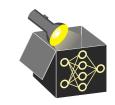
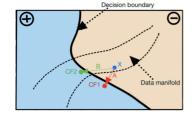
Interpretable Machine Learning

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
- ullet $y'\subset\mathbb{R}^g$: desired predi. (y'= "grant credit") or interval ($y'=[1000,\infty[)$



MATHEMATICAL PERSPECTIVE

Terminology:

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



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

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

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 ($y' = [1000, \infty[)$



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

• Prediction validity: CE's prediction $\hat{f}(\mathbf{x}')$ is equal to the desired pred. \mathbf{y}'

Proximity: CE x' is as close as possible to the original input x

Reformulate these two objectives as optimization problem:

$$\operatorname*{arg\,min}_{\mathbf{x'}} \lambda_{1} \textit{o}_{\textit{target}}(\hat{\textit{f}}(\mathbf{x'}), \textit{y'}) + \lambda_{2} \textit{o}_{\textit{proximity}}(\mathbf{x'}, \mathbf{x})$$

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

OBJECTIVE FUNCTIONS • "Dandl et al." 2020

Distance in target space o_{target} :

- Regression: L₁ distance $o_{target}(\hat{f}(\mathbf{x}'), y') = |\hat{f}(\mathbf{x}') y'|$
- Classification:
 - For predicted probabilities: $o_{target} = |\hat{f}(\mathbf{x}') y'|$
 - For predicted hard labels: $o_{target} = \mathbb{I}\{\hat{f}(\mathbf{x}') \neq y'\}$



OBJECTIVE FUNCTIONS • "Dandl et al." 2020

Distance in target space o_{target}:

- Regression: L₁ distance $o_{target}(\hat{f}(\mathbf{x}'), y') = |\hat{f}(\mathbf{x}') y'|$
- Classification:
 - For predicted probabilities: $o_{target} = |\hat{f}(\mathbf{x}') y'|$
 - For predicted hard labels: $o_{target} = \mathbb{I}\{\hat{f}(\mathbf{x}') \neq y'\}$

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

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

- $\delta_G(x_i', x_i) = \mathbb{I}\{x_i' \neq x_i\}$ if x_i is categorical
- $\delta_G(x'_j, x_j) = \frac{1}{\widehat{R}_i} |x'_j x_j|$ if x_j is numerical
 - $\rightsquigarrow \widehat{R}_i$: range of feature j in the training set to ensure $\delta_G(x_i', x_j) \in [0, 1]$



FURTHER OBJECTIVES: SPARSITY

Additional constraints can improve the explanation quality of the corresponding CEs

 \leadsto popular constraints include sparsity and plausibility

Sparsity Favor explanations that change few features

End-users often prefer short over long explanations



FURTHER OBJECTIVES: SPARSITY

Additional constraints can improve the explanation quality of the corresponding CEs

 \leadsto popular constraints include sparsity and plausibility

Sparsity Favor explanations that change few features

- End-users often prefer short over long explanations
- Sparsity could be integrated into o_{proximity}
 e.g., using L₀-norm (number of changed features) or L₁-norm (LASSO)



FURTHER OBJECTIVES: SPARSITY

Additional constraints can improve the explanation quality of the corresponding CEs

→ popular constraints include sparsity and plausibility



- End-users often prefer short over long explanations
- Sparsity could be integrated into o_{proximity}
 e.g., using L₀-norm (number of changed features) or L₁-norm (LASSO)
- Alternative: Include separate objective measuring sparsity, e.g., via L₀-norm

$$o_{sparse}(\mathbf{x}',\mathbf{x}) = \sum_{i=1}^{
ho} \mathcal{I}_{\{x_i'
eq x_j\}}$$



Plausibility:

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



Plausibility:

- CEs should suggest realistic (i.e., plausible) alternatives
 Implausible: increase income and become unemployed
- \bullet CEs should adhere to data manifold or originate from distribution of ${\mathcal X}$
 - Avoid unrealistic combinations of feature values



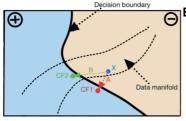
Plausibility:

- ◆ CEs should suggest realistic (i.e., plausible) alternatives
 → Implausible: increase income and become unemployed
- CEs should adhere to data manifold or originate from distribution of X
 → Avoid unrealistic combinations of feature values
- Estimating joint distribution is hard, especially for mixed feature spaces
 → Common proxy: ensure that x' is close to training data X



Plausibility:

- ◆ CEs should suggest realistic (i.e., plausible) alternatives
 → Implausible: increase income and become unemployed
- CEs should adhere to data manifold or originate from distribution of X
 → Avoid unrealistic combinations of feature values
- ullet Estimating joint distribution is hard, especially for mixed feature spaces \leadsto Common proxy: ensure that ${f x}'$ is close to training data ${f X}$



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



FURTHER OBJECTIVES

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}
- \bullet Use Gower distance between \boldsymbol{x}' and $\boldsymbol{x}^{[1]}$ to define plausibility objective:

$$o_{ extit{plausible}}(\mathbf{x}',\mathbf{X}) = d_G(\mathbf{x}',\mathbf{x}^{[1]}) = rac{1}{
ho} \sum_{j=1}^{
ho} \delta_G(x_j',x_j^{[1]})$$



FURTHER OBJECTIVES

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}
- ullet Use Gower distance between ${f x}'$ and ${f x}^{[1]}$ to define plausibility objective:

$$o_{ extit{plausible}}(\mathbf{x}',\mathbf{X}) = d_G(\mathbf{x}',\mathbf{x}^{[1]}) = rac{1}{
ho} \sum_{j=1}^{
ho} \delta_G(x_j',x_j^{[1]})$$

Extended optimization: Add sparsity and plausibility terms to the objective

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



REMARKS: THE RASHOMON EFFECT

Issue (Rashomon effect):

- Solution to the optimization problem might not be unique
- Many equally close CE might exist that obtain the desired prediction
 - \Rightarrow Many different equally good explanations for the same decision exist



REMARKS: THE RASHOMON EFFECT

Issue (Rashomon effect):

- Solution to the optimization problem might not be unique
- Many equally close CE might exist that obtain the desired prediction
 - \Rightarrow Many different equally good explanations for the same decision exist



Possible solutions:

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

REMARKS: THE RASHOMON EFFECT

Issue (Rashomon effect):

- Solution to the optimization problem might not be unique
- Many equally close CE might exist that obtain the desired prediction
 - \Rightarrow Many different equally good explanations for the same decision exist

0

Possible solutions:

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

Note:

- Nonlinear models can produce diverse and inconsistent CEs
 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
 Transfer of model explanations to explain real-world is generally not permitted



REMARKS: MODEL OR REAL-WORLD

- CEs explain model predictions, but may seem to explain real-world users
 Transfer of model explanations to explain real-world is generally not permitted

- Model drift: Bank's algorithm itself may change over time
 Past CEs may become invalid

