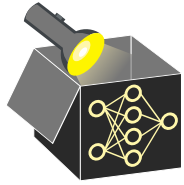
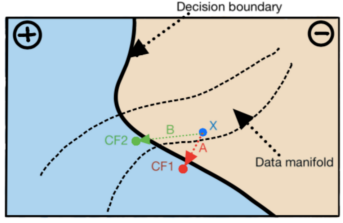
Interpretable Machine Learning



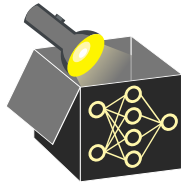
Counterfactual Explanations (CEs)
Optimization Problem and Objectives



Learning goals

- Formulate CEs as optimization problem
- Identify key objectives (proximity, sparsity)
- Understand trade-offs in CE generation

MATHEMATICAL PERSPECTIVE



Terminology:

- **x**: original/factual data point whose prediction we want to explain
- $y' \subset \mathbb{R}^g$: desired predi. ($y' =$ “grant credit") or interval ($y' = [1000, \infty[$)

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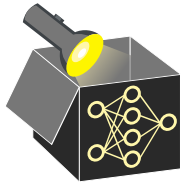

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A **valid** counterfactual $\mathbf{x}'$ satisfies two criteria:

1. **Prediction validity:** CE's prediction $\hat{f}(\mathbf{x}')$ is equal to the desired pred. y'
2. **Proximity:** CE $\mathbf{x}'$ is as close as possible to the original input **x**

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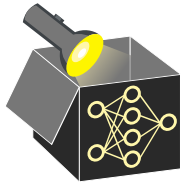

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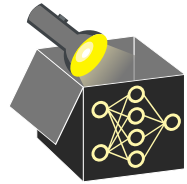
Reformulate these two objectives as optimization problem:

$$\arg\min_{\mathbf{x}'} \lambda_1 o_{target}(\hat{f}(\mathbf{x}'), y') + \lambda_2 o_{proximity}(\mathbf{x}', \mathbf{x})$$

- λ_1 and λ_2 balance the two objectives
- o_{target}: distance in target space
- $o_{proximity}$: distance in feature space

OBJECTIVE FUNCTIONS

▸ "Dandl et al." 2020



Distance in target space o_{target}:

- **Regression:** L_1 distance $o_{target}(\hat{f}(\mathbf{x}'), y') = |\hat{f}(\mathbf{x}') - y'|$
- **Classification:**
  - For predicted probabilities: $o_{target} = |\hat{f}(\mathbf{x}') - y'|$
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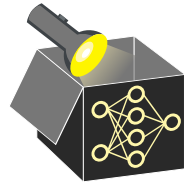

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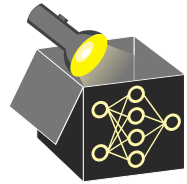
Distance in input space $o_{proximity}$: Gower distance (mixed feature types)

$$o_{proximity}(\mathbf{x}', \mathbf{x}) = d_G(\mathbf{x}', \mathbf{x}) = \frac{1}{p} \sum_{j=1}^{p} \delta_G(x_j', x_j) \in [0, 1], \text{ where}$$

- $\delta_G(x_j', x_j) = \mathbb{I}\left\{x_j' \neq x_j\right\}$ if x_j is categorical
- $\delta_G(x_j', x_j) = \frac{1}{\widehat{R}_j} |x_j' - x_j|$ if x_j is numerical

  $\rightsquigarrow$ $\widehat{R}_j$: range of feature j in the training set to ensure $\delta_G(x_j', x_j) \in [0, 1]$

FURTHER OBJECTIVES: SPARSITY



Additional constraints can improve the explanation quality of the corresponding CEs
$\rightsquigarrow$ popular constraints include **sparsity** and **plausibility**

Sparsity Favor explanations that change few features

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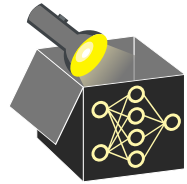

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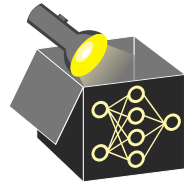

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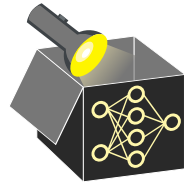
- Alternative: Include separate objective measuring sparsity, e.g., via L_0-norm

$$o_{sparse}(\mathbf{x}', \mathbf{x}) = \sum_{j=1}^{p} \mathcal{I}_{\{x'_j \neq x_j\}}$$

FURTHER OBJECTIVES: PLAUSIBILITY

Plausibility:

- CEs should suggest realistic (i.e., plausible) alternatives
  $\rightsquigarrow$ Implausible: increase income *and* become unemployed



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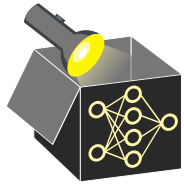

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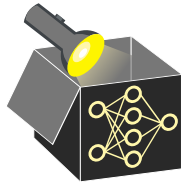

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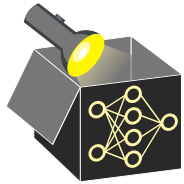

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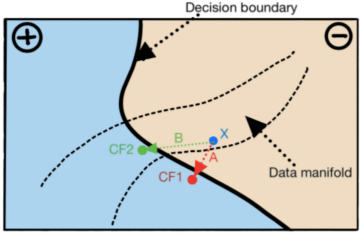

Example from ▸ "Verma et al." 2020

- Input **x** originally classified as ⊖
- Two valid CEs in class ⊕: CF1 and CF2
- Path **A** (CF1) is shorter (but unrealistic)
- Path **B** (CF2) is longer but in data manifold

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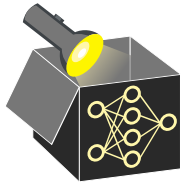

Plausibility term: Encourage counterfactuals close to observed data.

- Define $\mathbf{x}^{[1]}$ as the nearest neighbor of $\mathbf{x}'$ in the training set $\mathbf{X}$
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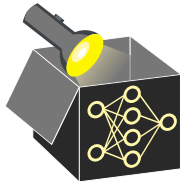

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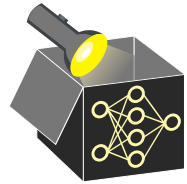
Extended optimization: Add sparsity and plausibility terms to the objective

$$\arg\min_{\mathbf{x}'} \lambda_1 o_{\text{target}}(\hat{f}(\mathbf{x}'), y') + \lambda_2 o_{\text{proximity}}(\mathbf{x}', \mathbf{x}) + \lambda_3 o_{\text{sparse}}(\mathbf{x}', \mathbf{x}) + \lambda_4 o_{\text{plausible}}(\mathbf{x}', \mathbf{X})$$

REMARKS: THE RASHOMON EFFECT



Issue (Rashomon effect):

- Solution to the optimization problem might not be unique
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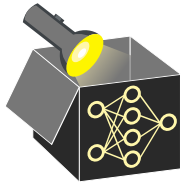

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- Present all CEs for $\mathbf{x}$ (but: time and human processing capacity is limited)
- Focus on one/few CEs (but: by which criterion should guide this choice?)

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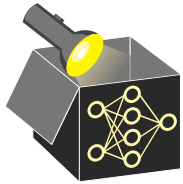

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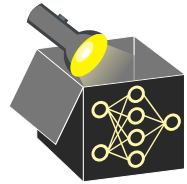
Note:

- Nonlinear models can produce diverse and inconsistent CEs
  $\rightsquigarrow$ suggest both increasing and decreasing credit duration
  (confusing for users)
- Handling this **Rashomon effect** remains an open problem in
  interpretable ML

REMARKS: MODEL OR REAL-WORLD



- CEs explain model predictions, but may seem to explain real-world users
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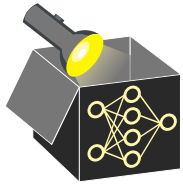

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- **Example:** CE suggests increasing age by 5 to receive a loan
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- **Problem:** Other features may change in the meantime (e.g., job status, income) $\rightsquigarrow$ ▸ "Karimi et al." 2020 propose CEs that respect causal structure
- **Model drift:** Bank's algorithm itself may change over time
  $\rightsquigarrow$ Past CEs may become invalid