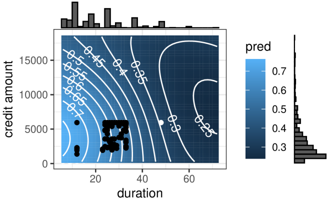
Interpretable Machine Learning

Methods & Discussion of CEs



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:

- **Target:** Most support classification; few extend to regression
  $\leadsto$ Recent work extends CEs to other ML tasks (un-, semi-, self-supervised)

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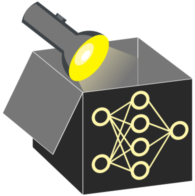

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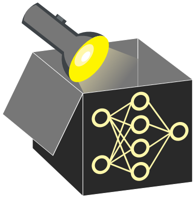

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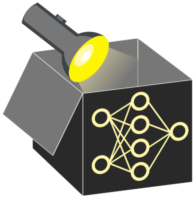

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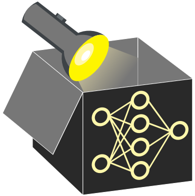

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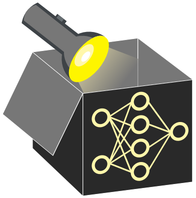

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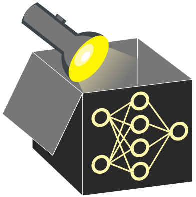

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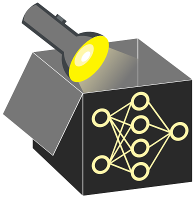
- **Rashomon Effect:** Many methods return one CE, some diverse sets of CEs, others prioritize CEs, or let the user choose

FIRST OPTIMIZATION-BASED CE METHOD

▸ Wachter et. al (2018)



Introduced CEs in context of ML predictions by solving

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

- o_{target} ensures prediction flips to y' (by increasing weight λ)
- $o_{proximity}$ penalizes deviations from $\mathbf{x}$, rescaled by median absolute deviation: $MAD_j = \text{med}_{i \in \{1,\ldots,n\}}(|x_j^{(i)} - \text{med}_{k \in \{1,\ldots,n\}}(x_j^{(k)})|)$

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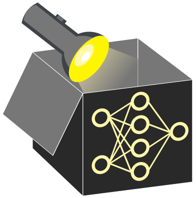

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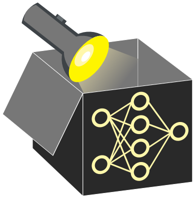
Approach: Alternating optimization over $\mathbf{x}'$ and λ

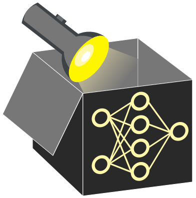
- Start with an initial λ (controls emphasis on o_{target} vs. $o_{proximity}$)
- Use a gradient-free optimizer (e.g., Nelder-Mead) to minimize over $\mathbf{x}'$
- If prediction constraint not satisfied ($\hat{f}(\mathbf{x}') \neq y'$), increase λ and repeat
  $\rightsquigarrow$ λ serves as soft constraint,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

LIMITATIONS OF WACHTER'S APPROACH



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

MULTI-OBJECTIVE CE ▸ Dandl et al. (2020)



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

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

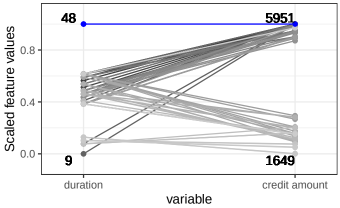
- Avoids using/tuning of weights (e.g., λ); returns Pareto-optimal set
- Uses an adjusted multi-objective genetic algorithm (NSGA-II) for mixed features
- Outputs diverse CEs representing different trade-offs between objectives

EXAMPLE: CREDIT DATA

- Model: SVM with RBF kernel
- **x**: First data point of credit data with $\mathbb{P}(y = \mathit{good}) = 0.34$
- 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 **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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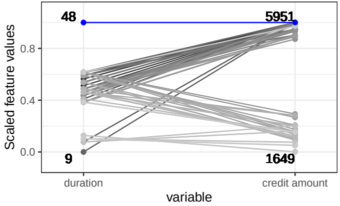
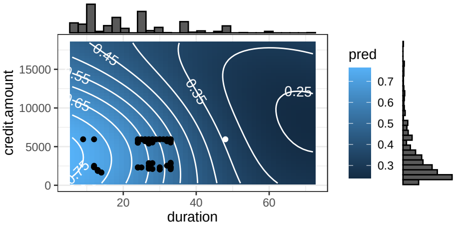
- Feature changes can be visualized using parallel and 2D surface plots
- Parallel plot: All CEs had values equal to or smaller than the values of $\mathbf{x}$
- Surface plot: CEs in lower-left appear distant, but lie in high-density regions near training data (as shown by histograms)





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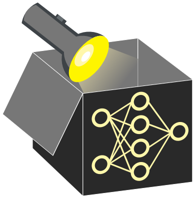
Surface plot: White dot = $\mathbf{x}$, black dots = CEs $\mathbf{x}'$.
Histograms: Marginal distribution of training data $\mathbf{X}$.

PROBLEMS, PITFALLS, & LIMITATIONS



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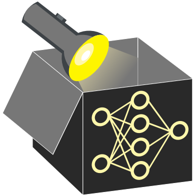

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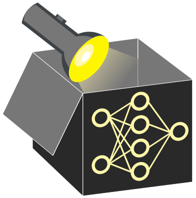

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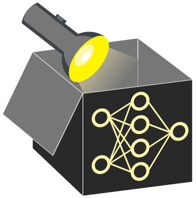

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- **Disclosing too much information:** CEs can reveal too much information about the model and help potential attackers

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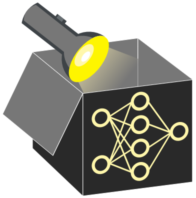

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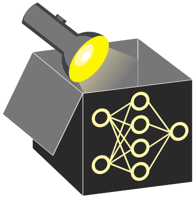

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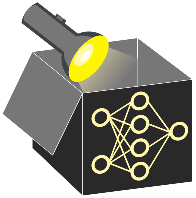

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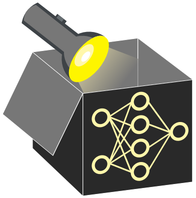

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- **Attacking CEs:** Researchers can create models with great performance, which generate arbitrary explanations specified by the ML developer
  $\rightsquigarrow$ how faithful are CEs to the models underlying mechanism?