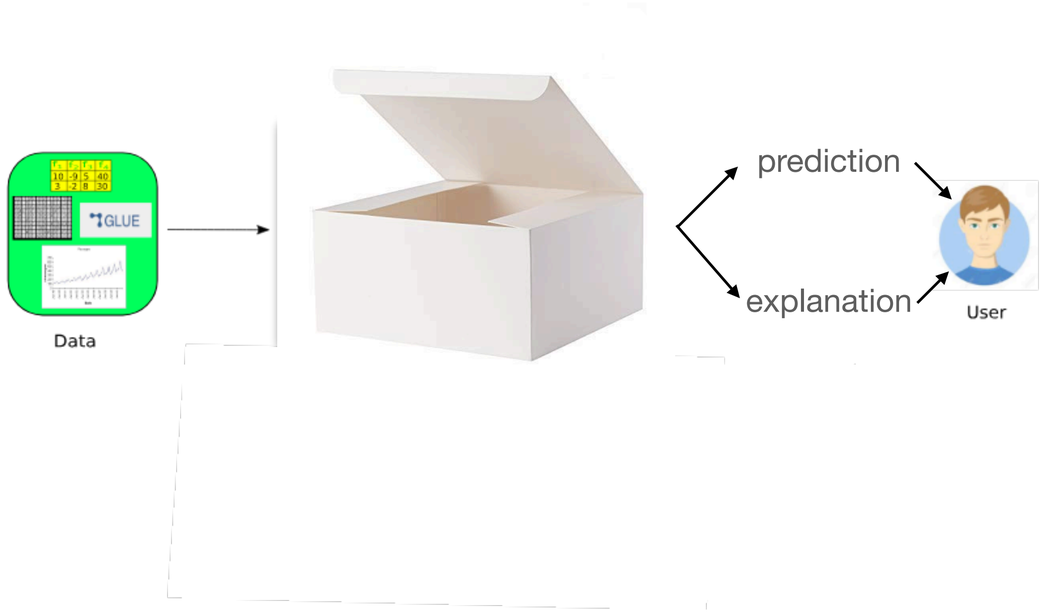
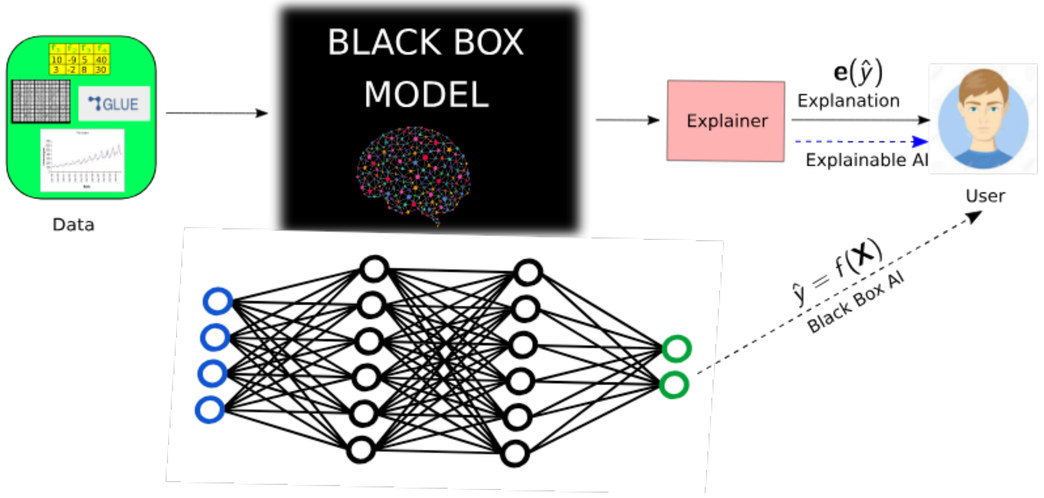


Explanations

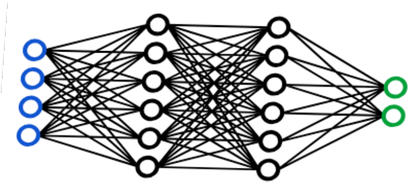
Ante-hoc Explanations



Post-hoc Explanations



Post-hoc Explanations



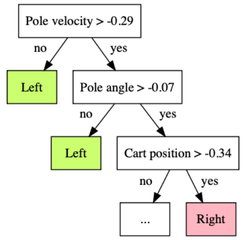
Explainers

Not today's talk

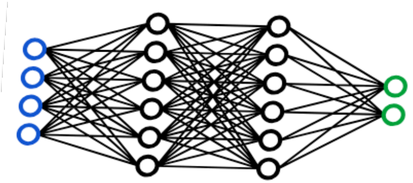
Global Explainers

Local Explainers

Model Distillation



Post-hoc Explanations



Explainers

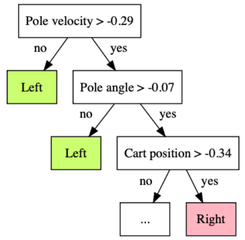
Input instance

Not today's talk

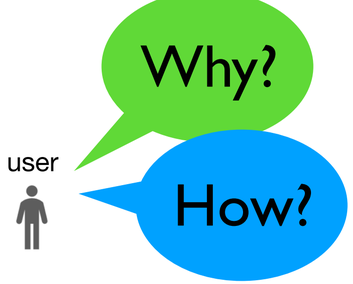
Global Explainers

Local Explainers

Model Distillation



Local Explanations



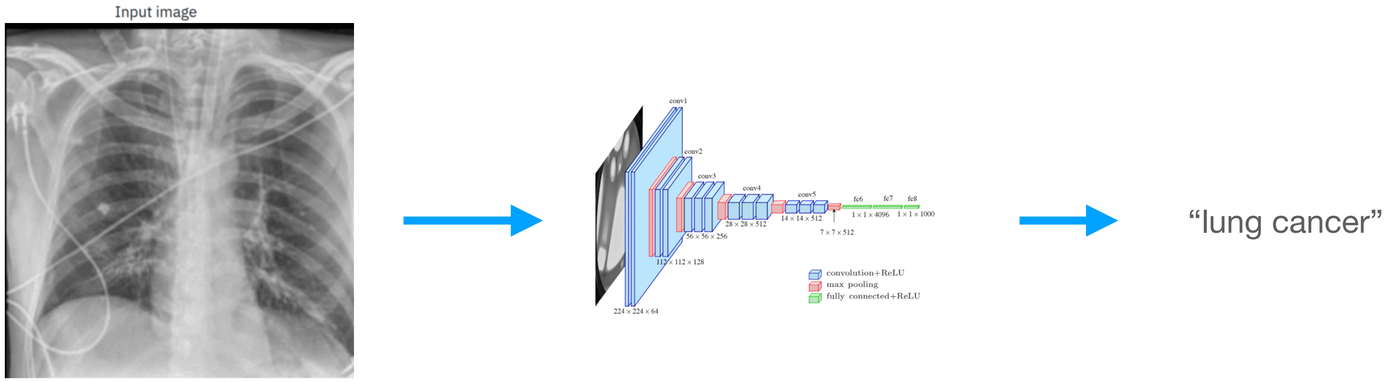
Local Explanations

Why?

user

Which features are important to make such a decision?

Saliency Map (e.g. GradCAM)



“lung cancer”

Local Explanations

Why?

user

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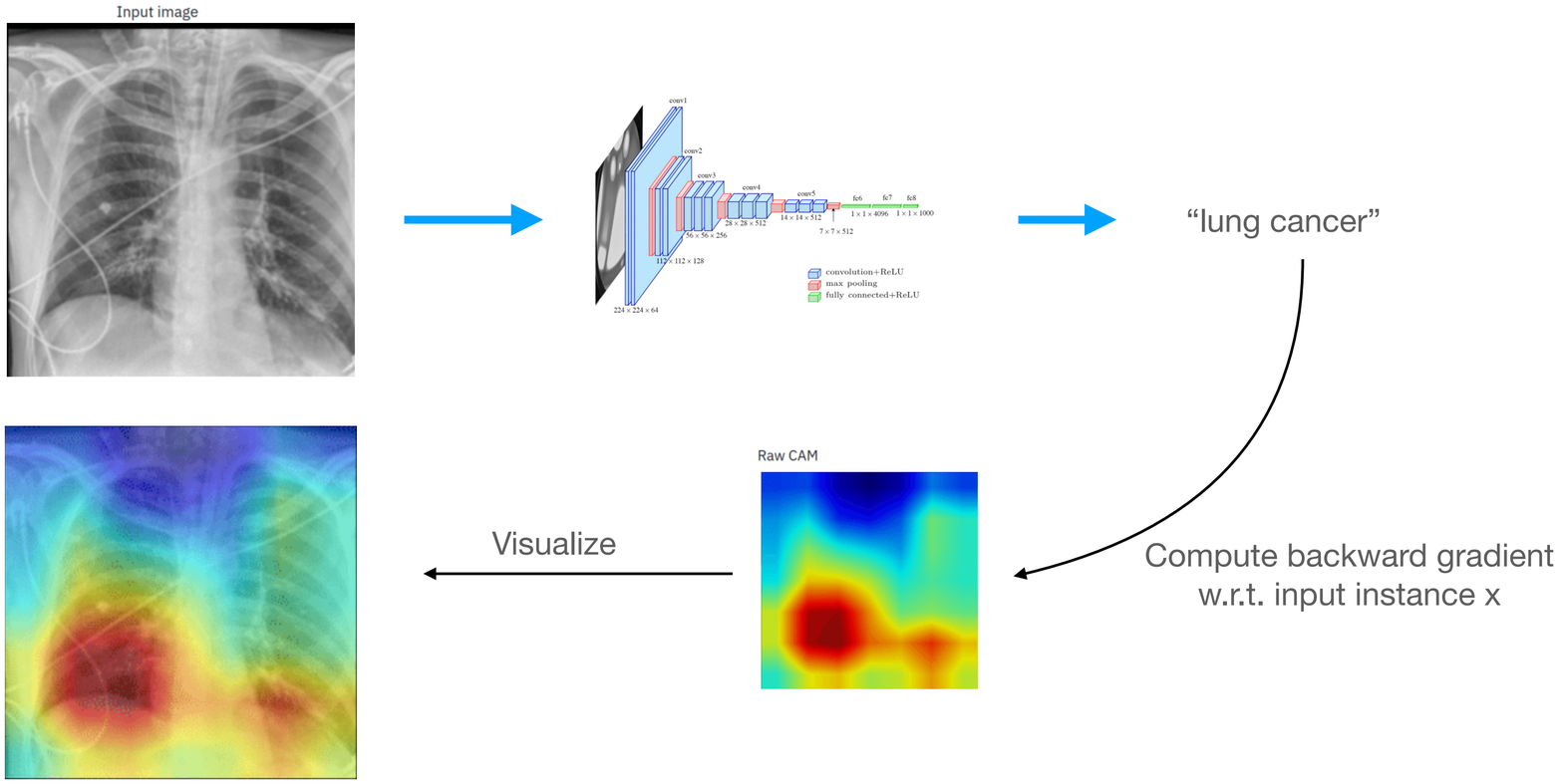

Local Explanations

user

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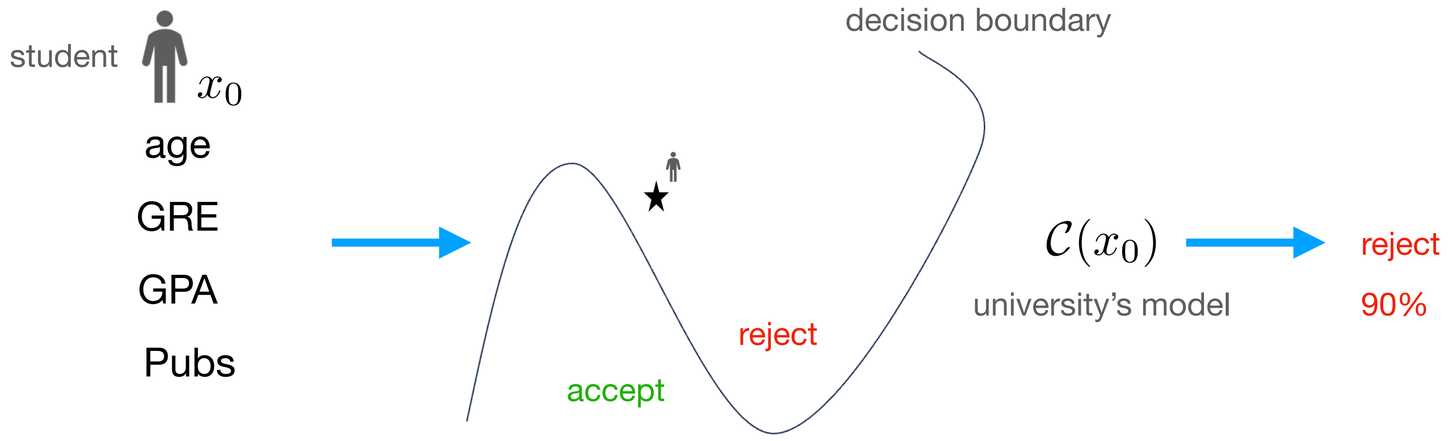
Which features are important to make such a decision?

Saliency Map (e.g. GradCAM)

Feature-based Attribution Methods (e.g. LIME, SHAP)



Local Explanations

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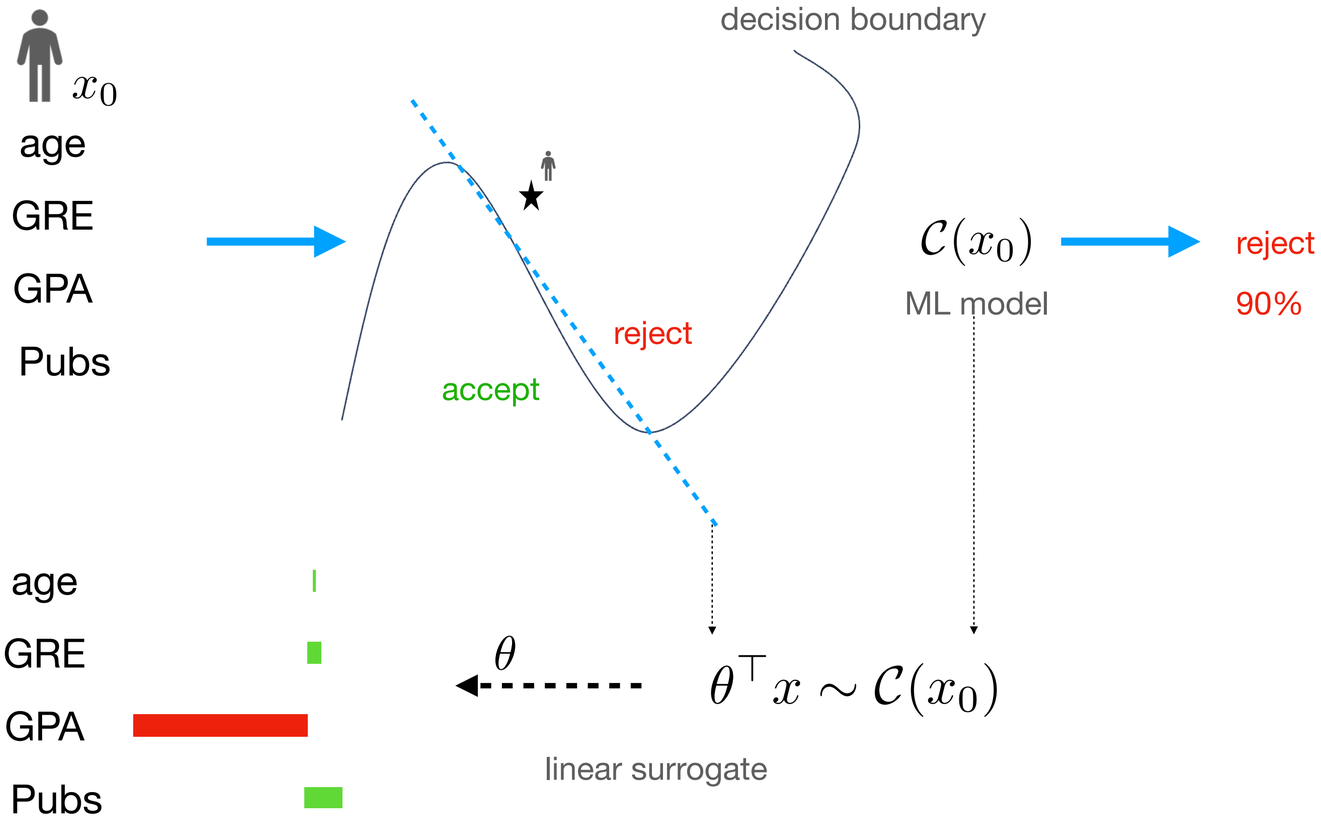
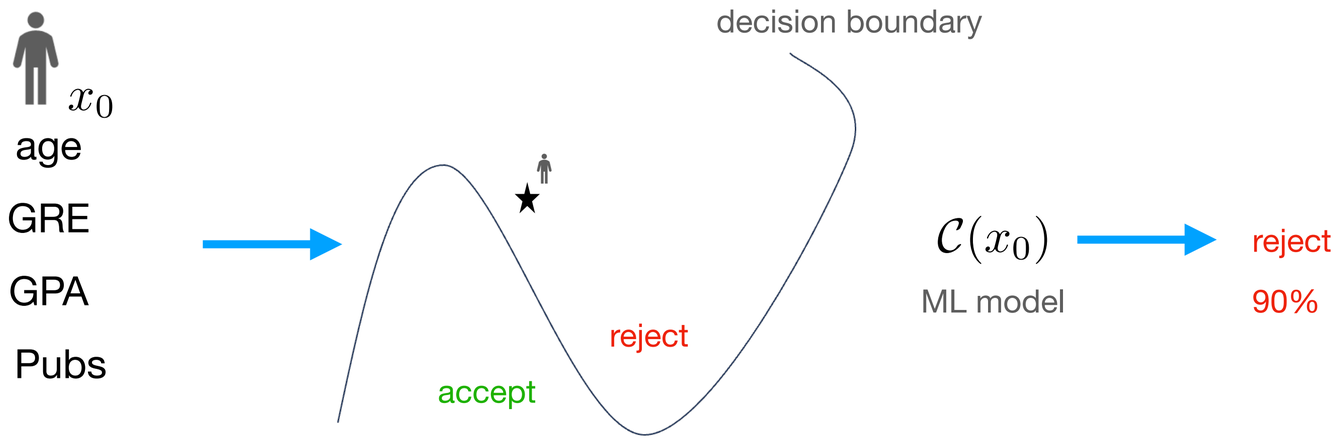


Local Explanations

How?

user

How can I improve to get a favorable result?



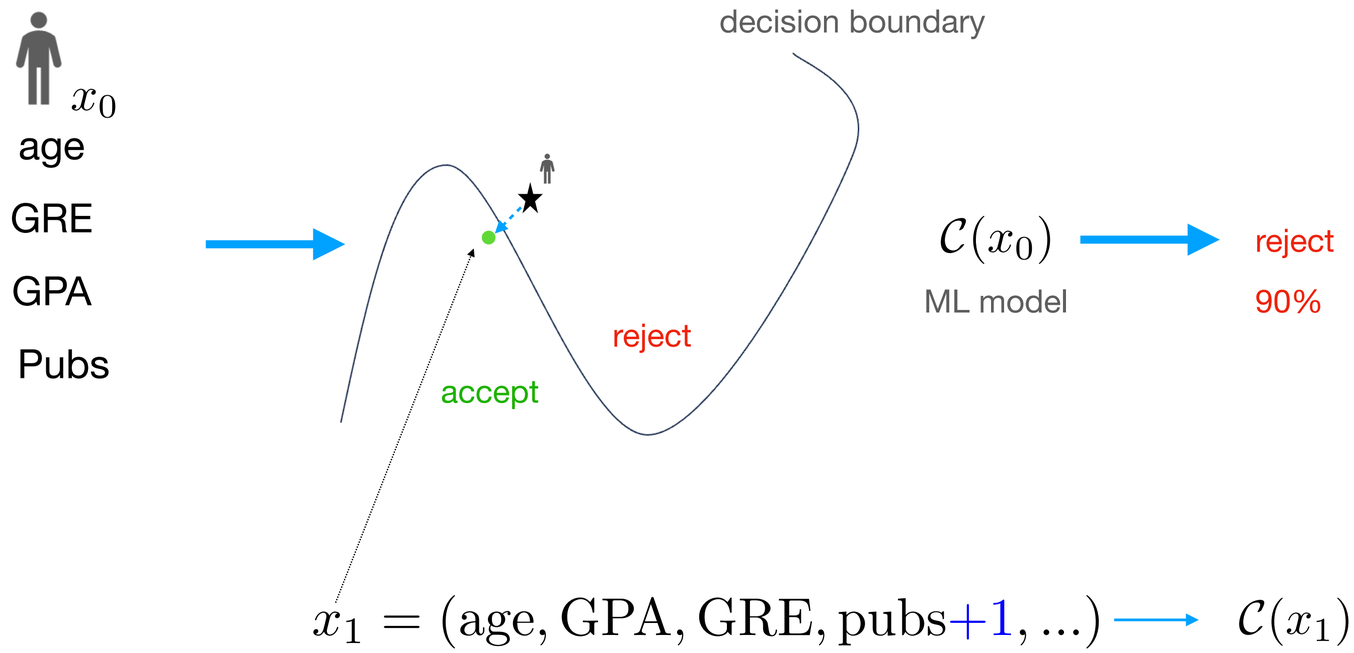
Local Explanations

How?

user

How can I improve to get a favorable result?

Counterfactual Explanations (a.k.a. Algorithmic Recourse):
examples that can flip the model's outcome



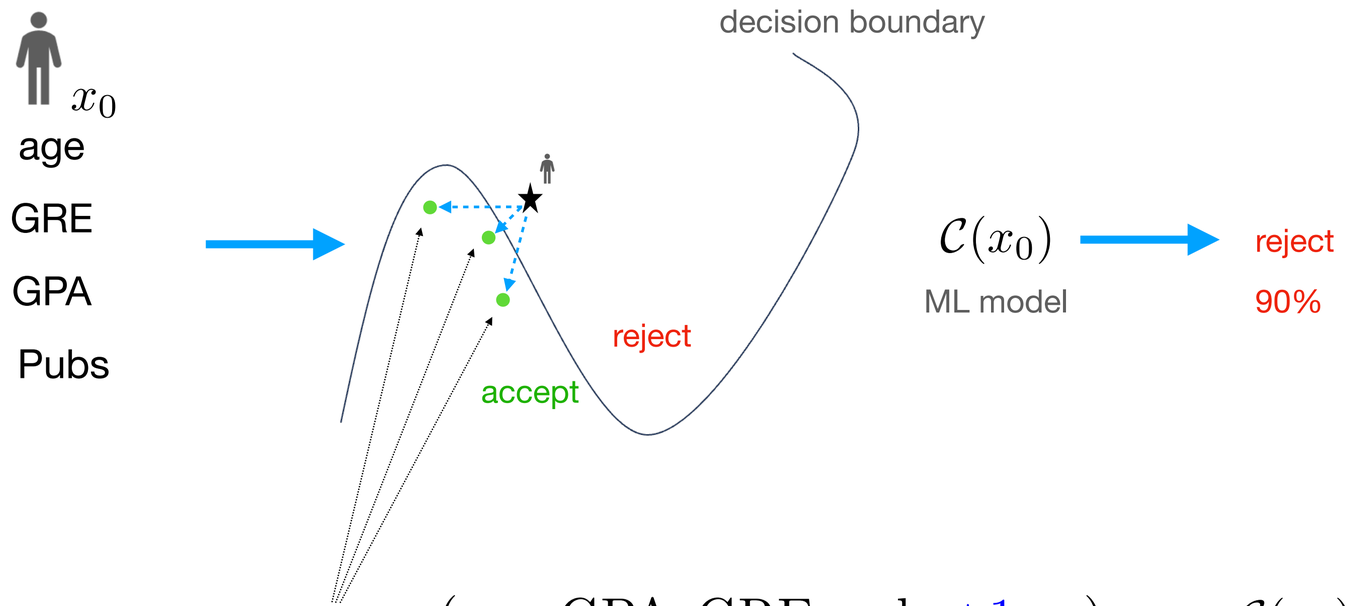
Local Explanations

How?

user

How can I improve to get a favorable result?

Counterfactual Plan: a set of counterfactual explanations



$x_1 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}{+}1, ...) \longrightarrow \mathcal{C}(x_1) \longrightarrow$ accept

$x_2 = (\text{age}, \text{GPA}, \text{GRE}{+}15, \text{pubs}, ...) \longrightarrow \mathcal{C}(x_2) \longrightarrow$ accept

$x_3 = (\text{age}, \text{GPA}{+}0.2, \text{GRE}, \text{pubs}, ...) \longrightarrow \mathcal{C}(x_3) \longrightarrow$ accept

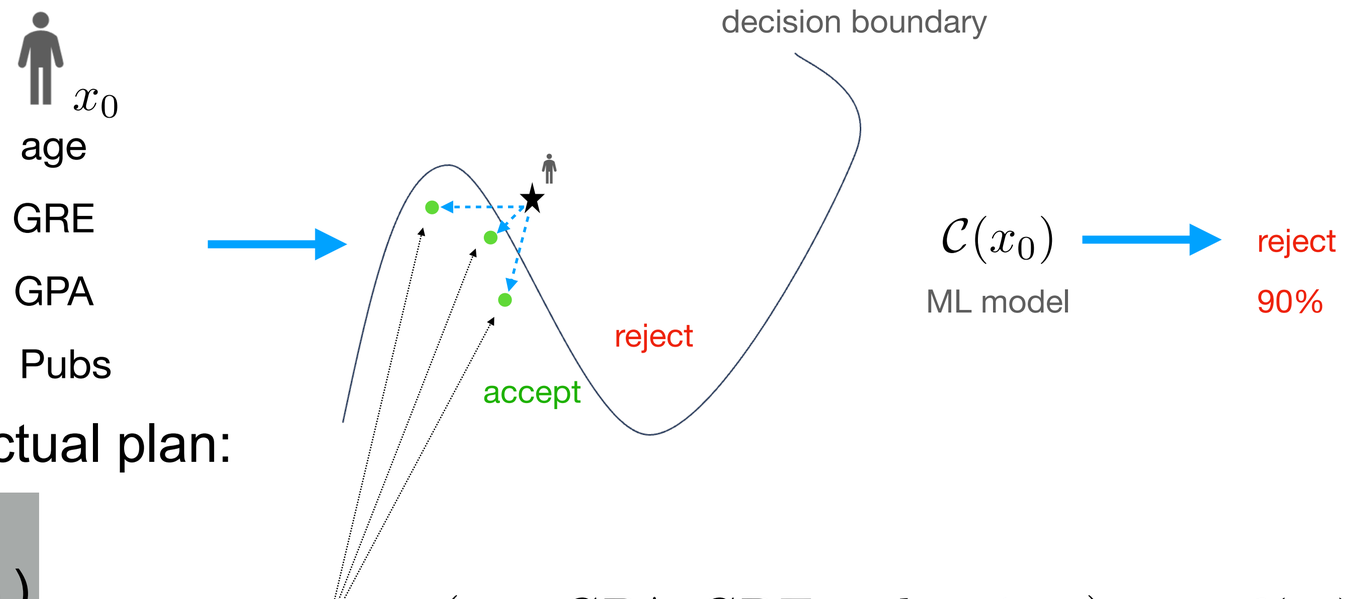
Local Explanations

How?

user

How can I improve to get a favorable result?

Counterfactual Plan: a set of counterfactual explanations



Criteria to construct counterfactual plan:

1. Validity
2. Proximity (closeness to x_0)
3. Diversity
4. Actionability

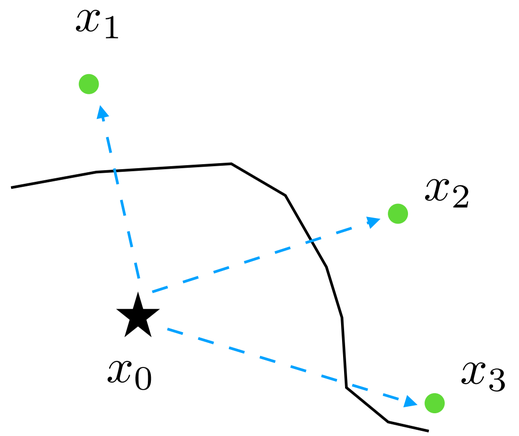
$x_1 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}+1, ...) \longrightarrow \mathcal{C}(x_1) \longrightarrow$ accept

$x_2 = (\text{age}, \text{GPA}, \text{GRE}+15, \text{pubs}, ...) \longrightarrow \mathcal{C}(x_2) \longrightarrow$ accept

$x_3 = (\text{age}, \text{GPA}+0.2, \text{GRE}, \text{pubs}, ...) \longrightarrow \mathcal{C}(x_3) \longrightarrow$ accept

Counterfactual Plan - Construction

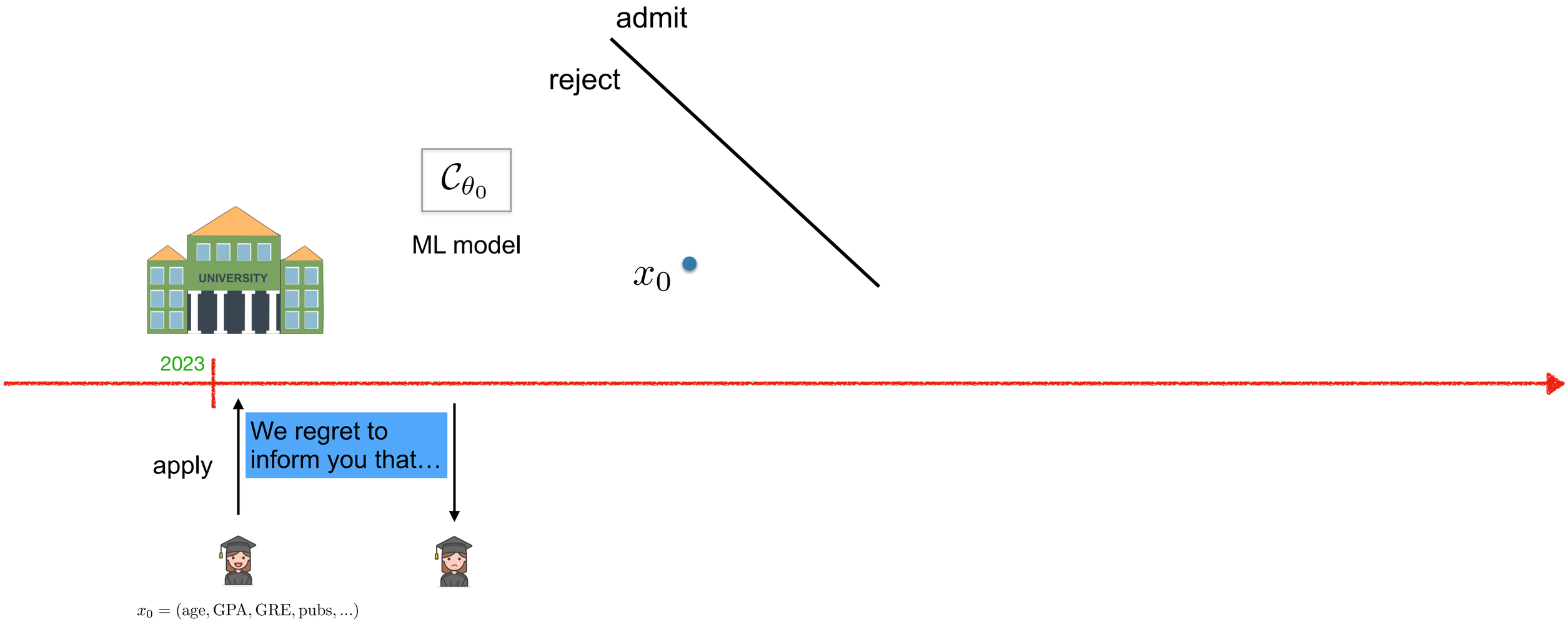
- Mixed-Integer Programming
  - Russell (2019) (for linear models)
    - Similar to Ustun (2018)
    - Promote diversity through diverse sets of constraints
- Multi-objective Evolutionary Algorithm
  - Dandl et al. (2020)
    - Universal but slow
    - Suitable to promote actionability
- Iterative, Gradient-based Optimization
  - Mothilal et al. (2020) (DICE)
    - A weighted sum of three objectives: validity, proximity, and diversity.
    - Solved by projected gradient descent



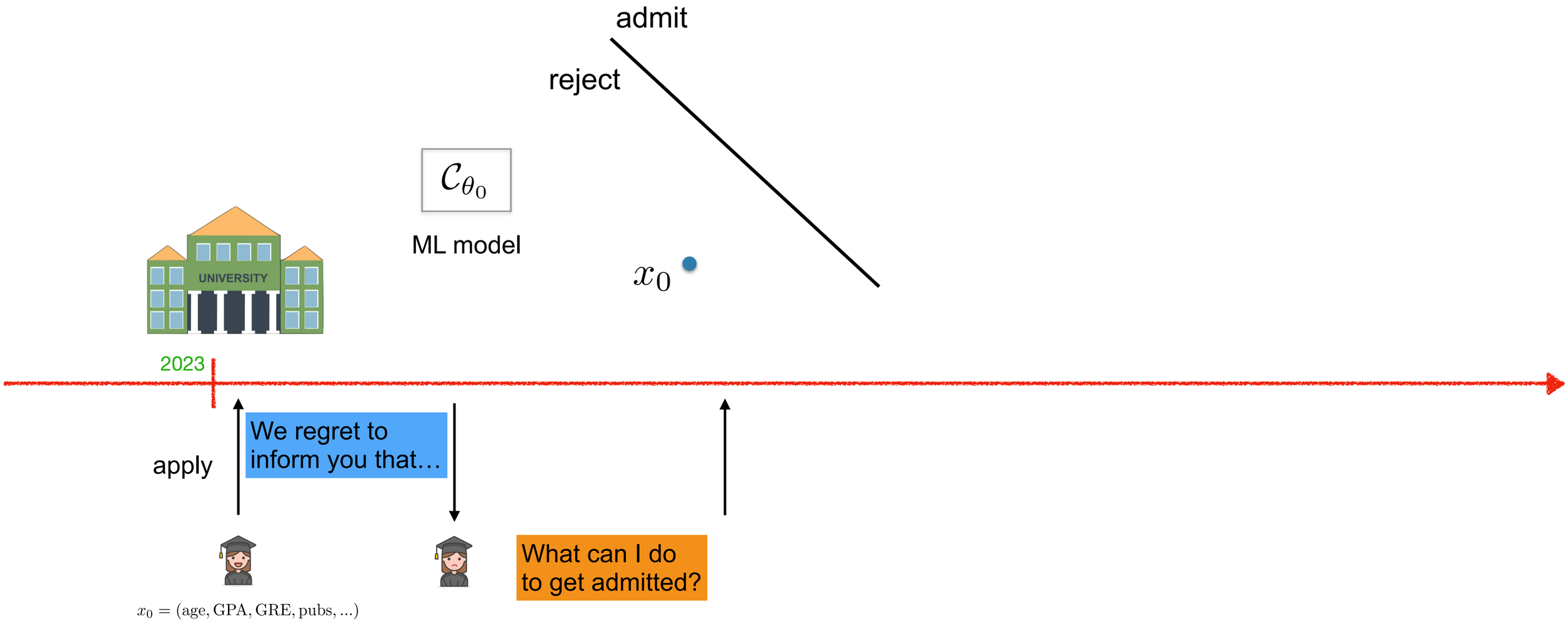
Counterfactual Explanations under Distributional Ambiguity

ICLR'22

Counterfactual Plan under Model Shifts



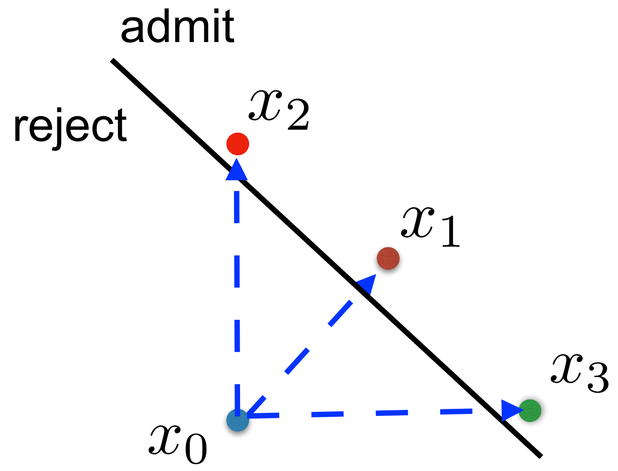
Counterfactual Plan under Model Shifts



Counterfactual Plan under Model Shifts

$\mathcal{C}_{\theta_0}$

ML model



2023

apply

We regret to inform you that…

$x_0 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}, ...)$

What can I do to get admitted?

$\{x_j\}_{j=1,\ldots,J}$

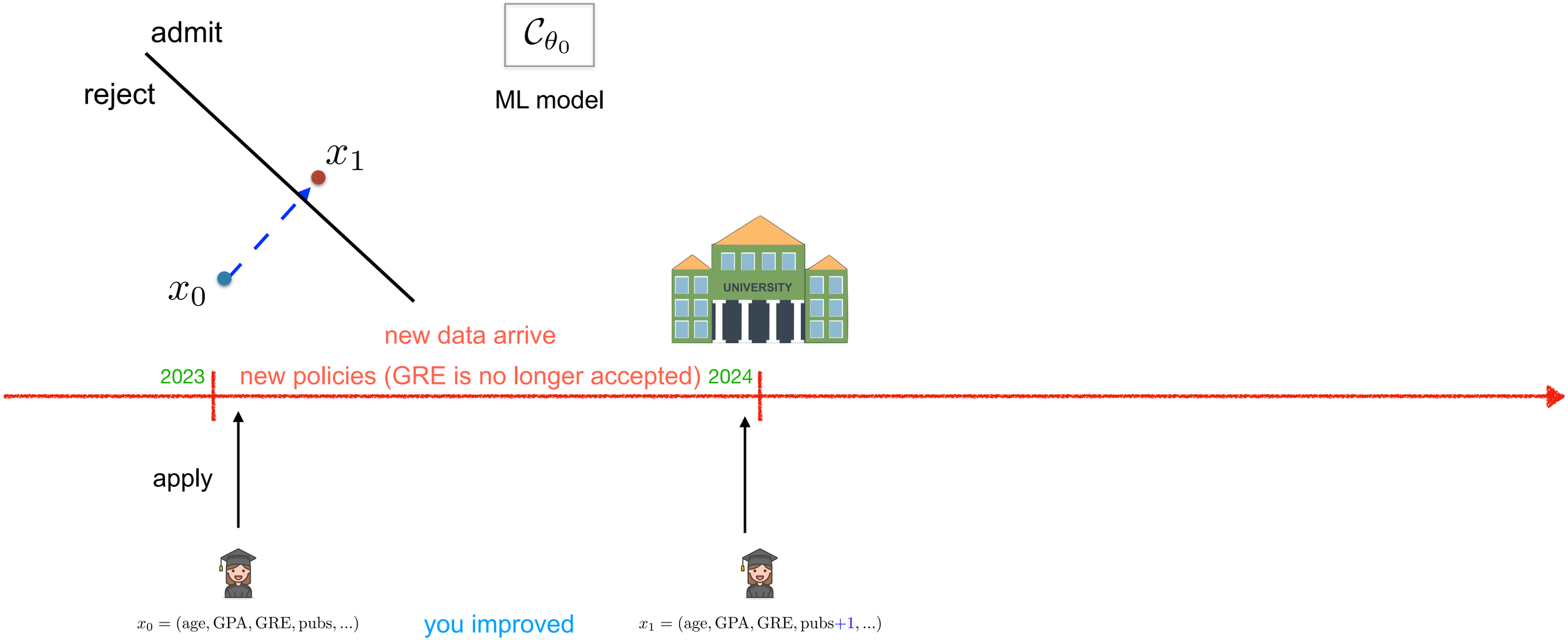
CF Plan

$x_1 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}{+}1, ...)$
$x_2 = (\text{age}, \text{GPA}, \text{GRE}{+}15, \text{pubs}, ...)$
$x_3 = (\text{age}, \text{GPA}{+}0.2, \text{GRE}, \text{pubs}, ...)$

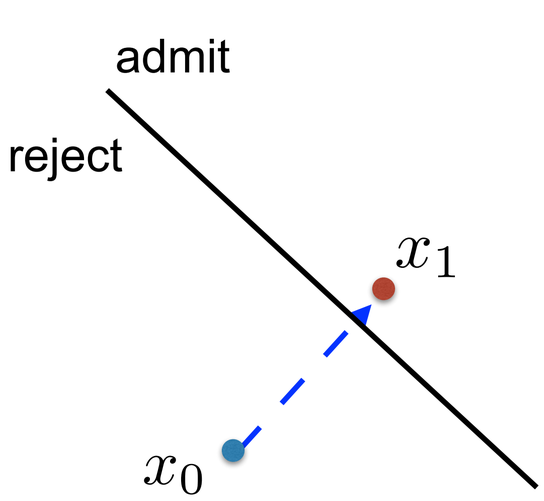
$x_1 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}{+}1, ...)$

Okay I will try to publish one more top-tier paper

Counterfactual Plan under Model Shifts



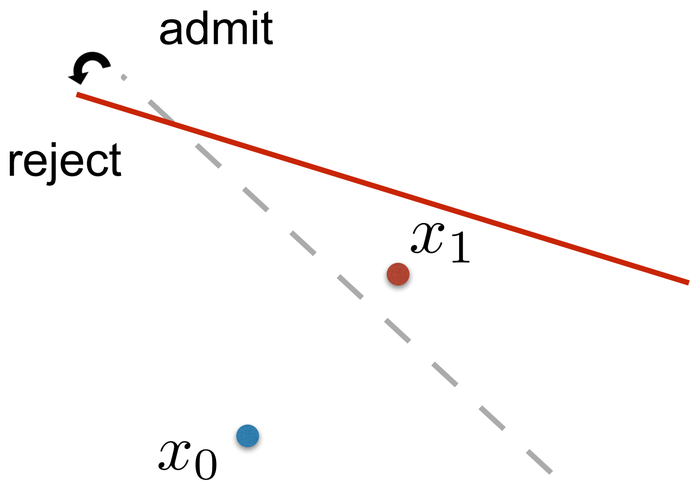
Counterfactual Plan under Model Shifts



$\mathcal{C}_{\theta_0}$ — retraining → $\mathcal{C}_{\tilde{\theta}}$

ML model (2023)

ML model



new data arrive

2023 new policies (GRE is no longer accepted) 2024

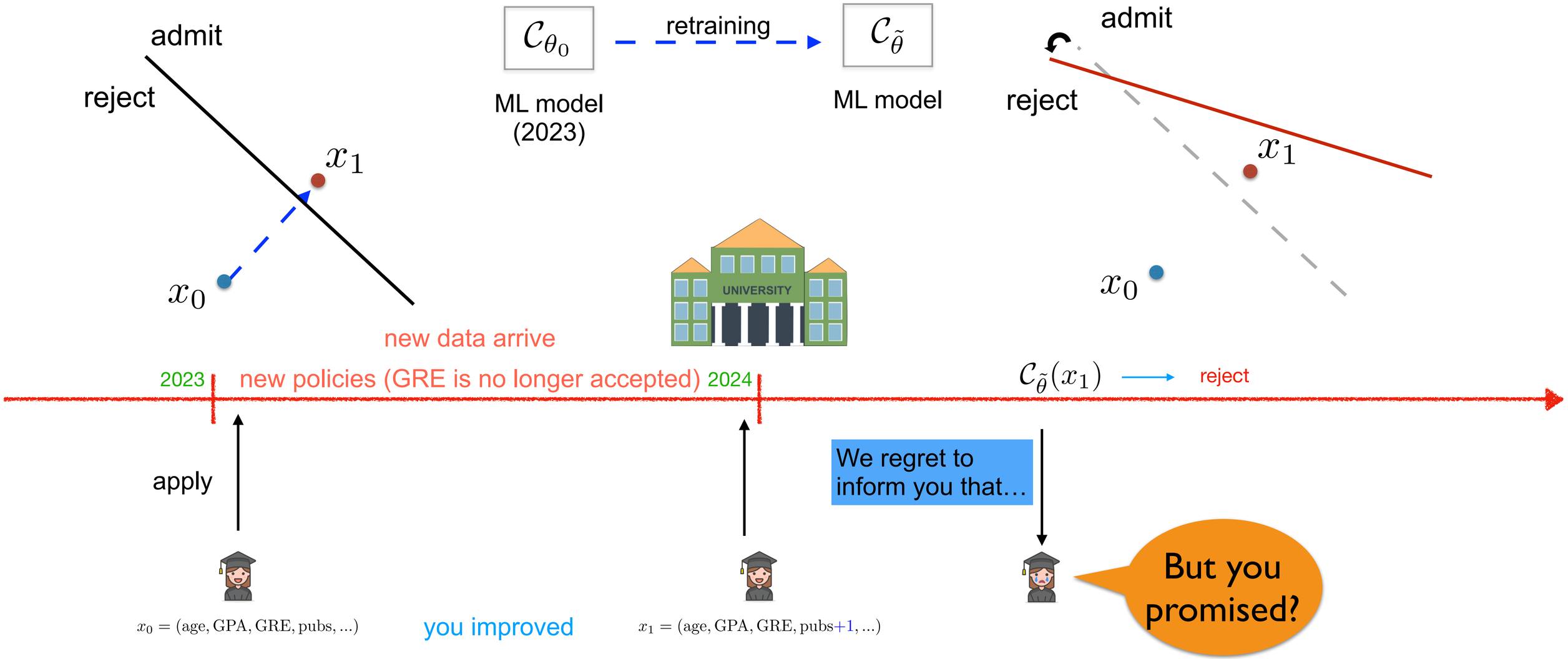
apply

$x_0 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}, ...)$

you improved

$x_1 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}{+}1, ...)$

Counterfactual Plan under Model Shifts



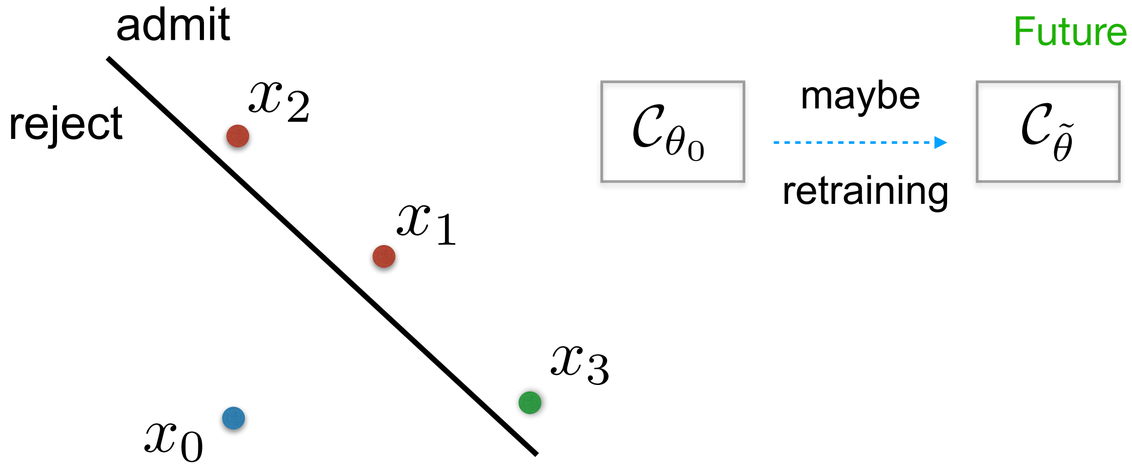
Settings

We are given:

- An ML model (assumed to be linear)

$$\mathcal{C}_{\theta_0}(x) = \begin{cases} 0 \Rightarrow \text{reject (unfavorable)} \\ 1 \Rightarrow \text{accept (favorable)} \end{cases}$$

- A CF plan $\{x_j\}_{j=1,\ldots,J}$



Definition: A plan $\{x_j\}_{j=1,\ldots,J}$ is valid w.r.t. $\tilde{\theta}$ if

$$\mathcal{C}_{\tilde{\theta}}(x_j) = 1 \qquad \forall j = 1, \ldots, J$$

$x_0 = (\text{age}, \text{GPA}, \text{GRE}, \text{pubs}, \ldots)$

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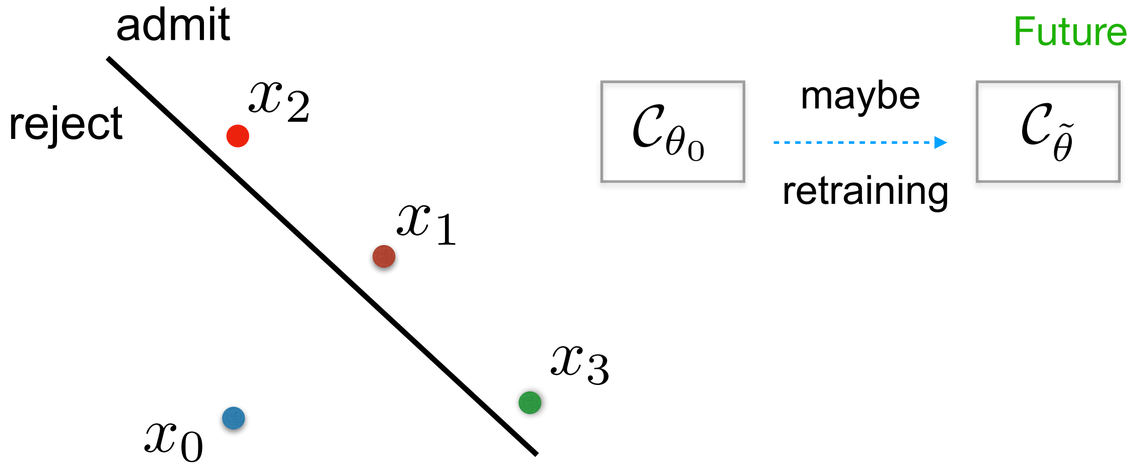
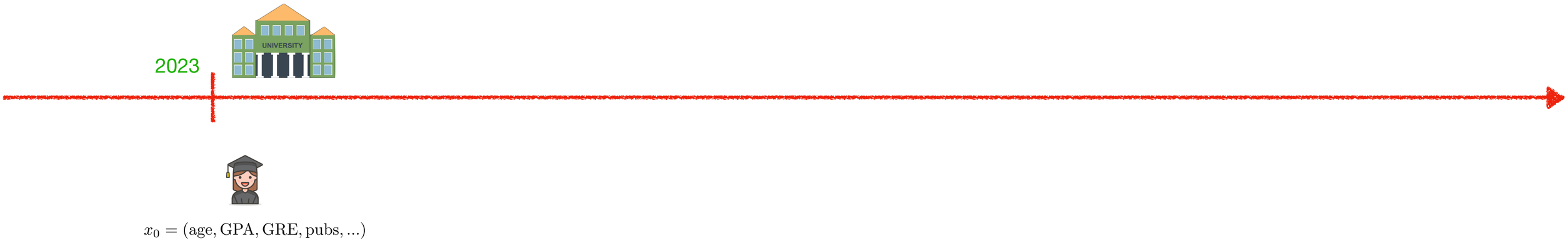


Q1. Given $\{x_j\}$, what is the probability that the plan is valid (w.r.t. $\tilde{\theta}$)?
Q2. Can we construct a counterfactual plan that is robust to model shifts?



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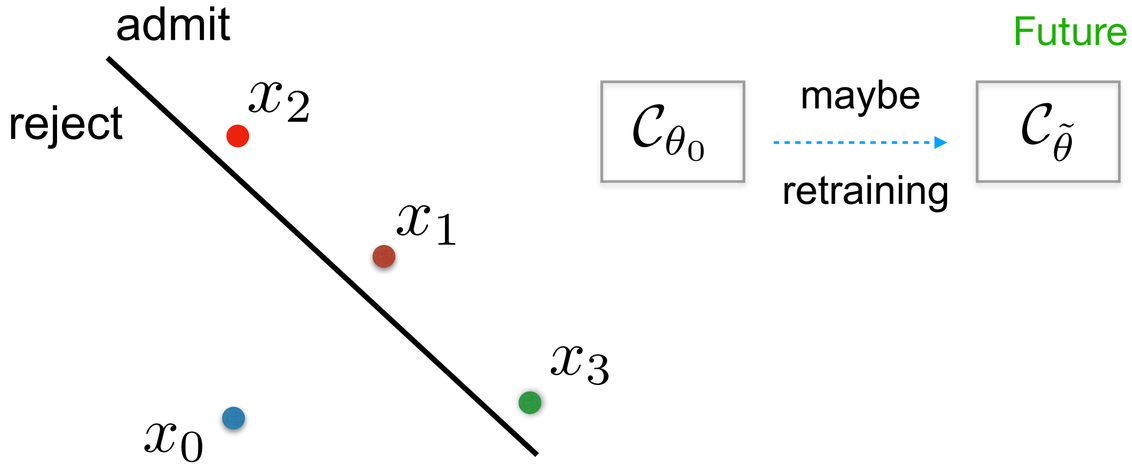
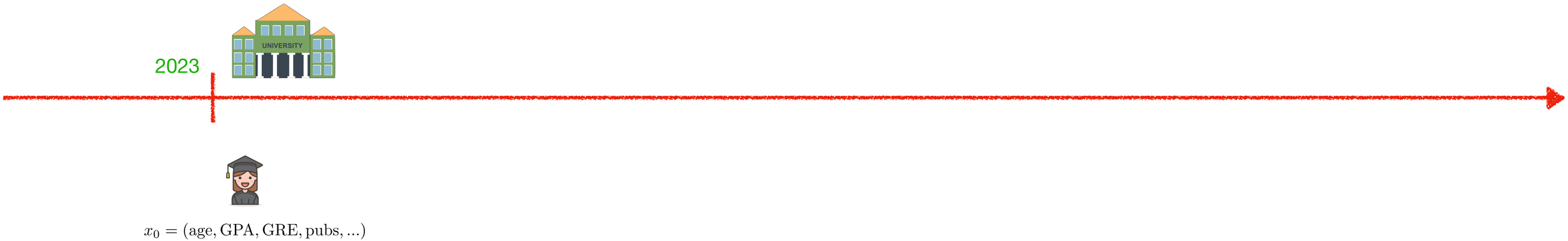
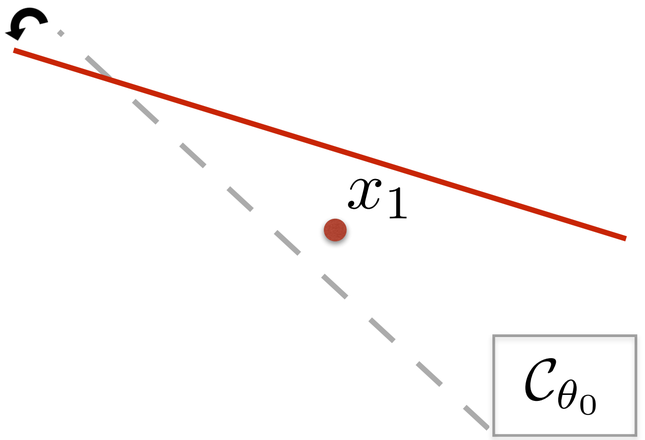


We don't know it

Q1. Given $\{x_j\}$, what is the probability that it is a valid plan (w.r.t. $\tilde{\theta}$)?
Q2. How can we construct a counterfactual plan that is robust to model shifts?



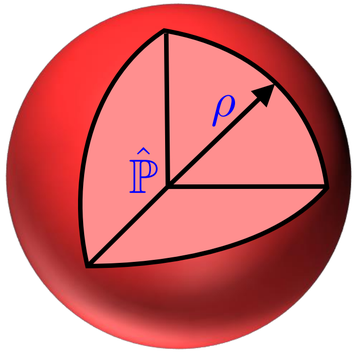
Uncertainty Modeling



Assume that the *future* parameter $\tilde{\theta} \sim \mathbb{P} \in \mathbb{B} = \{\mathbb{P} : \mathbb{G}(\mathbb{P}, \hat{\mathbb{P}}) \leq \rho\}$

Ambiguity set $\mathbb{B}$

- neighborhood around $\hat{\mathbb{P}} \sim (\hat{\mu}, \hat{\Sigma})$
- aims to contain the true distribution $\mathbb{P}$ with a high probability



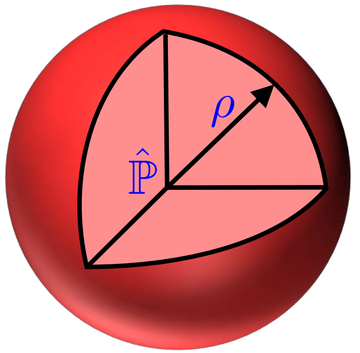
$\hat{\mathbb{P}} \sim (\hat{\mu}, \hat{\Sigma})$: estimated distribution (e.g. $\widehat{\mu} = \theta_0, \widehat{\Sigma} = I$)

$\mathbb{G}(\cdot\ , \cdot)$: distance between 2 distributions

ρ : uncertainty radius (controllable hyperparameter)

Uncertainty Modeling

$$\tilde{\theta} \sim \mathbb{P} \in \mathbb{B} = \{\mathbb{P} : \mathbb{G}(\mathbb{P}, \hat{\mathbb{P}}) \leq \rho\}$$



$\mathbb{G}(\cdot\,,\cdot)$: Gelbrich distance between two distributions

Definition: For $\mathbb{Q}_1 \sim (\mu_1, \Sigma_1)$ and $\mathbb{Q}_2 \sim (\mu_2, \Sigma_2)$

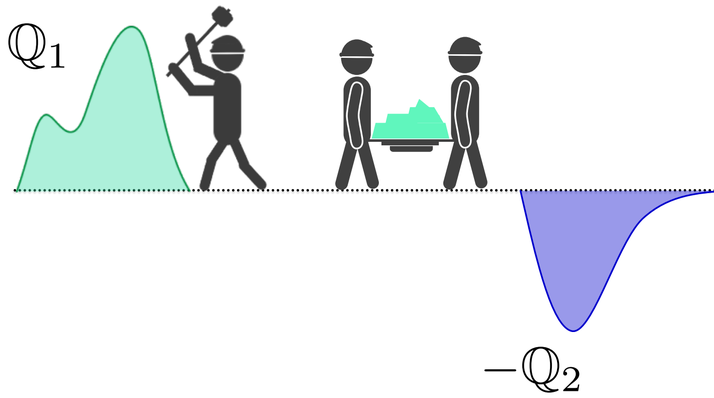
$$\mathbb{G}(\mathbb{Q}_1, \mathbb{Q}_2) = \sqrt{\|\mu_1 - \mu_2\|_2^2 + \mathrm{Tr}\left[\Sigma_1 + \Sigma_2 - 2\left(\Sigma_2^{\frac{1}{2}} \Sigma_1 \Sigma_2^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]}$$

Proposition (Connection to Type-2 Wasserstein distance)**:**

For $\mathbb{Q}_1 \sim (\mu_1, \Sigma_1)$ and $\mathbb{Q}_2 \sim (\mu_2, \Sigma_2)$

$$W(\mathbb{Q}_1, \mathbb{Q}_2) \geq \mathbb{G}(\mathbb{Q}_1, \mathbb{Q}_2)$$

$W^2(\mathbb{Q}_1, \mathbb{Q}_2) =$ minimum cost of moving $\mathbb{Q}_1$ to $\mathbb{Q}_2$



Gelbrich distance has a nice connection to Wasserstein distance but is much easier to compute.

Gelbrich (1990)

Uncertainty Quantification

- **Q1**. Given $\{x_j\}$, what is the probability that it is a valid plan (w.r.t. $\tilde{\theta}$)?

$$\mathcal{C}_\theta(x) = \begin{cases} 0 & \text{if } \theta^\top x < 0 \\ 1 & \text{if } \theta^\top x \geq 0 \end{cases}$$

Uncertainty Quantification

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$$\mathbb{P}(\mathcal{C}_{\tilde{\theta}}(x_j) = 1 \ \ \forall j)$$

True validity

Uncertainty Quantification

- **Q1**. Given $\{x_j\}$, what is the probability that it is a valid plan (w.r.t. $\tilde{\theta}$)?

$$\mathcal{C}_\theta(x) = \begin{cases} 0 & \text{if } \theta^\top x < 0 \\ 1 & \text{if } \theta^\top x \geq 0 \end{cases}$$

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True validity

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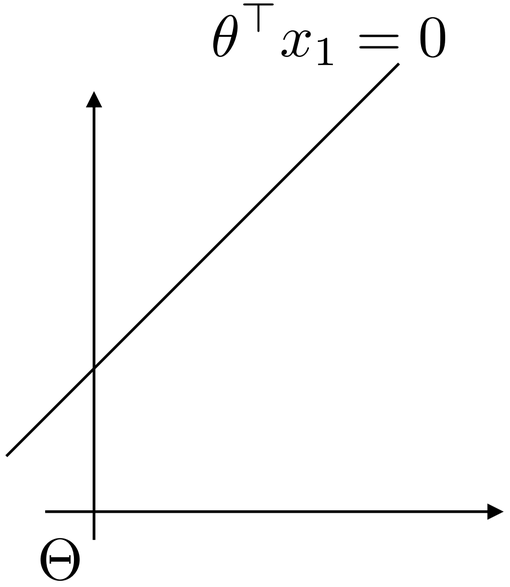

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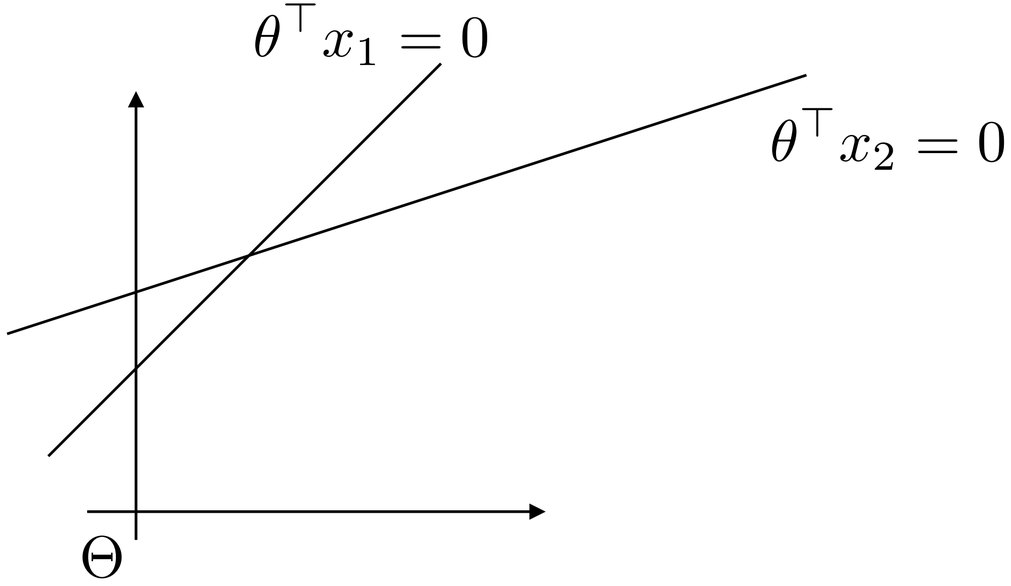

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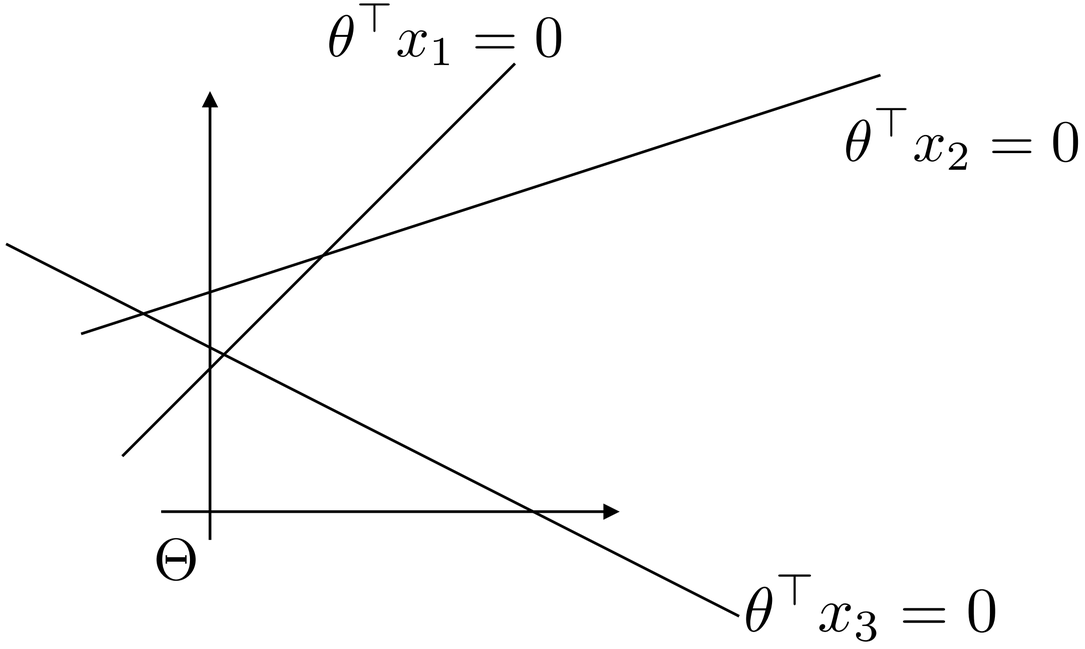

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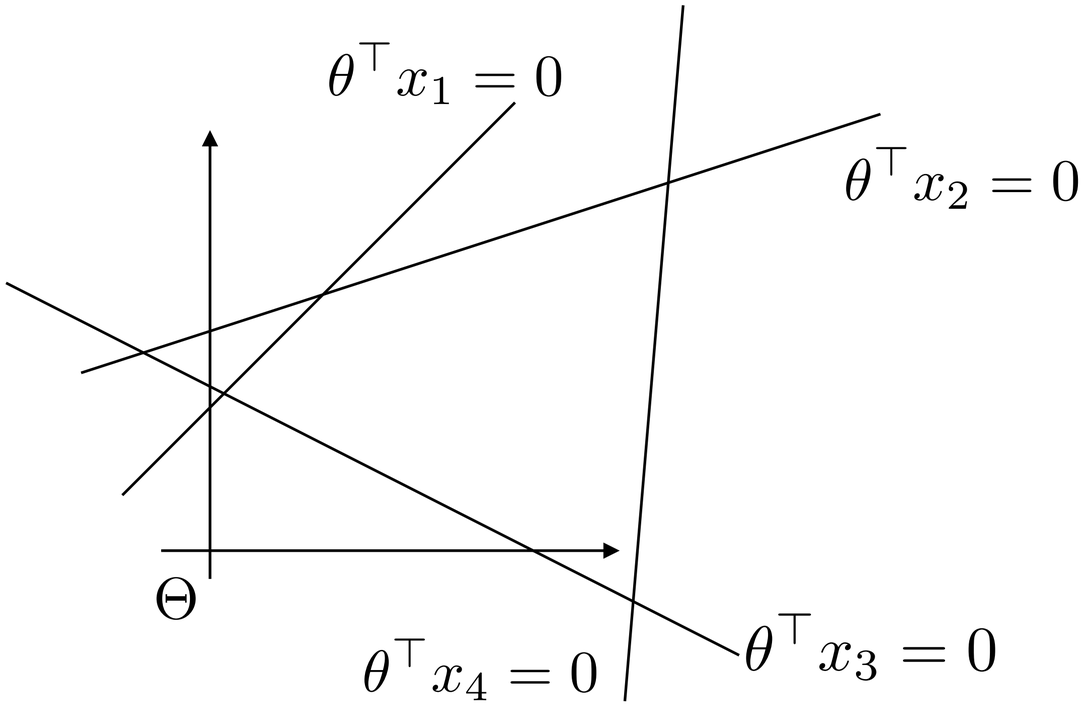

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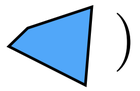
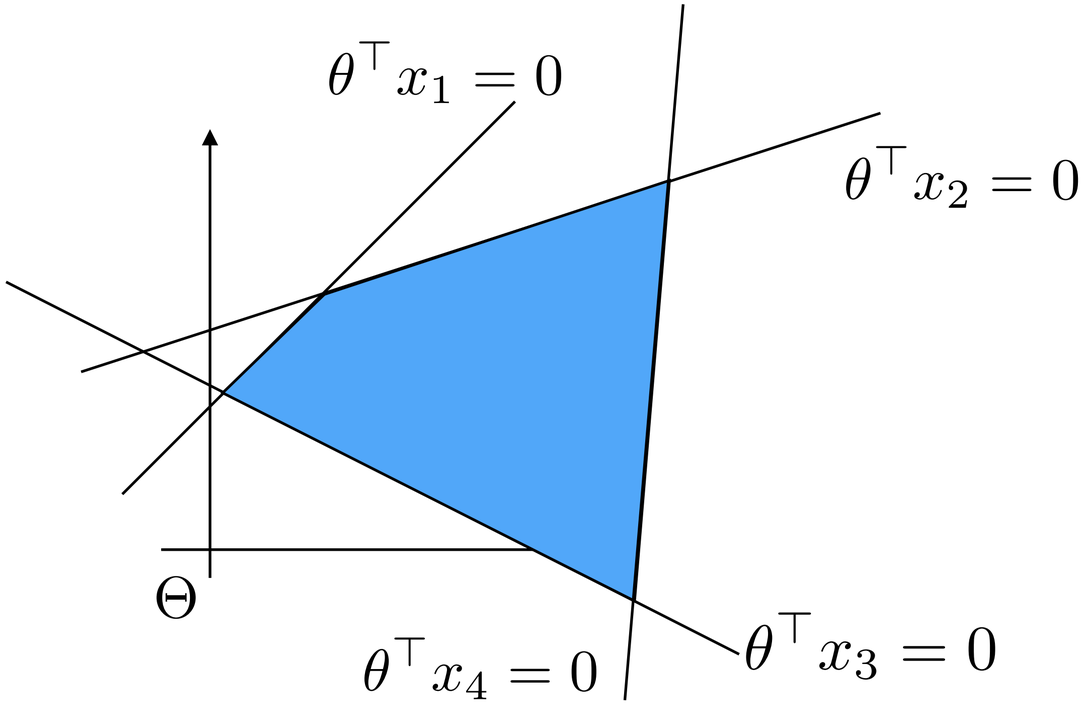
True validity $= \mathbb{P}(\tilde{\theta} \in$  $)$



Vandenberghe et al. (2007)

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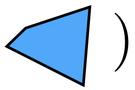
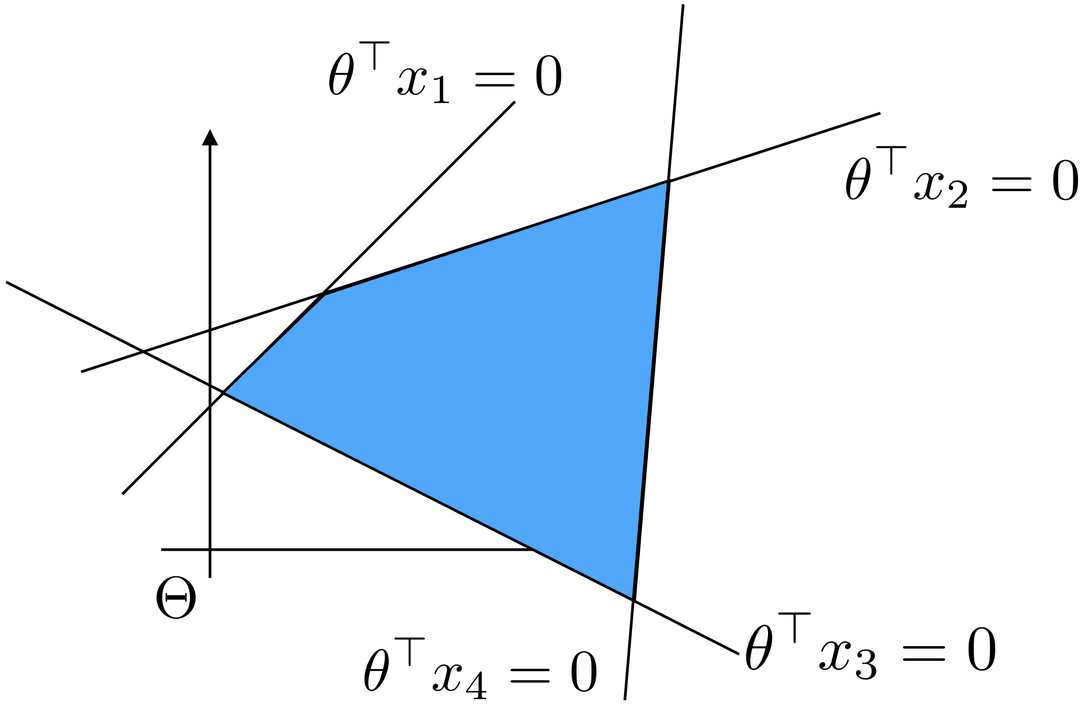
True validity $= \mathbb{P}(\tilde{\theta} \in$  $)$

We don't know



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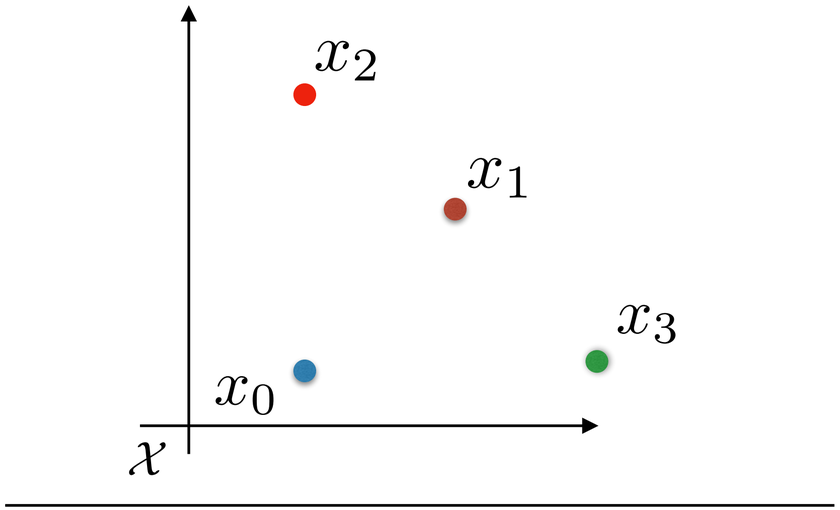

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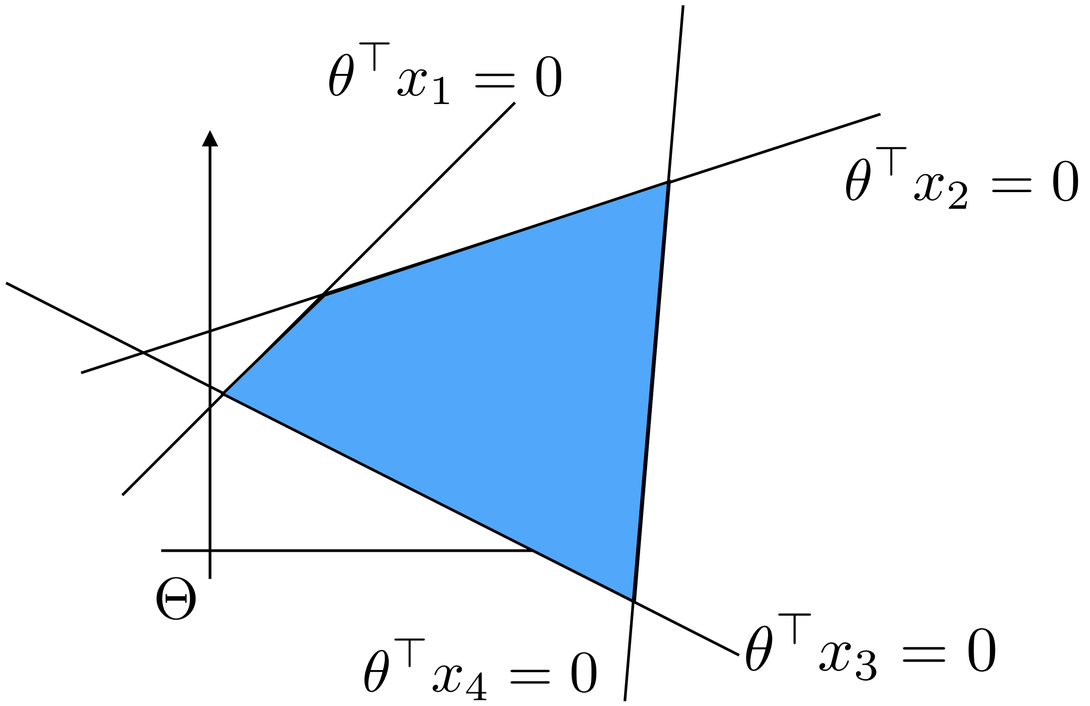
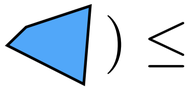
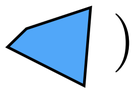
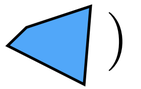


Vandenberghe et al. (2007)

Uncertainty Quantification

Assume that the *future* parameter $\tilde{\theta} \sim \mathbb{P} \in \mathbb{B} = \{\mathbb{P} : \mathbb{G}(\mathbb{P}, \hat{\mathbb{P}}) \leq \rho\}$

Lower bound $\leq$ True validity $\leq$ Upper bound

$\inf_{\mathbb{Q} \in \mathbb{B}} \mathbb{Q}(\tilde{\theta} \in$  $) \leq$ $\mathbb{P}(\tilde{\theta} \in$  $) \leq \sup_{\mathbb{Q} \in \mathbb{B}} \mathbb{Q}(\tilde{\theta} \in$  $)$

True validity of plan $\{x_j\}_{j=1,\ldots,J}$

Uncertainty Quantification

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Lower bound $\leq$ True validity $\leq$ Upper bound

$$L^\star \leq \inf_{\mathbb{Q} \in \mathbb{B}} \mathbb{Q}(\tilde{\theta} \in \blacktriangleleft) \leq \mathbb{P}(\tilde{\theta} \in \blacktriangleleft) \leq \sup_{\mathbb{Q} \in \mathbb{B}} \mathbb{Q}(\tilde{\theta} \in \blacktriangleleft) \leq U^\star$$

True validity of plan $\{x_j\}_{j=1,\ldots,J}$

Semi-definite program

Semi-definite program

Theorem: $L^\star$ and $U^\star$ can be computed by solving *linear* semidefinite programs.

- Computational tractability (solved effectively by MOSEK)
- Complementary information: either $L^\star = 0$ or $U^\star = 1$

Uncertainty Quantification

Theorem: We have

$$
L^\star = \left\{ \begin{array}{ll}
\inf & 1 - \sum_{j\in[J]} \lambda_j \\
\text{s.t.} & \mu \in \mathbb{R}^d,\ \Sigma \in \mathbb{S}_+^d,\ C \in \mathbb{R}^{d\times d},\ M \in \mathbb{S}_+^d \\
& \lambda_j \in \mathbb{R},\ z_j \in \mathbb{R}^d,\ Z_j \in \mathbb{S}^d \ \ \forall j \in [J] \\
& -x_j^\top z_j \geq 0, \ \begin{bmatrix} Z_j & z_j \\ z_j^\top & \lambda_j \end{bmatrix} \succeq 0 \qquad \forall j \in [J] \\
& \displaystyle\sum_{j\in[J]} \begin{bmatrix} Z_j & z_j \\ z_j^\top & \lambda_j \end{bmatrix} \preceq \begin{bmatrix} M & \mu \\ \mu^\top & 1 \end{bmatrix}, \ \begin{bmatrix} \Sigma & C \\ C^\top & \hat{\Sigma}_1 \end{bmatrix} \succeq 0, \ \begin{bmatrix} M-\Sigma & \mu \\ \mu^\top & 1 \end{bmatrix} \succeq 0 \\
& \|\hat{\mu}_1\|^2 - 2\hat{\mu}_1^\top \mu + \mathrm{Tr}\big[M + \hat{\Sigma}_1 - 2C\big] \leq \rho^2.
\end{array} \right.
$$

Proof ideas:

- Chebyshev bounds on an open polyhedron
- Rejoin a two-layer optimization problem

Uncertainty Quantification

Theorem: We have

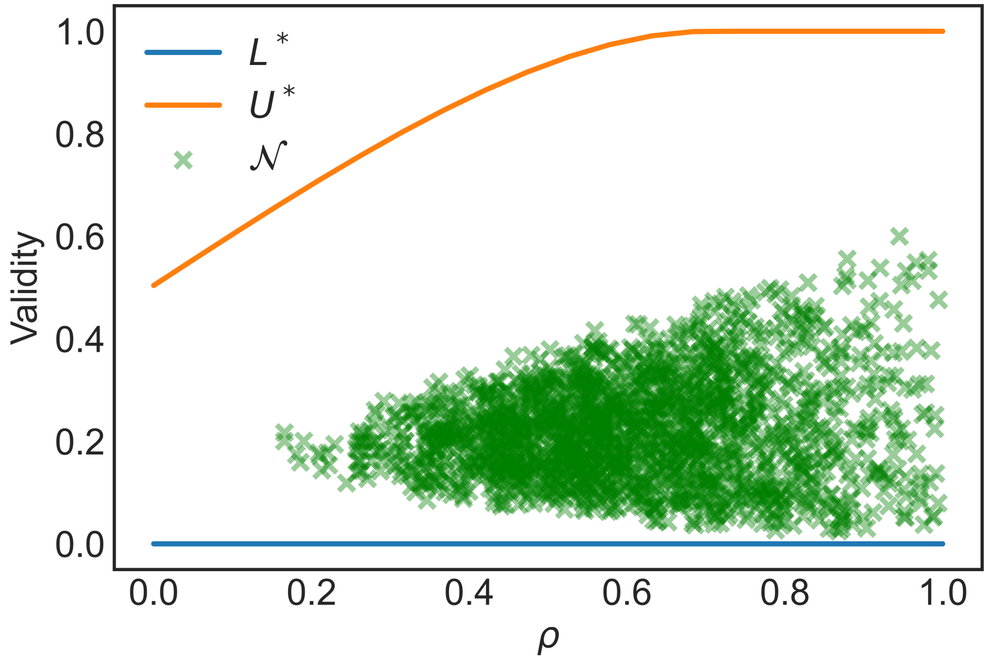
$$
U^\star = \left\{ \begin{array}{ll}
\inf & z_0 + \gamma(\rho^2 - \|\hat{\mu}_1\|_2^2 - \mathrm{Tr}\big[\hat{\Sigma}_1\big]) + q + \mathrm{Tr}\big[Q\big] \\
\text{s.t.} & \gamma \in \mathbb{R}_+,\ z_0 \in \mathbb{R},\ z \in \mathbb{R}^d,\ Z \in \mathbb{S}_+^d,\ q \in \mathbb{R}_+,\ Q \in \mathbb{S}_+^d,\ \lambda \in \mathbb{R}_+^J \\
& \begin{bmatrix} \gamma I - Z & \gamma \hat{\Sigma}_1^{\frac{1}{2}} \\ \gamma \hat{\Sigma}_1^{\frac{1}{2}} & Q \end{bmatrix} \succeq 0, \quad \begin{bmatrix} \gamma I - Z & \gamma \hat{\mu}_1 + z \\ \gamma \hat{\mu}_1^\top + z^\top & q \end{bmatrix} \succeq 0 \\
& \begin{bmatrix} Z & z \\ z^\top & z_0 \end{bmatrix} \succeq 0, \quad \begin{bmatrix} Z & z \\ z^\top & z_0 - 1 \end{bmatrix} \succeq \sum_{j \in [J]} \lambda_j \begin{bmatrix} 0 & \frac{1}{2} x_j \\ \frac{1}{2} x_j^\top & 0 \end{bmatrix}.
\end{array} \right.
$$

Proof ideas:

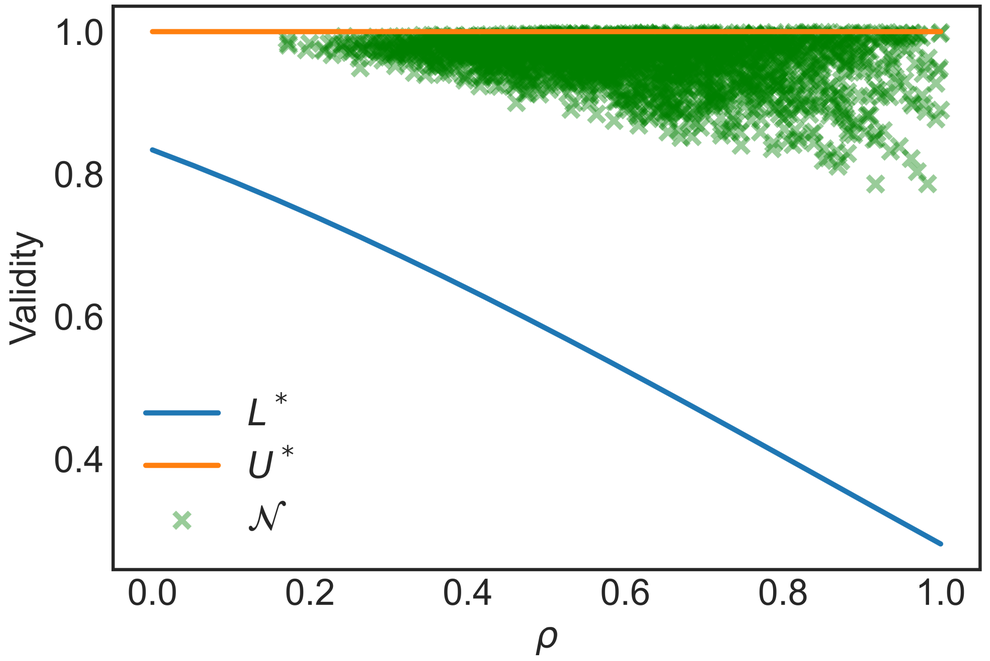
- Duality techniques from DRO
- Rejoin with the support function of the uncertainty set

Empirical Results

- fix a $\{x_j\}_J$
- fix $\hat{\mu} = \theta_0, \hat{\Sigma} = 0.5I$
- evaluate $L^\star$ and $U^\star$
- sample $\tilde{\theta} \sim \mathcal{N}(\mu_g, \Sigma_g)$, (μ_g, Σ_g) is chosen randomly



$\hat{\mu} \notin$



$\hat{\mu} \in$

Counterfactual Plan - Construction

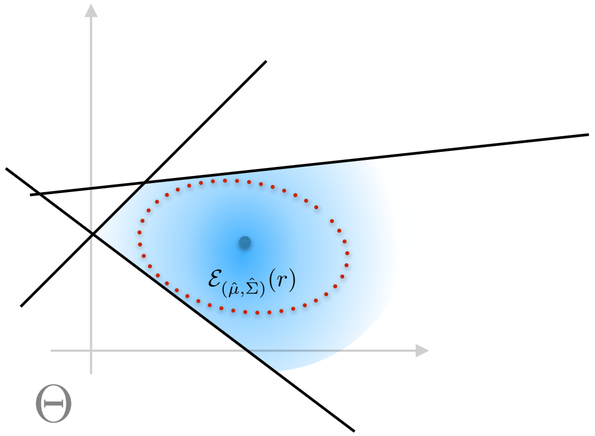
$$\min_{x_1,\ldots,x_J} \quad \text{Proximity}(\{x_j\}, x_0) - \lambda_1 \text{FutureValidity}(\{x_j\}) - \lambda_2 \text{Diversity}(\{x_j\})$$

Average L-1 distance

where $$\text{Proximity}(\{x_j\}, x_0) \triangleq \frac{1}{J}\sum_{j=1}^{J} \|x_j - x_0\|_1.$$

The maximum volume of the ellipsoid inscribed in a set of feasible parameters

$$\text{FutureValidity}(\{x_j\}) \triangleq \max\{r : r \geq 0,\ \mathcal{E}_{(\hat{\mu},\hat{\Sigma})}(r) \subseteq \Theta(\{x_j\})\}.$$



Determinantal point process (DPP)

$$\text{Diversity}(\{x_j\}) \triangleq \det(K), \text{ where } K_{i,j} = (1 + \|x_i - x_j\|_1)^{-1}\ \forall 1 \leq i, j \leq J.$$

Solved by projected gradient descent

Empirical Results

- each dataset contains two sets of data (present data and future data).
- generate counterfactuals w.r.t. the classifier trained on the present data.
- evaluate empirical validity w.r.t. the classifiers trained on the future data.

Dataset	Method	Proximity	Diversity	L^*	Empirical Validity
German credit	DiCE	0.986 ± 0.324	0.072 ± 0.050	0.649 ± 0.073	0.996 ± 0.008
	MahalanobisCrr	1.002 ± 0.323	0.064 ± 0.047	0.750 ± 0.064	0.999 ± 0.003
	COPA ($\lambda_1 = 0.2; \lambda_2 = 2.0$)	$\mathbf{0.916} \pm 0.178$	0.017 ± 0.058	0.944 ± 0.168	0.997 ± 0.018
	COPA ($\lambda_1 = 0.5; \lambda_2 = 5.0$)	1.154 ± 0.253	0.114 ± 0.101	$\mathbf{0.946} \pm 0.040$	$\mathbf{1.000} \pm 0.000$
	COPA ($\lambda_1 = 1.0; \lambda_2 = 10.0$)	1.351 ± 0.166	$\mathbf{0.225} \pm 0.045$	0.911 ± 0.022	$\mathbf{1.000} \pm 0.000$
SBA	DiCE	2.037 ± 0.470	0.089 ± 0.057	0.946 ± 0.014	0.801 ± 0.061
	MahalanobisCrr	2.014 ± 0.473	0.085 ± 0.055	0.966 ± 0.007	0.945 ± 0.062
	COPA ($\lambda_1 = 0.2; \lambda_2 = 2.0$)	$\mathbf{1.831} \pm 0.139$	0.253 ± 0.026	0.994 ± 0.000	1.000 ± 0.000
	COPA ($\lambda_1 = 0.5; \lambda_2 = 5.0$)	1.966 ± 0.112	0.363 ± 0.012	$\mathbf{0.995} \pm 0.000$	$\mathbf{1.000} \pm 0.000$
	COPA ($\lambda_1 = 1.0; \lambda_2 = 10.0$)	2.010 ± 0.124	$\mathbf{0.380} \pm 0.006$	0.995 ± 0.000	$\mathbf{1.000} \pm 0.000$
Student performance	DiCE	$\mathbf{1.486} \pm 0.325$	$\mathbf{0.136} \pm 0.044$	0.549 ± 0.307	0.408 ± 0.363
	MahalanobisCrr	1.497 ± 0.325	0.126 ± 0.044	0.864 ± 0.117	0.757 ± 0.284
	COPA ($\lambda_1 = 0.2; \lambda_2 = 2.0$)	1.779 ± 0.352	0.052 ± 0.047	$\mathbf{0.998} \pm 0.000$	$\mathbf{1.000} \pm 0.000$
	COPA ($\lambda_1 = 0.5; \lambda_2 = 5.0$)	1.882 ± 0.353	0.089 ± 0.032	0.998 ± 0.000	$\mathbf{1.000} \pm 0.000$
	COPA ($\lambda_1 = 1.0; \lambda_2 = 10.0$)	1.926 ± 0.349	0.109 ± 0.024	0.997 ± 0.000	$\mathbf{1.000} \pm 0.000$

Follow-up Questions

- Can we use the lower bound to construct a *robust* counterfactual plan?
  - No, we have to use a maximum ellipsoid to approximate it.
  - But, if there is only one counterfactual explanation, we can construct it efficiently -> ICLR'23

- Can we use it for nonlinear models?
  - Yes, but we must use a linear model (e.g., LIME) to construct a surrogate decision boundary before applying our technique.

- How does the linear surrogate affect the constructed explanation? (e.g., unfaithful to the decision boundary)
  - Analyzing and proposing a more faithful linear surrogate -> Rejected (4 times)

- I don't wanna use a linear surrogate.
  - Robust Bayesian Recourse -> UAI'22

The Shapley value

from game theory to machine learning

Cooperative games

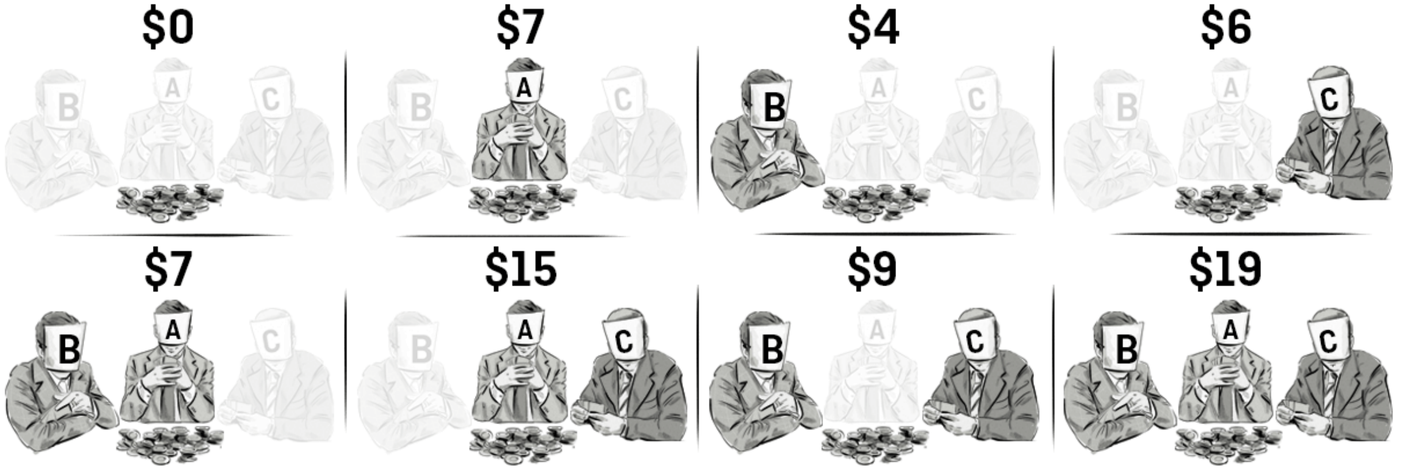
- Cooperative games model scenarios where
  - Agent can benefit by cooperating
  - Binding agreements are possible

Cooperative games

- How to construct a salary structure in a company or a football club?

Cooperative games

- How to construct a salary structure in a company or a football club?
- How to divide a surplus (profit) to shareholders so that everyone is satisfied?



Cooperative games

Cooperative game

- Players can benefit by cooperating
- Binding agreements are possible
- Answer the question: How to divide the surplus when joining the grand coalition?

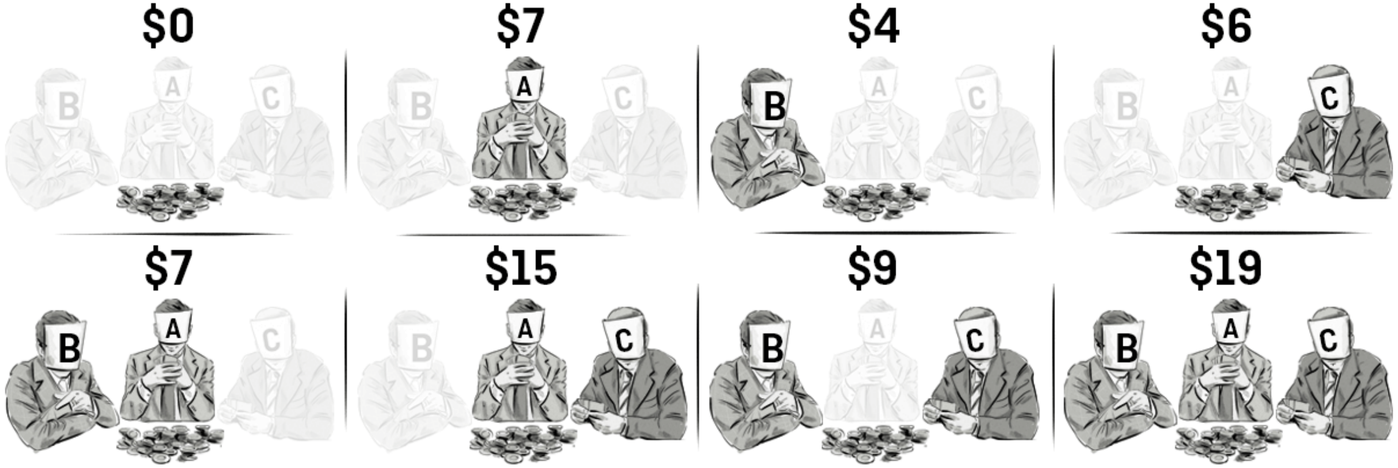
Non-cooperative game

- Players are independent
- No cooperation
- Answer the question: What is the “good” strategy for each player to maximize their return?

Nash equilibrium, zero-sum game

Cooperative games

- A cooperative game is described by a tuple (N, F) where $N = \{1, \ldots, n\}$ a set of players and $F : 2^N \to \mathbb{R}$, $F(\emptyset) = 0$ is a characteristic function.
  - By von Neumann and Morgenstern:
    - Superadditive game: $F(S \cup T) \geq F(S) + F(T)$ (relaxed by later works)
    - Transferable Utility (TU) game | non-Transferable Utility (NTU) game



John von Neumann and Oskar Morgenstern, *Theory of games and economic behavior. 1944*

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  - $\mathbb{G}$: set of all possible games

- How to divide a surplus (profit) to players?
  - $\psi : \mathbb{G} \to \mathbb{R}^n, \quad \psi((N, F)) \in \mathbb{R}^n$: a solution concept

When context is clear, I omit the player set *N* in *(N, F)*
and use *F* to denote the game and $\psi(F)$ to denote a solution concept of *F*

John von Neumann and Oskar Morgenstern, *Theory of games and economic behavior. 1944*

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$\psi((N, F))$	$4	$11	$9

Payoff vector

John von Neumann and Oskar Morgenstern, *Theory of games and economic behavior. 1944*

Several Solution Concepts

- **Imputation set** (von Neumann & Morgenstern, 1944): Includes all payoff vectors that are *efficient,* i.e., share the whole utility, and *individually rational*, i.e., assign to each player at least her standing alone worth.

$$\psi_{IS}((N,F)) = \left\{x \in \mathbb{R}^n : \sum_{i \in N} x_i = F(N), x_i \geq v(i), \forall i \in N\right\}$$

- **Core set** (Gillies, 1953): similar to imputation set but considering *coalitional rational* instead of individual rational.

$$\psi_{CS}((N,F)) = \left\{x \in \mathbb{R}^n : \sum_{i \in S} x_i \geq F(S), \forall S \subseteq N\right\}$$

Could be empty and not unique!

Chapman and Hall, *Handbook of the Shapley value.* 2019

The Shapley Value

- A solution concept for cooperative games that assigns payoffs for each player in the game and that is
  - unique for each game
  - efficient
  - fair

$\psi((N, F))$

$4	$8	$7

Payoff vector

The Shapley Value

Def 1.1 (*dividend*): The value of the player *i* is the sum of its dividend share to all possible coalitions to which he could be joined. The dividend of a coalition is shared equally by its members.

$$\phi_i((N,F)) = \sum_{S \subseteq N \setminus i} \frac{\Delta_F(S \cup i)}{s+1}, \quad \forall i \in N,$$

where $\Delta_F(T)$ is Harsanyi dividend of the game F to the coalition T:

$$\Delta_F(T) = \sum_{R \subseteq T} (-1)^{t-r} F(R), \quad \forall T \subseteq N$$

Harsanyi, *A bargaining model for cooperative n-person games*. 1959.

The Shapley Value

Def 1.2 (weighted *marginal contribution*): The value of player *i* is computed by its weighted average marginal contribution over all possible coalitions to which player *i could be joined*.

$$\phi_i((N,F)) = \frac{1}{n} \sum_{S \subseteq N \setminus i} \frac{1}{\binom{n-1}{s}} [F(S \cup i) - F(S)], \quad \forall i \in N$$

L.S. Shapley, *A value for n-person games*. 1953.

The Shapley Value

Def 1.3 (*random order*): The grand coalition is formed in a way that each player joins the coalition one-by-one, the value of player *i* is the average of its marginal contribution over all possible order.

$$\phi_i((N,F)) = \frac{1}{n!} \sum_{\pi \in \Pi(N)} [F(\pi^i \cup i) - F(\pi^i)]$$

where π^i is the set of players that precede player i in the permutation π.

Chapman and Hall, *Handbook of the Shapley value.* 2019

Axiomatic Characterization

We want to design a solution concept ψ that satisfies the following axioms:

- **Axiom 1** (*Linearity, L*)**:** for any two games F_1 and F_2,
$$\psi(F_1 + \alpha F_2) = \psi(F_1) + \alpha\psi(F_2)$$
- **Axiom 2** (*Dummy, D*): if $i \in N$ is a dummy player,
i.e., $F(S \cup i) = F(S) + F(i), \forall S \subseteq N$, then $\psi_i(F) = F(i)$.
- **Axiom 3** (*Symmetry, S*): For any permutation $\pi \in \Pi(N)$, $\psi_{\pi i}(\pi F) = \psi_i(F)$
- **Axiom 4** (*Efficiency, E*): $\sum_{i \in N} \psi_i(F) = F(N) - F(\emptyset)$

Alvin E. Roth, *The Shapley value.* 1988.

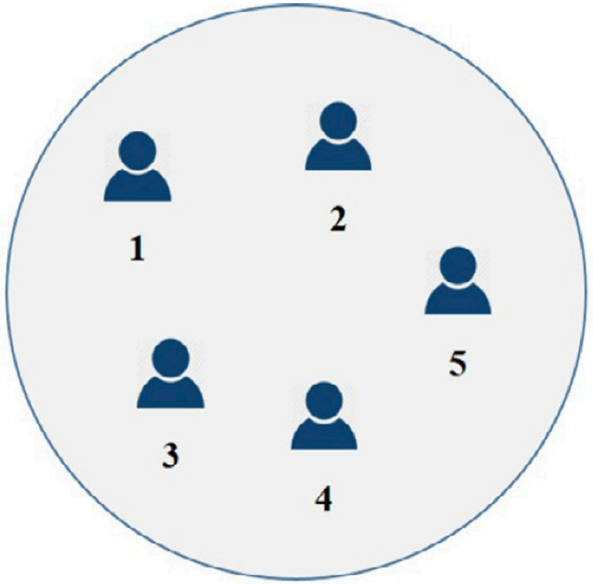
When context is clear, I omit the player set *N* in *(N, F)* and use *F* to denote the game

Main result

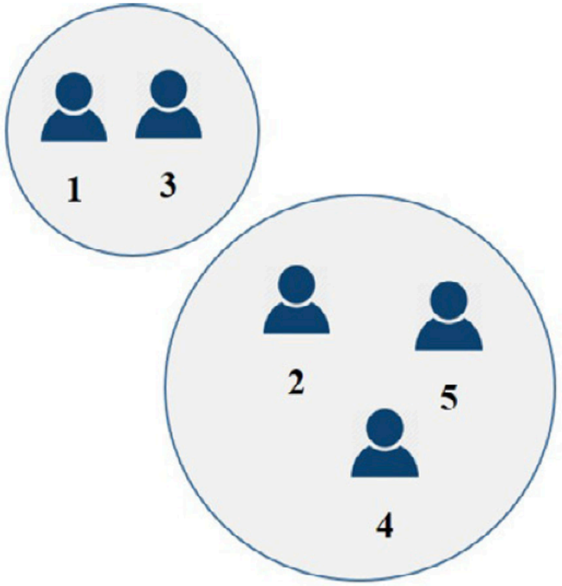
Theorem 1: Shapley value is a **unique** solution concept that satisfies four axioms *linearity, dummy, symmetry,* and *efficiency*.

L.S. Shapley, *A value for n-person games*. 1953.

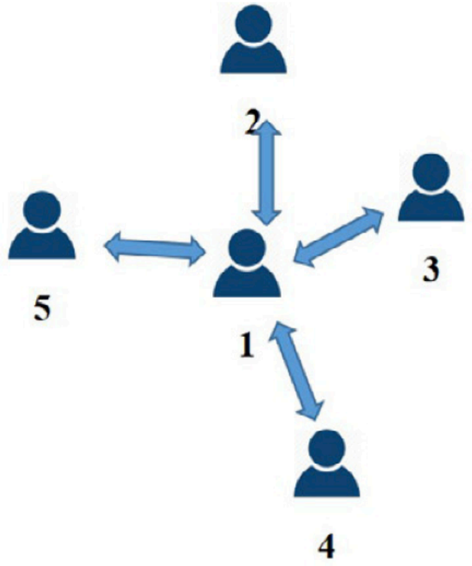
Types of Cooperative Games



Class I: Canonical Coalitional Games



Class II: Coalition Formation Games

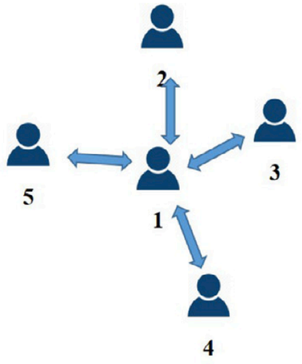


Class III: Coalitional Graph Games

Myerson, *Handbook of the Shapley value.* 1977

Coalitional Graph Games

- N is a set of nodes, $L = \{ij \mid i, j \in N\}$ is a set of edges. An edge represents a communication connection between two nodes.
- We omit the set N whenever the context is clear.
- $\zeta(N, L) = \{C_1, \ldots, C_r\}$ denotes a set of connected components of a graph (N, L).
- $L|_S$ is a set of edges induced by subset $S \subseteq N$, *i.e.*, $L|_S = \{ij \in L \mid i, j \in S\}$.



Class III: Coalitional Graph Games

- A communication-restricted function $f|_L$ is defined as

$$f|_L(T) = \sum_{R \in \zeta(T, L|_T)} f(R) \quad \forall T \subseteq N.$$

Myerson, *Handbook of the Shapley value.* 1977

The Myerson Value

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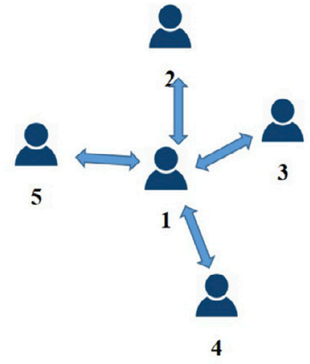

Class III: Coalitional Graph Games

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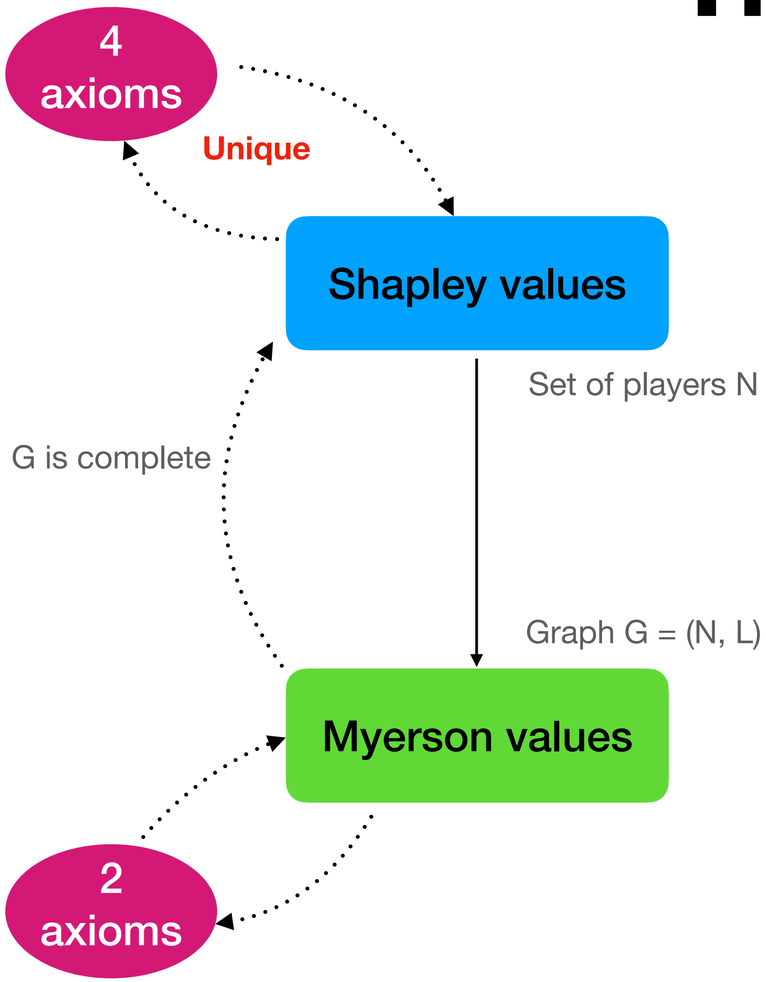
Definition 2.2 (Myerson value (Myerson, 1977))**.** *Given a graph* (N, L) *and a characteristic function* f*, Myerson value on a CO-game* (N, f, L) *is defined as*

$$\psi(f, L) = \phi(f|_L),$$

where $\phi(f|_L)$ *is Shapley value of a communication-restricted function* $f|_L$*.*

Myerson, *Handbook of the Shapley value.* 1977

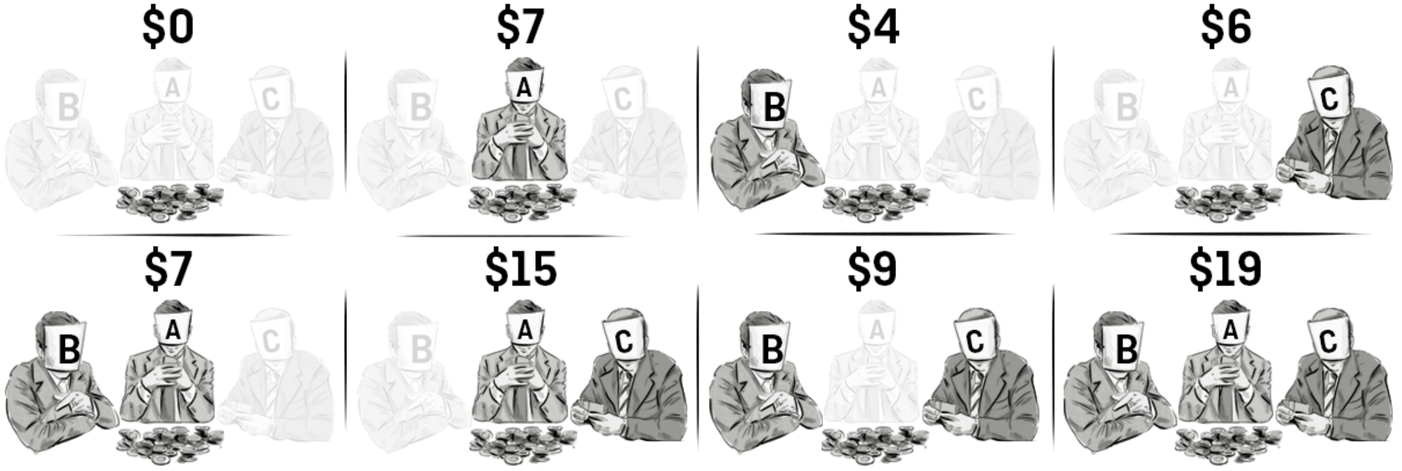
The Myerson Value



The Shapley Taylor Interaction Index

Definition 2.1 (Shapley-Taylor Interaction)**.** *The Shapley-Taylor index is defined as the expectation of* $\Phi^m_{S,\pi}(f)$ *over an ordering of* N *players chosen uniformly at random:*

$$\Phi^m_S(f) = \mathbb{E}_\pi(\Phi^m_{S,\pi}(f)) = \frac{m}{n} \sum_{T \subseteq N \setminus S} \delta_S f(T) \frac{1}{\binom{n-1}{t}}.$$



Myerson, *Handbook of the Shapley value.* 1977

The Myerson Value