# Counterfactual Explanations for Machine Learning

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Gabriele Tolomei

Department of Computer Science Sapienza University of Rome <u>tolomei@di.uniroma1.it</u>







UniPl (1999-2005)





UniPl (1999-2005)





UniVE (2008-2013)



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UniPD (2017-2019)

UniVE (2008-2013)



Sapienza (2019-)







#### Human-Explainable











#### Sounds cool?



#### Check out the lab's <u>home page</u> (still under construction, sic!)



## My Research Group: People

#### PhD Students



Cesare Campagnano Sapienza University of Rome PhD Student in Computer Science

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Edoardo Gabrielli Sapienza University of Rome PhD Student in

Cybersecurity

#### Collaborators



Flavio Giorgi

Sapienza University of Rome

PhD Student in Computer

Science

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PhD Student in Data

Giovanni Trappolini Sapienza University of Rome Postdoctoral Researcher Y 🖪 S 🙆 🗘





Sapienza University of Rome PhD Student in Data Science

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Ziheng Chen Walmart Labs, Sunnyvale, CA, USA **Research Scientist** 

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#### **HERCOLE** Lab



Fabio Pinelli IMT School for Advanced Studies Lucca Assistant Professor of Computer Science

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Fabrizio Silvestri Sapienza University of Rome Full Professor of

Computer Science **3 🚯 y 🛅 8 (0 ()** 

Federico Siciliano Sapienza University of Rome

Neural Networks MLP CNN LSTM Transformers GAN GNN Ensemble Random Forest XGBoost Performance SVM Decision K-NN Trees Graphical Models HMM CRF Linear Models Linkeg Logkeg

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Performance improvements often come at a cost of **compromised explainability** 



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This is partly due to the **increasing model complexity** (e.g., number of parameters, deep network architectures)



Simpler models may be **less accurate** but **more explainable** 

e.g., linear/logistic regression coefficients are interpretable by design

#### Explainability



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**Simple Decision Boundary Surface** 

#### Explainability



Complex models are **more expressive** but **opaque** 

e.g., multi-billion parameter NNs

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**Convoluted Decision Boundary Surface** 

#### Explainability



https://medium.com/@BonsaiAl/what-do-we-want-from-explainable-ai-5ed12cb36c07

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- In many domains, highly accurate predictions are not enough!
  - Healthcare: A physician must be able to tell their patient the rationale behind an AI/ML-based diagnosis
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- AI/ML-based predictions should be comprehensible to every stakeholder (including non-experts)

- Several attempts have been made to promote XAI as part of broader data privacy regulation initiatives
  - EU GDPR (General Data Protection Regulation)
  - HIPAA (Health Insurance Portability and Accountability Act) Privacy Rule
  - CCPA (California Consumer Privacy Act)
  - PCI DSS (Payment Card Industry Data Security Standard)
  - NIST AI Risk Management Framework

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#### **Taxonomy of XAI Methods**



### **Counterfactual Explanations: Intuition**

 Post-hoc local explanation method to interpret predictions of individual instances

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- Post-hoc local explanation method to interpret predictions of individual instances
- Search for modified versions of input samples that result in alternative output responses from the predictive model
- Explanations take the following form:

#### "If A had been different, B would not have occurred"



Will I have diabetes?





Will I have diabetes?









Will I have diabetes?

Yes/No + Explanation





FactualAge45

Age	Gender	Exercise Level	Fat Level
45	М	Low	High



Will I have diabetes?

Yes/No + Explanation





FactualAgeGenderExercise<br/>LevelFat Level45MLowHigh
### **Counterfactual Explanations: Example**



Will I have diabetes?

Yes/No + Explanation





Factual	Age	Gender	Exercise Level	Fat Level	f (. 🔗 ) — Vee
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Counterfactual	Age	Gender	Exercise Level	Fat Level
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Yes/No + Explanation





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Counterfactual	Age	Gender	Exercise Level	Fat Level	$f(\mathbf{s}) = \mathbf{No}$
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Yes/No + Explanation





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	45	М	Low	High	

Counterfactual<br/>LevelAgeGenderExercise<br/>LevelFat Level $f(\begin{bmatrix} f(\begin{bmatrix} f(\begin{bmatri$ 

#### **Explanation:**

You will not develop diabetes if you increase your exercise level and lower your fat level

### Finding Counterfactual Examples (CFs)



Given an input sample **x**, there may be (infinitely?) many counterfactual examples

We need to restrict our search to "some" of them!

### Finding the "Optimal" CF (for a given x)

$$\widetilde{\boldsymbol{x}}^* = \operatorname{argmin}_{\widetilde{\boldsymbol{x}}} \{ \ell_{\operatorname{CF}}(\boldsymbol{x}, \widetilde{\boldsymbol{x}}; f) + \lambda \ell_{\operatorname{dist}}(\boldsymbol{x}, \widetilde{\boldsymbol{x}}) \}$$

counterfactual loss penalizes if the CF goal is **not** met

CF goal: 
$$f(\widetilde{oldsymbol{x}}) 
eq f(oldsymbol{x})$$

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#### distance loss

discourages the CF to be too far away from the original input **x** 

e.g., L1-norm 
$$|\widetilde{x}-x|$$

#### Finding the "Optimal" CF (for a given **x**)

 $\widetilde{\boldsymbol{x}}^* = \operatorname{argmin}_{\widetilde{\boldsymbol{x}}} \{ \ell_{\operatorname{CF}}(\boldsymbol{x}, \widetilde{\boldsymbol{x}}; f) + \lambda \ell_{\operatorname{dist}}(\boldsymbol{x}, \widetilde{\boldsymbol{x}}) \}$ 

s.t.:  $1 \le p_{\max} \le m$ , where  $1 \le m \le |\mathcal{F}| \le n$ Limit on the number of Set of "actionable" "actionable" features to change features

#### **Evaluation Metrics for CFs**

Validity (1-Fidelity) Measures the ratio of generated CFs that actually meet the counterfactual goal (the higher the better)

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Computes the distance between a (valid) CF and the original input sample (the lower the better)

L1-norm or L2-norm

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Computes the distance between a (valid) CF and the original input sample (the lower the better)

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**Sparsity** 

Indicates the number of features modified to obtain the CF (the lower the better)

L0-norm

Sahil, V., Dickerson, J. and Hines, K., 2022. Counterfactual Explanations for Machine Learning: A Review. arXiv:2010.10596.

#### **Our Contributions to CF Explanations**



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### ReLAX: Reinforcement Learning Agent Explainer for Arbitrary Predictive Models

Chen, Z., Silvestri, F., Wang, J., Zhu, H., Ahn, H. and Tolomei, G., 2022, October. ReLAX: Reinforcement Learning Agent Explainer for Arbitrary Predictive Models. In Proceedings of the 31st ACM International Conference on Information & Knowledge Management (pp. 252-261).

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#### How Do We Find $g_{\theta^*}$ ?

$$\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} \left\{ \mathcal{L}(g_{\boldsymbol{\theta}}; \mathcal{D}, h_{\boldsymbol{\omega}}) \right\}$$
  
s.t.:  $p_{\max} \leq m$ 

$$\mathcal{L}(g_{\theta}; \mathcal{D}, h_{\omega}) = \frac{1}{|\mathcal{D}|} \sum_{\boldsymbol{x} \in \mathcal{D}} \ell_{\mathrm{CF}}(\boldsymbol{x}, g_{\theta}(\boldsymbol{x}); h_{\omega}) + \lambda \ell_{\mathrm{dist}}(\boldsymbol{x}, g_{\theta}(\boldsymbol{x}))$$

#### from *instance*-level (local) to *dataset*-level (global) explanations

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#### from optimizing to learning



 $\boldsymbol{x}$ 







# **1)** The RL Agent picks a feature to modify



**2)** The RL Agent chooses the magnitude of the feature change





**1)** The RL Agent picks a feature to modify



**2)** The RL Agent chooses the magnitude of the feature change





The RL Agent terminates when the CF goal is met!

We formulate the problem of finding the optimal CF generator  $g_{\theta^*}$  as an MDP

$$\mathcal{M} = \{\mathcal{S}, \mathcal{A}, \mathcal{T}, p_0, r, \gamma\}$$

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We find the **optimal policy** to apply the best sequence of actions to each input

### **Our Proposed Framework**



#### 2024 MT4H International Workshop – Valencia, Spain

#### **Experiments: Datasets and Tasks**

Dataset	N. of Instances	N. of Features	Task
Breast Cancer [5]	699	10 (numerical)	classification
Diabetes [2]	768	8 (numerical)	classification
Sonar [3]	208	60 (numerical)	classification
Wave [4]	5,000	21 (numerical)	classification
Boston Housing [1]	506	14 (mixed)	regression

### Experiments: (Black-Box) Models

Dataset [Best Model]	Structure	Acc. (▲)/RMSE (♦)
Breast Cancer [RF]	{#trees=100}	0.99 (▲)
Diabetes [AdaBoost]	{#trees=100}	0.79 (▲)
Wave [XGBoost]	{#trees=100}	0.95 (▲)
Breast Cancer [MLP]	{#L1=64, #L2=128}	1.00 (▲)
Sonar [MLP]	{#L1=256, #L2=256}	0.90 (▲)
Wave [MLP]	{#L1=100, #L2=200}	0.97 (▲)
Boston Housing [MLP-ReG]	{#L1=50, #L2=128}	3.36 (♦)
#### Experiments: Sparsity vs. Validity





ReLAX achieves the **best trade-off** between sparsity and validity of the generated CFs

Sparsity

	Validity (Sparsity)			
Threshold ( $\delta$ )	ReLAX-Global	<b>RELAX-LOCAL</b>		
0.20	$0.81 \pm 0.09 \ (3.02 \pm 0.17)$	$0.87 \pm 0.05 \ (3.10 \pm 0.18)$		
0.40	$0.74 \pm 0.06 \ (3.09 \pm 0.16)$	$0.81 \pm 0.05 \ (3.18 \pm 0.16)$		
0.60	$0.70 \pm 0.06$ (3.21 $\pm$ 0.12)	$0.77 \pm 0.03 (3.28 \pm 0.09)$		

Dataset-level Explainer

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Instance-level Explainer

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Threshold ( $\delta$ )	ReLAX-Global	<b>RELAX-LOCAL</b>		
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In the case of regression task, the CF goal must be adapted with a validity threshold ( $\delta$ ):  $|h_{\omega}(\tilde{x}) - h_{\omega}(x)| \ge \delta, \ \delta \in \mathbb{R}_{>0}$ 

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The higher the threshold the harder is for ReLAX to find a valid CF

# Experiments: Proximity vs. Generation Time

Metric	Dataset [Models]	CF Generation Methods			
		RELAX-GLOBAL	RELAX-LOCAL	LORE	MACE
Proximity	Breast Cancer [RF, MLP]	[4.46, 5.92]	[4.49, 5.87]	[4.63, 5.63]	[4.47, N/A]
	Diabetes [ADABOOST]	[4.41]	[4.50]	[4.76]	[N/A]
	Sonar [MLP]	[7.32]	[7.66]	[7.36]	[N/A]
	Wave [XGBoost, MLP]	[5.93, 6.38]	[6.02, 6.50]	[6.60, 6.41]	[N/A, N/A]
	Boston Housing [MLP-Reg]	[5.10]	[5.36]	[N/A]	[N/A]
Generation Time (secs.)	*	1500	1320	2100	2280

**ReLAX-Global** generates CFs that are closer to the original input instance but **ReLAX-Local** takes less time on average

### Experiments: The Hyperparameter $\lambda$

 $\lambda$  controls the balance between sparsity and validity

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Larger values of λ force the agent to prefer sparser CFs at the expense of lower validity

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The complex network structure of a DRL policy learned for CF generation poses a challenge for understanding the decision logic of the agent

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The complex network structure of a DRL policy learned for CF generation poses a challenge for understanding the decision logic of the agent

To explain the decision process of a learned policy, we **distill** knowledge from the policy to a naturally-interpretable **decision tree** 



We apply ReLAX to generate CF explanations for a binary classifier (XGBoost with 500 trees) trained to predict the risk of mortality for COVID-19

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- Decrease death rate
- Decrease unemployment rate
- Increase nurse rate per 10,000 people
- Decrease urban population rate
- Decreasing obesity prevalence

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As obvious as they sound, many countries have suggested or enacted similar strategies to counter the COVID-19 pandemic (see <u>here</u> and <u>here</u>)

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- If we don't want to trade accuracy for explainability, we need to develop post-hoc explainers for complex, black-box models
- Counterfactual examples (CFs) are promising tools to generate actionable explanations
- We present a state-of-the-art CF generation method based on reinforcement learning and its application to a real use case

- Counterfactual explanation is a very trendy research topic! A few possible open challenges are:
  - Developing new CF generation methods (e.g., based on/inspired by diffusion models)

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  - Generating CFs for new prediction settings (e.g., sequential recommender systems, anomaly detection tools)
  - Incorporating personalization into CFs (not every actionable feature has the same weight across different input samples)
  - Extracting natural language explanations from generated CFs

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## Let's Collaborate!