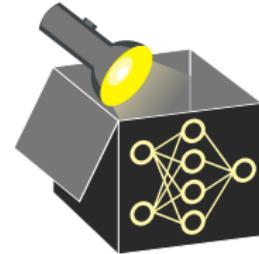
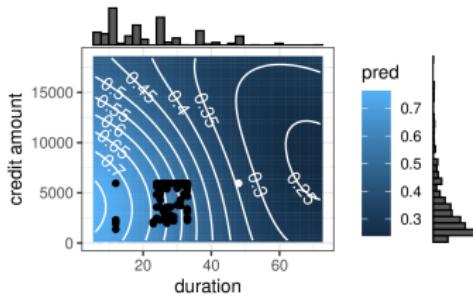


Interpretable Machine Learning



Counterfactual Explanations (CEs) Methods & Discussion



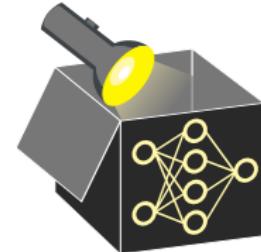
Learning goals

- See two strategies to generate CEs
- Know problems and limitations of CEs

OVERVIEW OF COUNTERFACTUAL METHODS

Many methods exist to generate counterfactuals, they mainly differ in:

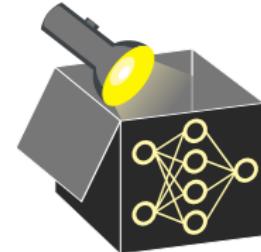
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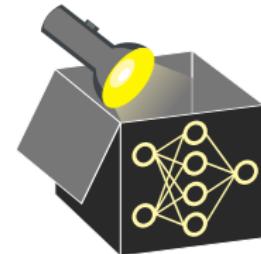
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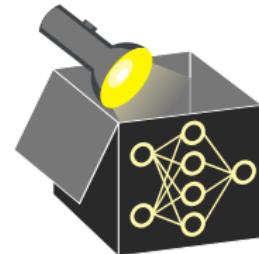
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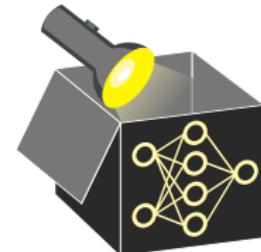
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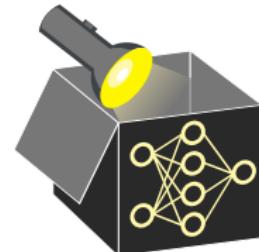
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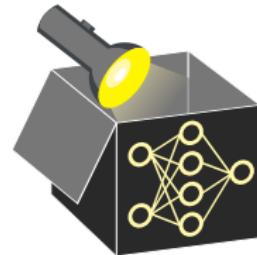
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- **Optimization:** From gradient-based (differentiable models) and mixed-integer programming (linear models) to gradient-free methods (e.g., genetic algorithms)
- **Rashomon Effect:** Many methods return one CE, some diverse sets of CEs, others prioritize CEs, or let the user choose

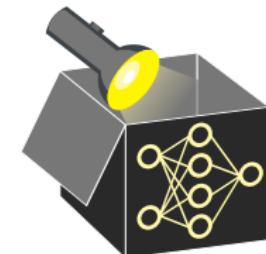


FIRST OPTIMIZATION-BASED CE METHOD

► "Wachter et. al" 2018

Introduced CEs in context of ML predictions by solving

$$\arg \min_{\mathbf{x}'} \max_{\lambda} \underbrace{\lambda (\hat{f}(\mathbf{x}') - y')^2}_{o_{target}(\hat{f}(\mathbf{x}'), y')} + \underbrace{\sum_{j=1}^p \frac{|x'_j - x_j|}{MAD_j}}_{o_{proximity}(\mathbf{x}', \mathbf{x})}$$



- o_{target} ensures prediction flips to y' (by increasing weight λ)
- $o_{proximity}$ penalizes deviations from \mathbf{x} , rescaled by median abs. deviation:

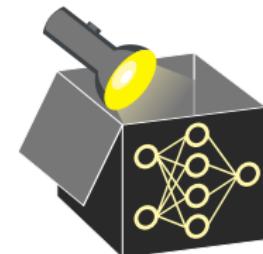
$$MAD_j = \text{med}_{i \in \{1, \dots, n\}} (|x_j^{(i)} - \text{med}_{k \in \{1, \dots, n\}} (x_j^{(k)})|)$$

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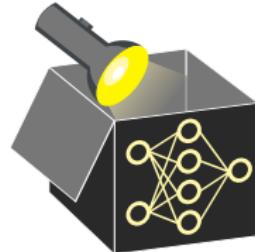
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Approach: Alternating optimization over \mathbf{x}' and λ

- Start with an initial λ (controls emphasis on o_{target} vs. $o_{proximity}$)
- Use a gradient-free optimizer (e.g., Nelder-Mead) to minimize over \mathbf{x}'
- If prediction constraint not satisfied ($\hat{f}(\mathbf{x}') \neq y'$), increase λ and repeat
~~~  $\lambda$  serves as soft constraint, gradually enforcing prediction validity  
 $\hat{f}(\mathbf{x}') = y'$
- Iteratively shift focus: 1. achieve prediction validity, 2. minimize proximity

# LIMITATIONS OF WACHTER'S APPROACH

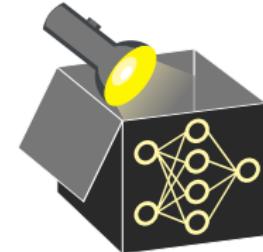
- **Manual tuning:** No principled way to set  $\lambda$ ; requires iterative increase
- **Asymmetric focus:** Early iterations dominated by minimizing target loss
- **Limited feature support:** Proximity term defined only for numerical feats
- **No additional objectives:** Ignores sparsity, plausibility, fairness, diversity
- **Single solution:** Returns one CE; no support for diverse or ranked CEs



- **Multi-Objective Counterfactual Explanations (MOC):** Instead of collapsing objectives into a single obj., optimize all 4 obj. simultaneously

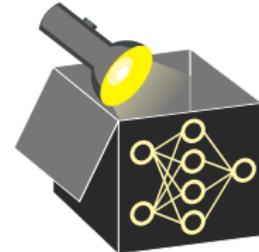
$$\arg \min_{\mathbf{x}'} \left( o_{target}(\hat{f}(\mathbf{x}'), y'), o_{proximity}(\mathbf{x}', \mathbf{x}), o_{sparse}(\mathbf{x}', \mathbf{x}), o_{plausible}(\mathbf{x}', \mathbf{X}) \right).$$

- Avoids using/tuning of weights (e.g.,  $\lambda$ ); returns Pareto-optimal set
- Uses an adjusted multi-objective genetic algo. (NSGA-II) for mixed feats
- Outputs diverse CEs representing different trade-offs between objectives



# EXAMPLE: CREDIT DATA

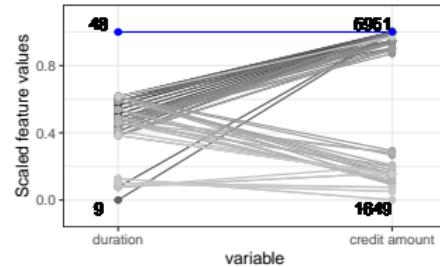
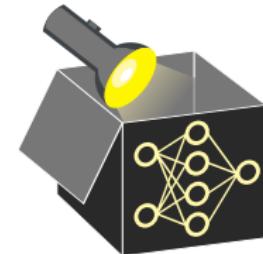
- Model: SVM with RBF kernel
- $\mathbf{x}$ : First data point of credit data with  $\mathbb{P}(y = \text{good}) = 0.34$
- Goal: Increase the probability to desired outcome [0.5, 1]
- MOC (with default parameters) returned 69 valid CEs after 200 iterations
- All CEs modified credit duration; many also adjusted credit amount



# EXAMPLE: CREDIT DATA

► "Dandl et al." 2020

- Feature changes can be visualized using parallel and 2D surface plots
- Parallel plot: All CEs had values equal to or smaller than the values of  $\mathbf{x}$



Parallel plot: Grey lines = CEs  $\mathbf{x}'$ , blue line =  $\mathbf{x}$ .

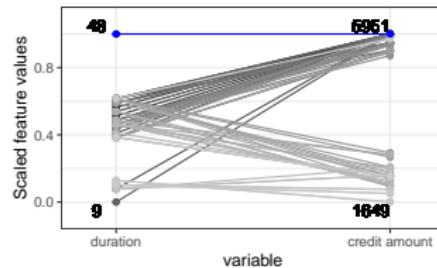
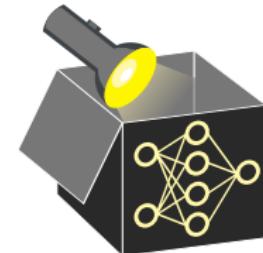
Features without changes omitted.

Bold numbers denote numeric ranges.

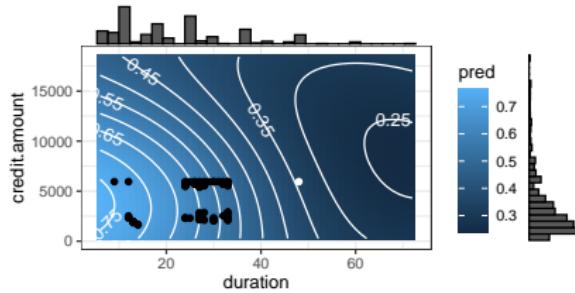
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- Feature changes can be visualized using parallel and 2D surface plots
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- Surface plot: CEs in lower-left appear distant, but lie in high-density regions near training data (as shown by histograms)



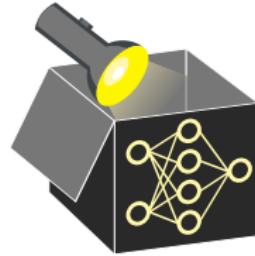
**Parallel plot:** Grey lines = CEs  $\mathbf{x}'$ , blue line =  $\mathbf{x}$ .  
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**Surface plot:** White dot =  $\mathbf{x}$ , black dots = CEs  $\mathbf{x}'$ .  
**Histograms:** Marginal distribution of training data  $\mathbf{X}$ .

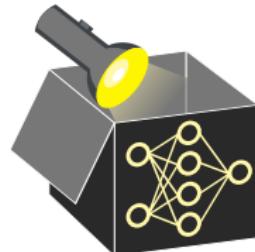
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  - ~~ Psychologists have shown that although perceived model understanding of end-users increases, the objective model understanding remains unchanged



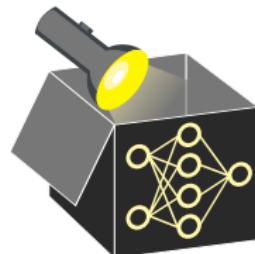
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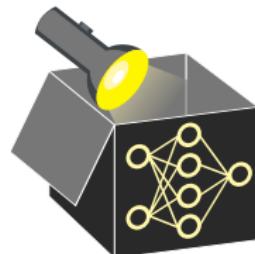
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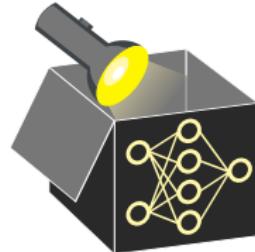
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- **Disclosing too much information:** CEs can reveal too much information about the model and help potential attackers



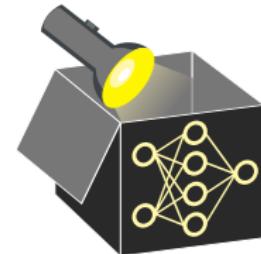
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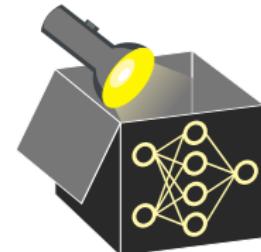
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- **Attacking CEs:** Researchers can create models with great performance, which generate arbitrary explanations specified by the ML developer
  - ~~ how faithful are CEs to the models underlying mechanism?

