

Pitfalls of Confound Regression in Machine Learning

Holger Schwender⁴, Simon B. Eickhoff^{1,2} & Kaustubh R. Patil^{1,2}

Sami Hamdan^{1,2}, Bradley C. Love³, Georg G. von Polier², Susanne Weis^{1,2},

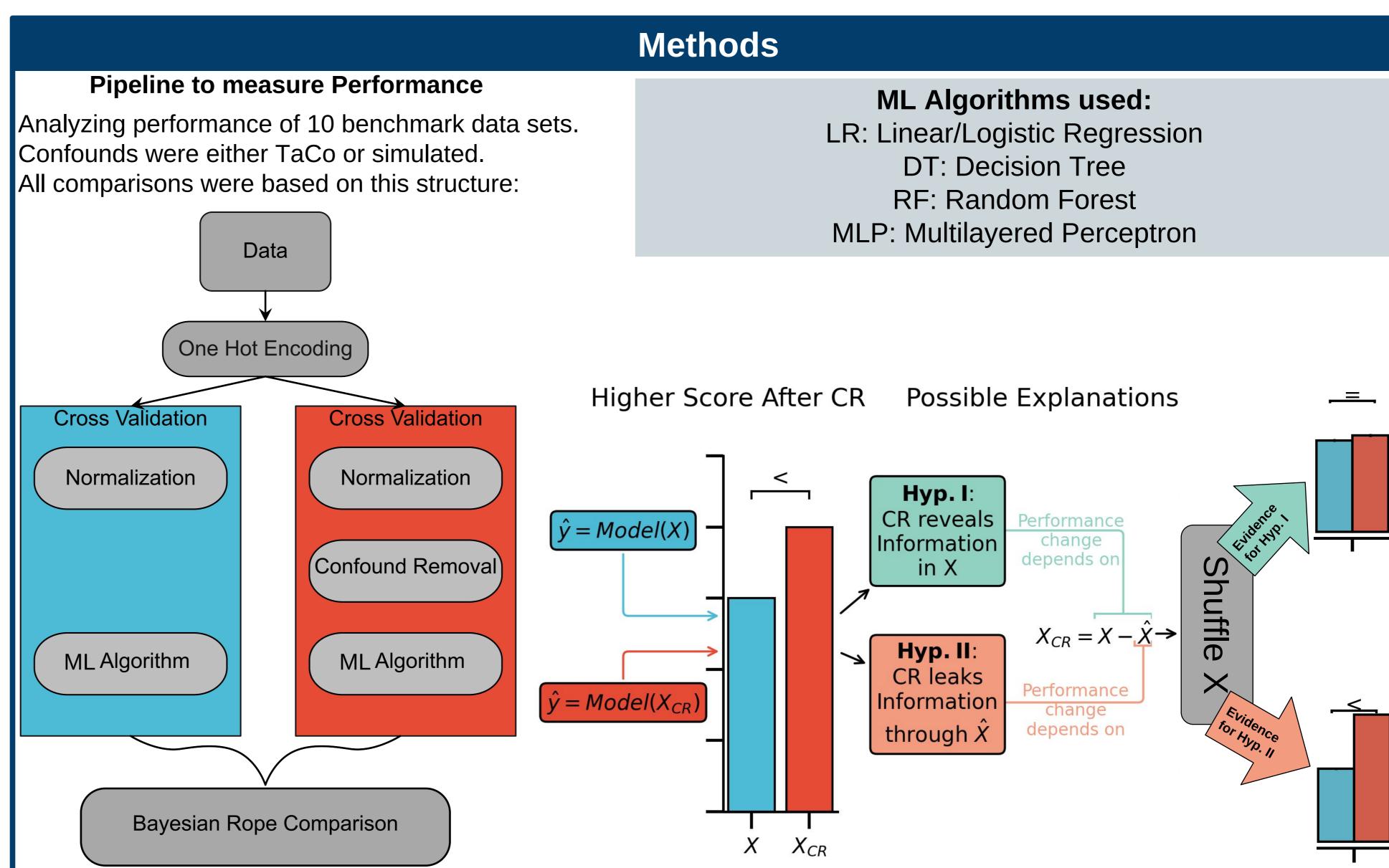
JÜLICH Forschungszentrum

Poster Number: 236

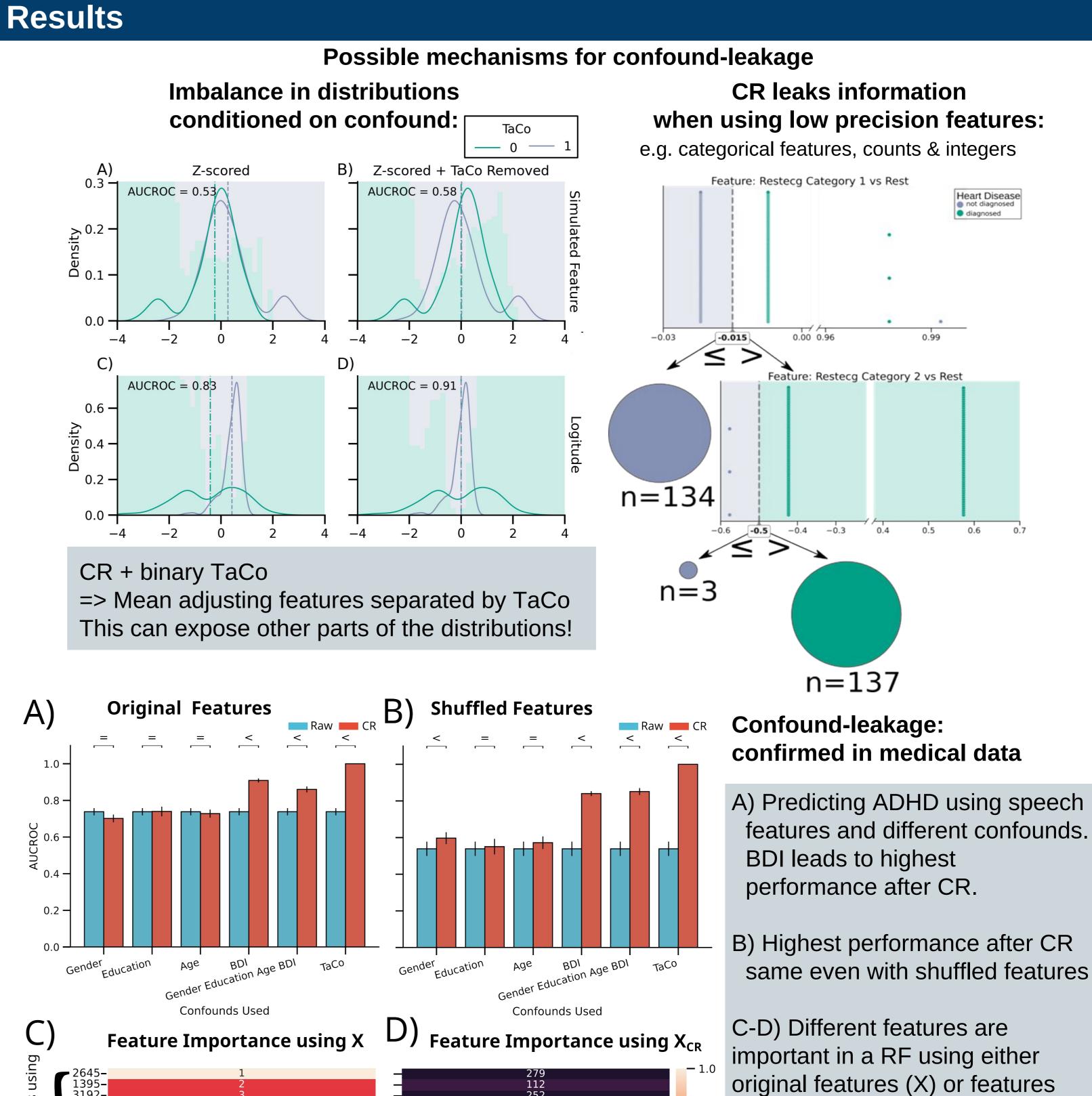
¹Institute of Systems Neuroscience, Heinrich Heine University Düsseldorf, Düsseldorf, Germany ²Institute of Neuroscience and Medicine (INM-7: Brain and Behaviour), Research Centre Jülich, Jülich, Germany, ³University College London, Department of Experimental Psychology, London, UK

⁴Heinrich-Heine University Düsseldorf, Institute of Mathematics, Germany

Introduction **Pipeline to measure Performance** Not dealing with confounding can threaten the interpretability & Analyzing performance of 10 benchmark data sets. meaningfulness of machine learning (ML) models. Confounds were either TaCo or simulated. This can lead to: untrustworthy predictions & questionable insights.¹ All comparisons were based on this structure: Therefore, researchers often remove them using Confound Regression (CR).² Data **Typical Confound:** Linear Predictability Linear Predictability One Hot Encoding Residualized Features X Target y Target y Features X_n **Cross Validation** Cross Validation Confounds C Normalization Normalization Confounds C **Target as a Confound (TaCo):** Confound Removal TaCo shares all variance any confound could share with features & the target. Therefore, the TaCo represents the most extreme case of confounding, which helps revealing pitfalls of CR. ML Algorithm ML Algorithm No Linear Predictability Linear Predictability Target as Target as Confound Features > Confound Features X TaCo TaCo Bayesian Rope Comparison



Performance after CR increases before applying non-linear ML Features: TaCo CR TaCo CR Shuffled CR Simulated Confounds ² 0.5 − 1.0 -~ 0.5 − AUR 0.5 MLP MLP DT DT **Confound Target** Model Model Correlation CR can increase performance Performance increase Shuffling possible with weaker when using TaCo? => Non-informative features Is this leakage of information? Still performance increase confounds (non TaCo) Here: Only leakage possible Or revealing real information? Confound removal using CR can leak information into your features! => confound-leakage Confound-leakage: CR increases information usable by (here non-linear) ML models inside of the features. => Danger for interpretability & meaningfulness of all CR-ML workflows



Discussion

Recommendations CR-ML Workflows Summary

We show confound-leakage in

- Benchmark data Simulations
- Medical data

We found possible mechanisms

- imbalance in distributions conditioned on confound
- low precision features

- 1) Check performance without CR
- If CR-ML higher proceed. 2) Assess confounding strength

Stronger confounds to target relationship pose greater danger of confound-leakage.

- 3) Gain evidence for/against confound-leakage
 - TaCo + shuffling of features
- 4) Carefully choose alternatives other procedures may also entail unknown pitfalls.

Feature Importance Rank

Limitations

after CR (X_{CR})

Summary CR changes:

=> performance 1

=> feature importance

No full-proof method for detection & elimination of confound leakage.

Several complex combinations of:

- Features
- Target
- Confounds

Feature Importance Rank

could lead to confound-leakage

References:

1) Mehrabi, N., Morstatter, F., Saxena, N., Lerman, K. & Galstyan, A. A survey on bias and fairness in machine learning. ACM Comput. Surv. 54, 1-35 (2021). 2) Snoek, L., Miletić, S. & Scholte, H. S. How to control for confounds in decoding analyses of neuroimaging data. Neuroimage 184, 741–760 (2019).