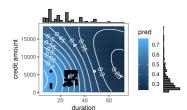
Interpretable Machine Learning

Counterfactual Explanations (CEs) Methods & Discussion





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



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

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



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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

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



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

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Approach: Alternating optimization over x' and λ

- Start with an initial λ (controls emphasis on o_{target} vs. $o_{proximitv}$)
- Use a gradient-free optimizer (e.g., Nelder-Mead) to minimize over x'
- If prediction constraint not satisfied $(\hat{f}(\mathbf{x}') \neq y')$, increase λ and repeat $\rightsquigarrow \lambda$ 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

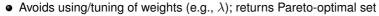
- Manual tuning: No principled way to set λ ; requires iterative increase
- Asymmetric focus: Early iterations dominated by minimizing target loss
- Limited feature support: Proximity term defined only for numerical feats
- No additional objectives: Ignores sparsity, plausibility, fairness, diversity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



MULTI-OBJECTIVE CE • "Dandl et al." 2020

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

$$\operatorname*{arg\,min}_{\boldsymbol{x}'}\left(o_{\textit{target}}(\hat{f}(\boldsymbol{x}'),y'),o_{\textit{proximity}}(\boldsymbol{x}',\boldsymbol{x}),o_{\textit{sparse}}(\boldsymbol{x}',\boldsymbol{x}),o_{\textit{plausible}}(\boldsymbol{x}',\boldsymbol{X})\right).$$



- 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

• **x**: First data point of credit data with $\mathbb{P}(y = good) = 0.34$

• Goal: Increase the probability to desired outcome [0.5, 1]

MOC (with default parameters) returned 69 valid CEs after 200 iterations

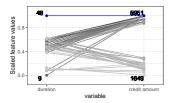
• All CEs modified credit duration; many also adjusted credit amount



EXAMPLE: CREDIT DATA • "Dandl et al." 2020

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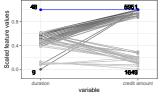




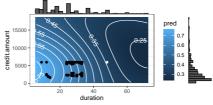
Parallel plot: Grey lines = CEs x', blue line = x.
Features without changes omitted.
Bold numbers denote numeric ranges.

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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 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 = x, black dots = CEs x'. Histograms: Marginal distribution of training data X.



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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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- 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?

