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# COUNTERFACTUAL TRAINING: TEACHING MODELS PLAUSIBLE AND ACTIONABLE EXPLANATIONS

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## ABSTRACT

Counterfactual Explanations have emerged as a popular tool to explain predictions made by opaque machine learning models: they explain how factual inputs need to change in order for some fitted model to produce some desired output. Much existing research has focused on identifying explanations that are not only valid but also deemed plausible and desirable with respect to the underlying data and stakeholder requirements. Recent work has shown that under this premise, the task of learning plausible explanations is effectively reassigned from the model itself to the (post-hoc) counterfactual explainer. Building on that work, we propose a novel model objective that leverages counterfactuals during the training phase (ad-hoc) in order to minimize the divergence between learned representations and plausible explanations. Through extensive experiments, we demonstrate that our proposed methodology facilitates training models that inherently deliver plausible explanations while maintaining high predictive performance.

**Keywords** Counterfactual Explanations • Explainable AI • Representation Learning

## 1 Introduction

Today's prominence of artificial intelligence (AI) has largely been driven by advances in **representation learning**: instead of relying on features and rules that are carefully hand-crafted by humans, modern machine learning (ML) models are tasked with learning these representations from scratch, guided by narrow objectives such as predictive accuracy (I. Goodfellow, Bengio, and Courville 2016). Modern advances in computing have made it possible to provide such models with ever greater degrees of freedom to achieve that task, which has often led them to outperform traditionally more parsimonious models. Unfortunately, in doing so they also learn increasingly complex and highly sensitive representations that we can no longer easily interpret.

This trend towards complexity for the sake of performance has come under serious scrutiny in recent years. At the very cusp of the deep learning revolution, Szegedy et al. (2013) showed that artificial neural networks (ANN) are sensitive

23 to adversarial examples: counterfactuals of model inputs that yield vastly different model predictions despite being  
 24 “imperceptible” in that they are semantically indifferent from their factual counterparts. Despite partially effective  
 25 mitigation strategies such as **adversarial training** (I. J. Goodfellow, Shlens, and Szegedy 2014), truly robust deep  
 26 learning (DL) remains unattainable even for models that are considered shallow by today’s standards (Kolter 2023).

27 Part of the problem is that high degrees of freedom provide room for many solutions that are locally optimal with  
 28 respect to narrow objectives (Wilson 2020)<sup>1</sup>. Based purely on predictive performance, these solutions may seem to  
 29 provide compelling explanations for the data, when in fact they are based on purely associative, semantically mean-  
 30 ingless patterns. This poses two related challenges: firstly, it makes these models inherently opaque, since humans  
 31 cannot simply interpret what type of explanation the complex learned representations correspond to; secondly, even  
 32 if we could resolve the first challenge, it is not obvious how to mitigate models from learning representations that  
 33 correspond to meaningless and implausible explanations.

34 The first challenge has attracted an abundance of research on **explainable AI** (XAI) which aims to develop tools to  
 35 derive explanations from complex model representations. This can mitigate a scenario in which we deploy opaque  
 36 models and blindly rely on their predictions. On countless occasions, this scenario has already occurred in practice  
 37 and caused real harm to people who were affected adversely and often unfairly by automated decision-making systems  
 38 (ADMS) involving opaque models (O’Neil 2016). Effective XAI tools can aide us in monitoring models and providing  
 39 recourse to individuals to turn adverse outcomes (e.g. “loan application rejected”) into positive ones (“application  
 40 accepted”). Wachter, Mittelstadt, and Russell (2017) propose **counterfactual explanations** as an effective approach  
 41 to achieve this: they explain how factual inputs need to change in order for some fitted model to produce some desired  
 42 output, typically involving minimal perturbations.

43 To our surprise, the second challenge has not yet attracted any consolidated research effort. Specifically, there has  
 44 been no concerted effort towards improving model **explainability**, which we define here as the degree to which learned  
 45 representations correspond to explanations that are interpretable and deemed **plausible** by humans (see Definition 3.1).  
 46 Instead, the choice has typically been to improve the capacity of XAI tools to identify the subset explanations that are  
 47 both plausible and valid for any given model, independent of whether the learned representations are also compatible  
 48 with implausible explanations (Altmeyer et al. 2024). Fortunately, recent findings indicate that explainability can arise  
 49 as byproduct of regularization techniques aimed at other objectives such as robustness, generalization and generative  
 50 capacity Altmeyer et al. (2024).

51 Building on these findings, we introduce **counterfactual training**: a novel regularization technique geared explicitly  
 52 towards aligning model representations with plausible explanations. Our contributions are as follows:

- 53 • We discuss existing related work on improving models and consolidate it through the lens of counterfactual  
 54 explanations (Section 2).
- 55 • We present our proposed methodological framework that leverages faithful counterfactual explanations during  
 56 the training phase of models to achieve the explainability objective (Section 3).
- 57 • Through extensive experiments we demonstrate the counterfactual training improve model explainability  
 58 while maintaining high predictive performance. We run ablation studies and grid searches to understand  
 59 how the underlying model components and hyperparameters affect outcomes. (Section 4).

60 Despite limitations of our approach discussed in Section 5, we conclude that counterfactual training provides a practi-  
 61 cal framework for researchers and practitioners interested in making opaque models more trustworthy Section 6. We  
 62 also believe that this work serves as an opportunity for XAI researchers to reevaluate the premise of improving XAI  
 63 tools without improving models.

## 64 2 Related Literature

65 To the best of our knowledge, our proposed framework for counterfactual training represents the first attempt to use  
 66 counterfactual explanations during training to improve model explainability. In high-level terms, we define model  
 67 explainability as the extent to which valid explanations derived for an opaque model are also deemed plausible with  
 68 respect to the underlying data and stakeholder requirements. To make this more concrete, we follow Augustin, Meinke,  
 69 and Hein (2020) in tieing the concept of explainability to the quality of counterfactual explanations that we can  
 70 generate for a given model. The authors show that counterfactual explanations—understood here as minimal input  
 71 perturbations that yield some desired model prediction—are generally more meaningful if the underlying model is  
 72 more robust to adversarial examples. We can make intuitive sense of this finding when looking at adversarial training  
 73 (AT) through the lens of representation learning with high degrees of freedom: by inducing models to “unlearn”

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<sup>1</sup>For clarity: we follow standard ML convention in using “degrees of freedom” to refer to the number of parameters estimated from data.

74 representations that are susceptible to worst-case counterfactuals (i.e. adversarial examples), AT effectively removes  
 75 some implausible explanations from the solution space.

## 76 2.1 Adversarial Examples are Counterfactual Explanations

77 This interpretation of the link between explainability through counterfactuals on one side, and robustness to adversarial  
 78 examples on the other, is backed by empirical evidence. Sauer and Geiger (2021) demonstrate that using counterfactual  
 79 images during classifier training improves model robustness. Similarly, Abbasnejad et al. (2020) argue that counterfactuals  
 80 represent potentially useful training data in machine learning, especially in supervised settings where inputs may  
 81 be reasonably mapped to multiple outputs. They, too, demonstrate the augmenting the training data of image classifi-  
 82 cers can improve generalization. Teney, Abbasnejad, and Hengel (2020) propose an approach using counterfactuals  
 83 in training that does not rely on data augmentation: they argue that counterfactual pairs typically already exist in train-  
 84 ing datasets. Specifically, their approach relies on, firstly, identifying similar input samples with different annotations  
 85 and, secondly, ensuring that the gradient of the classifier aligns with the vector between pairs of counterfactual inputs  
 86 using the cosine distance as a loss function. In the natural language processing (NLP) domain, counterfactuals have  
 87 similarly been used to improve models through data augmentation: Wu et al. (2021), propose *POLYJUICE*, a general-  
 88 purpose counterfactual generator for language models. They demonstrate empirically that augmenting training data  
 89 through *POLYJUICE* counterfactuals improves robustness in a number of NLP tasks. Luu and Inoue (2023) introduce  
 90 Counterfactual Adversarial Training (CAT), which also aims at improving generalization and robustness of language  
 91 models. Specifically, they propose to proceed as follows: firstly, they identify training samples that are subject to  
 92 high predictive uncertainty; secondly, they generate counterfactual explanations for those samples; and, finally, they  
 93 fine-tune the given language model on the augmented dataset that includes the generated counterfactuals.

94 There have also been several attempts at formalizing the relationship between counterfactual explanations (CE) and  
 95 adversarial examples (AE). Pointing to clear similarities in how CE and AE are generated, Freiesleben (2022) makes  
 96 the case for jointly studying the opaqueness and robustness problem in representation learning. Formally, AE can  
 97 be seen as the subset of CE, for which misclassification is achieved (Freiesleben 2022). Similarly, Pawelczyk et  
 98 al. (2022) show that CE and AE are equivalent under certain conditions and derive theoretical upper bounds on the  
 99 distances between them.

100 Two recent works are closely related to ours in that they use counterfactuals during training with the explicit goal  
 101 of affecting certain properties of post-hoc counterfactual explanations. Firstly, Ross, Lakkaraju, and Bastani (2024)  
 102 propose a way to train models that are guaranteed to provide recourse for individuals to move from an adverse outcome  
 103 to some positive target class with high probability. The approach proposed by Ross, Lakkaraju, and Bastani (2024)  
 104 builds on adversarial training, where in this context susceptibility to targeted adversarial examples for the positive  
 105 class is explicitly induced. The proposed method allows for imposing a set of actionability constraints ex-ante: for  
 106 example, users can specify that certain features (e.g. *age*, *gender*, ...) are immutable. Secondly, Guo, Nguyen, and  
 107 Yadav (2023) are the first to propose an end-to-end training pipeline that includes counterfactual explanations as part  
 108 of the training procedure. In particular, they propose a specific network architecture that includes a predictor and CE  
 109 generator network, where the parameters of the CE generator network are learnable. Counterfactuals are generated  
 110 during each training iteration and fed back to the predictor network. In contrast to Guo, Nguyen, and Yadav (2023),  
 111 we impose no restrictions on the neural network architecture at all.

## 112 2.2 Beyond Robustness

113 Improving the adversarial robustness of models is not the only path towards aligning representations with plausible  
 114 explanations. In a work closely related to this one, Altmeyer et al. (2024) show that explainability can be improved  
 115 through model averaging and refined model objectives. The authors propose a way to generate counterfactuals that  
 116 are maximally **faithful** to the model in that they are consistent with what the model has learned about the underlying  
 117 data. Formally, they rely on tools from energy-based modelling to minimize the divergence between the distribution  
 118 of counterfactuals and the conditional posterior over inputs learned by the model. Their proposed counterfactual  
 119 explainer, *ECCo*, yields plausible explanations if and only if the underlying model has learned representations that  
 120 align with them. They find that both deep ensembles (Lakshminarayanan, Pritzel, and Blundell 2017) and joint energy-  
 121 based models (JEMs) (Grathwohl et al. 2020) tend to do well in this regard.

122 Once again it helps to look at these findings through the lens of representation learning with high degrees of freedom.  
 123 Deep ensembles are approximate Bayesian model averages, which are most called for when models are underspecified  
 124 by the available data (Wilson 2020). Averaging across solutions mitigates the aforementioned risk of relying on a  
 125 single locally optimal representations that corresponds to semantically meaningless explanations for the data. Previous  
 126 work by Schut et al. (2021) similarly found that generating plausible (“interpretable”) counterfactual explanations is  
 127 almost trivial for deep ensembles that have also undergone adversarial training. The case for JEMs is even clearer:  
 128 they involve a hybrid objective that induces both high predictive performance and generative capacity (Grathwohl et al.

129 This is closely related to the idea of aligning models with plausible explanations and has inspired our proposed  
 130 counterfactual training objective, as we explain in Section 3.

### 131 3 Counterfactual Training

132 Counterfactual training combines ideas from adversarial training, energy-based modelling and counterfactuals expla-  
 133 nations with the explicit objective of aligning representations with plausible explanations that comply with user re-  
 134 quirements. In the context of CE, plausibility has broadly been defined as the degree to which counterfactuals comply  
 135 with the underlying data generating process (Poyiadzi et al. 2020; Guidotti 2022; Altmeyer et al. 2024). Plausibility  
 136 is a necessary but insufficient condition for using CE to provide algorithmic recourse (AR) to individuals affected by  
 137 opaque models in practice. This is because for recourse recommendations to be **actionable**, they need to not only  
 138 result in plausible counterfactuals but also be attainable. A plausible CE for a rejected 20-year-old loan applicant, for  
 139 example, might reveal that their application would have been accepted, if only they were 20 years older. Ignoring all  
 140 other features, this complies with the definition of plausibility if 40-year-old individuals are in fact more credit-worthy  
 141 on average than young adults. But of course this CE does not qualify for providing actionable recourse to the applicant  
 142 since *age* is not a mutable feature. For our intents and purposes, counterfactual training aims at improving model ex-  
 143 plainability by aligning models with counterfactuals that meet both desiderata, plausibility and actionability. Formally,  
 144 we define explainability as follows:

145 **Definition 3.1** (Model Explainability). Let  $\mathbf{M}_\theta : \mathcal{X} \mapsto \mathcal{Y}$  denote a supervised classification model that maps from the  
 146  $D$ -dimensional input space  $\mathcal{X}$  to representations  $\phi(\mathbf{x}; \theta)$  and finally to the  $K$ -dimensional output space  $\mathcal{Y}$ . Assume that  
 147 for any given input-output pair  $\{\mathbf{x}, \mathbf{y}\}_i$  there exists a counterfactual  $\mathbf{x}' = \mathbf{x} + \Delta : \mathbf{M}_\theta(\mathbf{x}') = \mathbf{y}^+ \neq \mathbf{y} = \mathbf{M}_\theta(\mathbf{x})$  where  
 148  $\mathbf{y}^+$  denotes some target output. We say that  $\mathbf{M}_\theta$  is **explainable** to the extent that faithfully generated counterfactuals  
 149 are plausible (i.e. consistent with the data) and actionable. Formally, we define these properties as follows:

- 150 1. (Plausibility)  $\int^A p(\mathbf{x}|\mathbf{y}^+) d\mathbf{x} \rightarrow 1$  where  $A$  is some small region around  $\mathbf{x}'$ .  
 151 2. (Actionability) Permutations  $\Delta$  are subject to actionability constraints.

152 We consider counterfactuals as faithful to the extent that they are consistent with what the model has learned about the  
 153 input data. Let  $p_\theta(\mathbf{x}|\mathbf{y}^+)$  denote the conditional posterior over inputs, then formally:

- 154 3. (Faithfulness)  $\int^A p_\theta(\mathbf{x}|\mathbf{y}^+) d\mathbf{x} \rightarrow 1$  where  $A$  is defined as above.

155 The definitions of faithfulness and plausibility in Definition 3.1 are the same as in Altmeyer et al. (2024), with adapted  
 156 notation. Actionability constraints in Definition 3.1 vary and depend on the context in which  $\mathbf{M}_\theta$  is deployed. In this  
 157 work, we focus on domain and mutability constraints for individual features  $x_d$  for  $d = 1, \dots, D$ . We limit ourselves  
 158 to classification tasks for reasons discussed in Section 5.

#### 159 3.1 Our Proposed Objective

160 To train models with high explainability as defined in Definition 3.1, we propose the following objective,

$$\text{yloss}(\mathbf{M}_\theta(\mathbf{x}), \mathbf{y}) + \lambda_{\text{div}} \text{div}(\mathbf{x}, \mathbf{x}', \mathbf{y}; \theta) + \lambda_{\text{adv}} \text{advloss}(\mathbf{M}_\theta(\mathbf{x}'), \mathbf{y}) \quad (1)$$

161 where  $\text{yloss}(\cdot)$  denotes any conventional classification loss function (e.g. cross-entropy) that induces discriminative  
 162 (predictive) performance. The two additional components in Equation 1 are explained in more detail below. For now,  
 163 they can be sufficiently described as inducing explainability directly and indirectly by penalizing: 1) the contrastive  
 164 divergence,  $\text{div}(\cdot)$ , between counterfactuals  $x'$  and observed samples  $x$  and, 2) the adversarial loss,  $\text{advloss}(\cdot)$ , with  
 165 respect to counterfactuals. The tradeoff between the different components can be governed by adjusting the strengths  
 166 of the penalties  $\lambda_{\text{div}}$  and  $\lambda_{\text{adv}}$ .

##### 167 3.1.1 Directly Inducing Explainability through Contrastive Divergence

168 Grathwohl et al. (2020) observe that any classifier can be re-interpreted as a joint energy-based model (JEM)  
 169 that learns to discriminate output classes conditional on inputs and generate inputs. They show that JEMs can be  
 170 trained to perform well at both tasks by directly maximizing the joint log-likelihood factorized as  $\log p_\theta(\mathbf{x}, \mathbf{y}) =$   
 171  $\log p_\theta(\mathbf{y}|\mathbf{x}) + \log p_\theta(\mathbf{x})$ . The first factor can be optimized using conventional cross-entropy as in Equation 1. To  
 172 optimize  $\log p_\theta(\mathbf{x})$  Grathwohl et al. (2020) minimize the contrastive divergence between samples drawn from  $p_\theta(\mathbf{x})$   
 173 and training observations, i.e. samples from  $p(\mathbf{x})$ .

174 A key empirical finding in Altmeyer et al. (2024) was that JEMs tend to do well with respect to the plausibility objec-  
 175 tive in Definition 3.1. If we consider samples drawn from  $p_\theta(\mathbf{x})$  as counterfactuals, this is an expected finding, because

176 the JEM objective effectively minimizes the divergence between the conditional posterior and  $p(\mathbf{x}|\mathbf{y}^+)$ . To generate  
 177 samples, Grathwohl et al. (2020) rely on Stochastic Gradient Langevin Dynamics (SGLD) using an uninformative  
 178 prior for initialization. This is where we depart from their methodology: instead of generating samples through SGLD,  
 179 we propose using counterfactual explainers to generate counterfactuals for observed training samples. Specifically, we  
 180 have

$$\text{div}(\mathbf{x}, \mathbf{x}', y; \theta) = \mathcal{E}_\theta(\mathbf{x}, y) - \mathcal{E}_\theta(\mathbf{x}', y) \quad (2)$$

181 where  $\mathcal{E}_\theta(\cdot)$  denotes the energy function. We generate samples  $\mathbf{x}'$  by first randomly sampling the target class  $y^+ \sim$   
 182  $p(y)$  and then generating a counterfactual explanation for that target, similar to how conditional sampling is used to  
 183 draw from  $p_\theta(\mathbf{x})$  in Grathwohl et al. (2020). In particular, we set  $\mathcal{E}_\theta(\mathbf{x}, y) = -\mathbf{M}_\theta(\mathbf{x})[y^+]$  where  $y^+$  denotes the  
 184 index of the target class.

185 Intuitively, the gradient of Equation 2 decreases the energy of observed training samples (positive samples) while at  
 186 same time increasing the energy of counterfactuals (negative samples) (Du and Mordatch 2020). As the generated  
 187 counterfactuals get more plausible (Definition 3.1) over the cause of training, these two opposing effects gradually  
 188 balance each out (Lippe 2024).

189 The departure from SGLD allows us to tap into the vast repertoire of explainers that have been proposed in the literature  
 190 to meet different desiderata. Typically, these methods facilitate the imposition of domain and mutability constraints,  
 191 for example. In principle, any existing approach for generating counterfactual explanations is viable, so long as it does  
 192 not violate the faithfulness condition. Like JEMs (Murphy 2022), counterfactual training can be considered as a form  
 193 of contrastive representation learning.

### 194 3.1.2 Indirectly Inducing Explainability through Adversarial Robustness

195 Based on our analysis in Section 2, counterfactuals  $\mathbf{x}'$  can be repurposed as additional training samples (Luu and Inoue  
 196 2023) or adversarial examples (Freiesleben 2022; Pawelczyk et al. 2022). This leaves some flexibility with respect to  
 197 the exact choice for  $\text{advloss}(\cdot)$  in Equation 1. An intuitive functional form to use, though likely not the only reasonable  
 198 choice, is inspired by adversarial training:

$$\text{advloss}(\mathbf{M}_\theta(\mathbf{x}'), \mathbf{y}; \varepsilon) = \begin{cases} \text{yloss}(\mathbf{M}_\theta(\mathbf{x}'), \mathbf{y}) & \text{if } \|\Delta\|_\infty \leq \varepsilon \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

199 Under this choice we treat the counterfactual  $\mathbf{x}'$  as an adversarial example iff it is imperceptible, i.e. the magnitude of  
 200 the perturbation of any individual feature is upper-bounded at  $\varepsilon$ .

### 201 3.2 Encoding Actionability Constraints

202 Many existing counterfactual explainers support domain and mutability constraints out-of-the-box. In fact, both types  
 203 of constraints can be implemented for any counterfactual explainer that relies on gradient descent in the feature space  
 204 for optimization (Altmeyer, Deursen, et al. 2023). In this context, domain constraints can be imposed by simply  
 205 projecting counterfactuals back to the specified domain, if the previous gradient step resulted in updated feature values  
 206 that were out-of-domain. Mutability constraints can similarly be enforced by setting partial derivatives to zero to  
 207 ensure that features are only mutated in the allowed direction, if at all.

208 Since actionability constraints are binding at test time, we should also impose them when generating  $\mathbf{x}'$  during each  
 209 training iteration to align model representations with user requirements. Through their effect on  $\mathbf{x}'$ , both types of  
 210 constraints influence model outcomes through Equation 2. Here it is crucial that we avoid penalizing implausibility  
 211 that arises due to mutability constraints. For any mutability-constrained feature  $d$  this can be achieved by enforcing  
 212  $\mathbf{x}[d] - \mathbf{x}'[d] := 0$  whenever perturbing  $\mathbf{x}'[d]$  in the direction of  $\mathbf{x}[d]$  would violate mutability constraints. Specifically,  
 213 we set  $\mathbf{x}[d] := \mathbf{x}'[d]$  if

- 214 1. Feature  $d$  is strictly immutable in practice.
- 215 2. We have  $\mathbf{x}[d] > \mathbf{x}'[d]$  but feature  $d$  can only be decreased in practice.
- 216 3. We have  $\mathbf{x}[d] < \mathbf{x}'[d]$  but feature  $d$  can only be increased in practice.

217 From a Bayesian perspective, setting  $\mathbf{x}[d] := \mathbf{x}'[d]$  can be understood as assuming a point mass prior for  $p(\mathbf{x})$  with  
 218 respect to feature  $d$ . Intuitively, we think of this simply in terms ignoring implausibility costs with respect to immutable  
 219 features, which effectively forces the model to instead seek plausibility with respect to the remaining features. This  
 220 in turn results in lower overall sensitivity to immutable features, which we demonstrate empirically for different  
 221 classifiers in Section 4. Under certain conditions, this results holds theoretically[For the proof, see the supplementary  
 222 appendix.].

223 **Theorem 3.1** (Protecting Immutable Features). Let  $f_\theta(\mathbf{x}) = \mathcal{S}(\mathbf{M}_\theta(\mathbf{x})) = \mathcal{S}(\Theta\mathbf{x})$  denote a linear classifier with  
 224 softmax activation  $\mathcal{S}$  (i.e. multinomial logistic regression) where  $y \in \{1, \dots, K\} = \mathcal{K}$  and  $\mathbf{x} \in \mathbb{R}^D$ . If we assume  
 225 multivariate Gaussian class densities with common diagonal covariance matrix  $\Sigma_k = \Sigma$  for all  $k \in \mathcal{K}$ , then protecting  
 226 an immutable feature from the contrastive divergence penalty (Equation 2) will result in lower classifier sensitivity to  
 227 that feature relative to the remaining features, provided that at least one of those is mutable.

228 It is worth highlighting that Theorem 3.1 assumes independence of features. This raises a valid concern about the  
 229 effect of protecting immutable features in the presence of proxy features that remain unprotected. We discuss this  
 230 limitation in Section 5.

### 231 3.3 Illustration

232 To better convey the intuition underlying our proposed method, we illustrate different model outcomes in Example 3.1.

233 **Example 3.1** (Prediction of Consumer Credit Default). Suppose we are interested in predicting the likelihood that  
 234 loan applicants default on their credit. We have access to historical data on previous loan takers comprised of a binary  
 235 outcome variable ( $y \in \{1 = \text{default}, 2 = \text{no default}\}$ ) two input features: 1) the subjects' *age*, which we define as  
 236 immutable, and 2) the subjects' existing level of *debt*, which we define as mutable.

237 We have simulated this scenario using synthetic data with independent features and Gaussian class-conditional densities in Figure 1. The four panels in Figure 1 show the outcomes for different training procedures using the same model  
 238 architecture each time (a linear classifier). In each case, we show the linear decision boundary (green) and the training  
 239 data colored according to their ground-truth label: orange points belong to the target class,  $y^+ = 2$ , blue points belong  
 240 to the non-target class,  $y^- = 1$ . Stars indicate counterfactuals in the target class generated at test time using generic  
 241 gradient descent for a fixed number of iterations.

243 In panel (a), we have trained our model conventionally, and we do not impose mutability constraints at test time. The  
 244 generated counterfactuals are all valid, but not plausible: they are clearly distinguishable from the ground-truth data. In  
 245 panel (b), we have trained our model with counterfactual training, once again not imposing mutability constraints at test  
 246 time. We observe that the counterfactuals are clearly plausible, therefore meeting the first objective of Definition 3.1.

247 In panel (c), we have used conventional training again, this time imposing the mutability constraint on *age* at test  
 248 time. Counterfactuals are valid but involve some substantial reductions in *debt* for some individuals, in particular  
 249 very young applicants. By comparison, counterfactual paths are shorter on average in panel (d), where we have used  
 250 counterfactual training and protected immutable features as described in Section 3.2. In particular, we observe that due  
 251 to the classifier's lower sensitivity to *age*, recourse recommendations with respect to *debt* are much more homogenous,  
 252 in that they do not disproportionately punish younger individuals. The counterfactuals are also plausible with respect  
 253 to the mutable feature. Thus, we consider the model in panel (d) as the most explainable according to Definition 3.1.

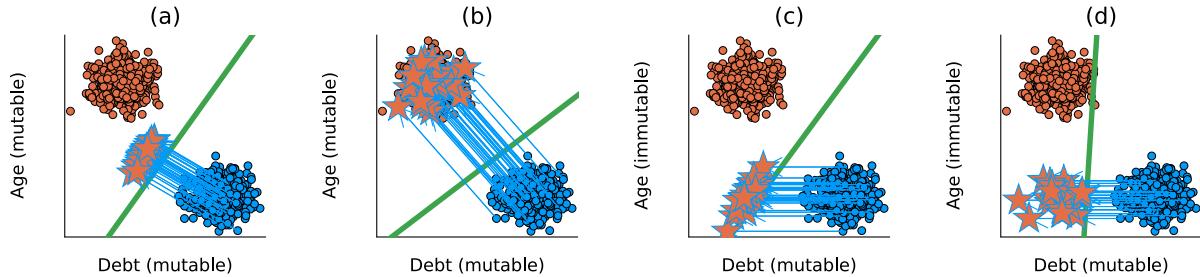


Figure 1: Visual illustration of how counterfactual training improves explainability. See Example 3.1 for details.

## 254 4 Experiments

255 In this section, we present experiments that we have conducted in order to answer the following research questions:

256 **Research Question 4.1** (Plausibility). Does our proposed counterfactual training objective (Equation 1) induce mod-  
 257 els to learn plausible explanations?

258 **Research Question 4.2** (Actionability). Does our proposed counterfactual training objective (Equation 1) yield more  
 259 favorable algorithmic recourse outcomes in the presence of actionability constraints?

260 Beyond this, we are also interested in understanding how robust our answers to RQ 4.1 and RQ 4.2 are:

261 **Research Question 4.3** (Hyperparameters). *What are the effects of different hyperparameter choices with respect to*  
 262 *Equation 1?*

263 **4.1 Experimental Setup**

264 **4.2 Experimental Results**

265 **5 Discussion**

- 266 1. Limited to classification models.  
 267 2. Proxy attributes of immutable features.

268 **6 Conclusion**

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338 **A Notation**

- 339 •  $y^+$ : The target class and also the index of the target class.
- 340 •  $y^-$ : The non-target class and also the index of non-the target class.
- 341 •  $\mathbf{y}^+$ : The one-hot encoded output vector for the target class.
- 342 •  $\theta$ : Model parameters (unspecified).
- 343 •  $\Theta$ : Matrix of parameters.

344 **B Technical Details of Our Approach**

345 **B.1 Protecting Mutability Constraints with Linear Classifiers**

346 In Section 3.2 we explain that to avoid penalizing implausibility that arises due to mutability constraints, we impose a  
 347 point mass prior on  $p(\mathbf{x})$  for the corresponding feature. We argue in Section 3.2 that this approach induces models to  
 348 be less sensitive to immutable features and demonstrate this empirically in Section 4. Below we derive the analytical  
 349 results in Theorem 3.1.

350 *Proof.* Let  $d_{\text{mtbl}}$  and  $d_{\text{immmtbl}}$  denote some mutable and immutable feature, respectively. Suppose that  $\mu_{y^-, d_{\text{immmtbl}}} <$   
 351  $\mu_{y^+, d_{\text{immmtbl}}}$  and  $\mu_{y^-, d_{\text{mtbl}}} > \mu_{y^+, d_{\text{mtbl}}}$ , where  $\mu_{k,d}$  denotes the conditional sample mean of feature  $d$  in class  $k$ . In words,  
 352 we assume that the immutable feature tends to take lower values for samples in the non-target class  $y^-$  than in the  
 353 target class  $y^+$ . We assume the opposite to hold for the mutable feature.

354 Assuming multivariate Gaussian class densities with common diagonal covariance matrix  $\Sigma_k = \Sigma$  for all  $k \in \mathcal{K}$ , we  
 355 have for the log likelihood ratio between any two classes  $k, m \in \mathcal{K}$  (Hastie, Tibshirani, and Friedman 2009):

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \mathbf{x}^\top \Sigma^{-1} (\mu_k - \mu_m) + \text{const} \quad (4)$$

356 By independence of  $x_1, \dots, x_D$ , the full log-likelihood ratio decomposes into:

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \sum_{d=1}^D \frac{\mu_{k,d} - \mu_{m,d}}{\sigma_d^2} x_d + \text{const} \quad (5)$$

357 By the properties of our classifier (*multinomial logistic regression*), we have:

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \sum_{d=1}^D (\theta_{k,d} - \theta_{m,d}) x_d + \text{const} \quad (6)$$

358 where  $\theta_{k,d} = \Theta[k, d]$  denotes the coefficient on feature  $d$  for class  $k$ .

359 Based on Equation 5 and Equation 6 we can identify that  $(\mu_{k,d} - \mu_{m,d}) \propto (\theta_{k,d} - \theta_{m,d})$  under the assumptions we  
 360 made above. Hence, we have that  $(\theta_{y^-, d_{\text{immmtbl}}} - \theta_{y^+, d_{\text{immmtbl}}}) < 0$  and  $(\theta_{y^-, d_{\text{mtbl}}} - \theta_{y^+, d_{\text{mtbl}}}) > 0$

361 Let  $\mathbf{x}'$  denote some randomly chosen individual from class  $y^-$  and let  $y^+ \sim p(y)$  denote the randomly chosen target  
 362 class. Then the partial derivative of the contrastive divergence penalty Equation 2 with respect to coefficient  $\theta_{y^+, d}$  is  
 363 equal to

$$\frac{\partial}{\partial \theta_{y^+, d}} (\text{div}(\mathbf{x}, \mathbf{x}', \mathbf{y}; \theta)) = \frac{\partial}{\partial \theta_{y^+, d}} ((-\mathbf{M}_\theta(\mathbf{x})[y^+]) - (-\mathbf{M}_\theta(\mathbf{x}')[y^+])) = x'_d - x_d \quad (7)$$

364 and equal to zero everywhere else.

365 Since  $(\mu_{y^-, d_{\text{immmtbl}}} < \mu_{y^+, d_{\text{immmtbl}}})$  we are more likely to have  $(x'_{d_{\text{immmtbl}}} - x_{d_{\text{immmtbl}}}) < 0$  than vice versa at initialization.  
 366 Similarly, we are more likely to have  $(x'_{d_{\text{mtbl}}} - x_{d_{\text{mtbl}}}) > 0$  since  $(\mu_{y^-, d_{\text{mtbl}}} > \mu_{y^+, d_{\text{mtbl}}})$ .

367 This implies that if we do not protect feature  $d_{\text{immmtbl}}$ , the contrastive divergence penalty will push down on  $\theta_{y^-, d_{\text{immmtbl}}}$   
 368 thereby exacerbating the existing effect  $(\theta_{y^-, d_{\text{immmtbl}}} - \theta_{y^+, d_{\text{immmtbl}}}) < 0$ . In words, not protecting the immutable feature  
 369 would have the undesirable effect of making the classifier more sensitive to this feature, in that it would be more likely  
 370 to predict class  $y^-$  as opposed to  $y^+$  for lower values of  $d_{\text{immmtbl}}$ .

371 By the same rationale, the contrastive divergence penalty can generally be expected to push up on  $\theta_{y^-, d_{\text{mtbl}}}$  exacerbating  
 372  $(\theta_{y^-, d_{\text{mtbl}}} - \theta_{y^+, d_{\text{mtbl}}}) > 0$ . In words, this has the effect of making the classifier more sensitive to the mutable feature, in  
 373 that it would be more likely to predict class  $y^-$  as opposed to  $y^+$  for higher values of  $d_{\text{mtbl}}$ .

374 Thus, our proposed approach of protecting feature  $d_{\text{immtbl}}$  has the net affect of decreasing the classifier's sensitivity  
 375 to the immutable feature relative to the mutable feature (i.e. no change in sensitivity for  $d_{\text{immtbl}}$  relative to increased  
 376 sensitivity for  $d_{\text{mtbl}}$ ).  $\square$

### ⚠ Warning

@Cynthia, @Arie, I have tentatively phrased the above in terms of a theorem and proof. This is something I've so far shied away from because I feel a bit out of my depth when it comes to mathematical proofs. The above makes intuitive sense to me, but I don't know for sure if it's correct.

377

## C Detailed Results

### ⚠ Warning

@Cynthia, @Arie, I'm including some preliminary results here but will rerun experiments in the coming days. You'll notice some odd outlier results (huge values) for the initial grid search (Section C.2). My belief is that this is once again due to *ECCo* overshooting for some hyperparameter choices, that we have discussed before. A simple solution to this story is to actually impose domain constraints. Let's see what the final results show us (I also still plan to make slight changes to the implementation), but in any case I think it might even be worth to report results for the initial grid search in the final appendix (they do include good results for CT for certain hyperparameter ranges and highlight limitations inherited from energy-based modelling).

379

### C.1 Qualitative Findings for Image Data

### ℹ Note

@Cynthia, @Arie, Figure A1 shows much more plausible (faithful) counterfactuals for a model with CT than the model with conventional training (Figure A2). In fact, this is not even using *ECCo+* and still showing better results than the best results we achieved in our AAAI paper for JEM ensembles.

381

### C.2 Initial Grid Search

383 For the initial round of experiments we

#### C.2.1 Generator Parameters

385 The hyperparameter grids for the first investigation of the effect of generator parameters are shown in Parameters C.1  
 386 and Parameters C.2.

#### 387 Parameters C.1 (Training Phase).

- 388 • Generator Parameters:

- 389 –  $\lambda_{\text{cost}}$ : 0.0, 0.001, 0.1
- 390 –  $\lambda_{\text{div}}$ : 0.01, 0.05, 0.1, 0.5, 1.0, 5.0, 10.0, 15.0
- 391 – Learning Rate: 1.0
- 392 – Maximum Iterations: 20, 50, 100
- 393 – Optimizer: sgd

- 394 • Generator: ecco, generic, omni, revise
- 395 • Training Parameters:

- 396 – Objective: full, vanilla

#### 397 Parameters C.2 (Evaluation Phase).

- 398 • Counterfactual Parameters:

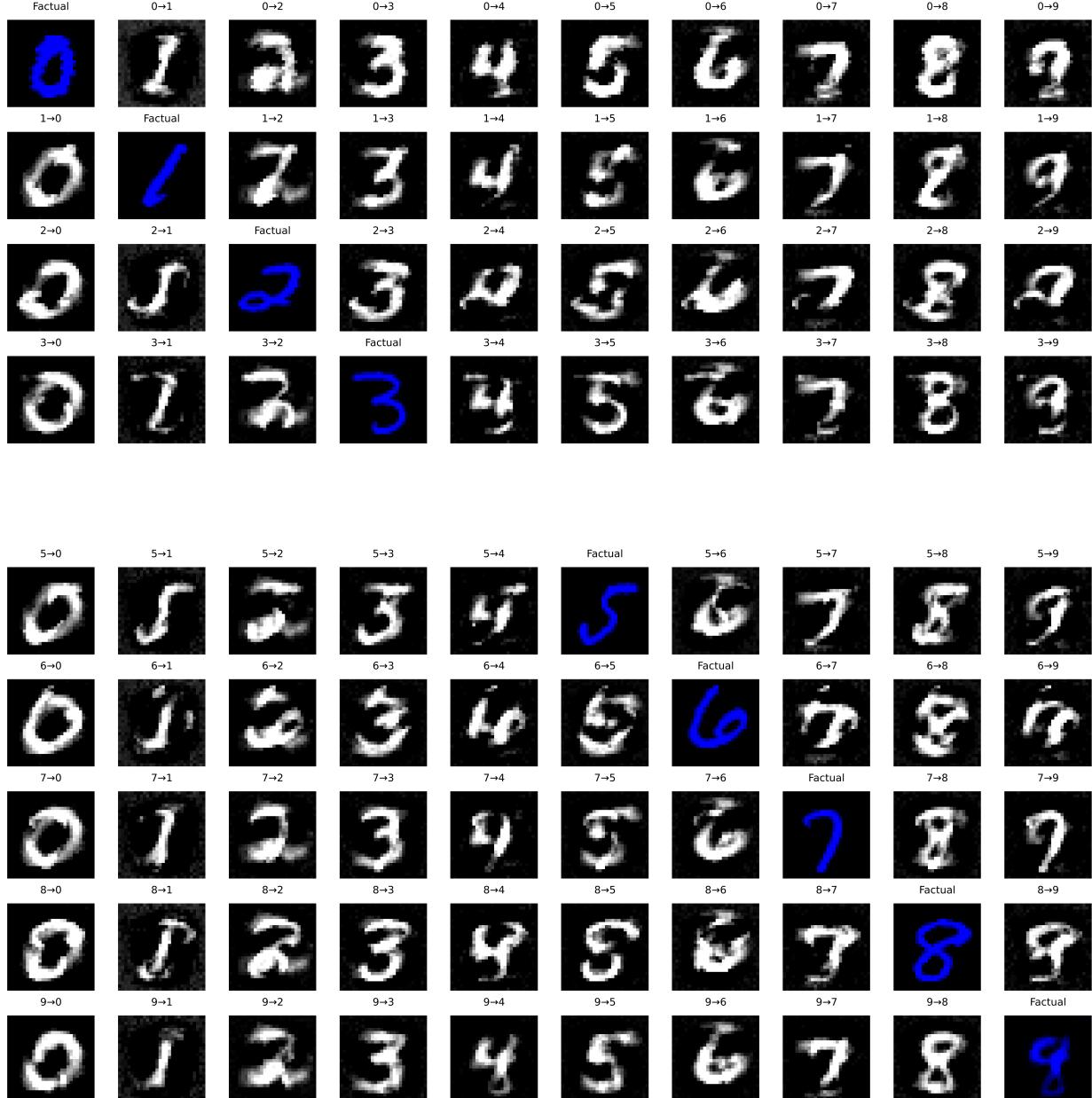


Figure A1: Counterfactual images for *MLP* with counterfactual training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

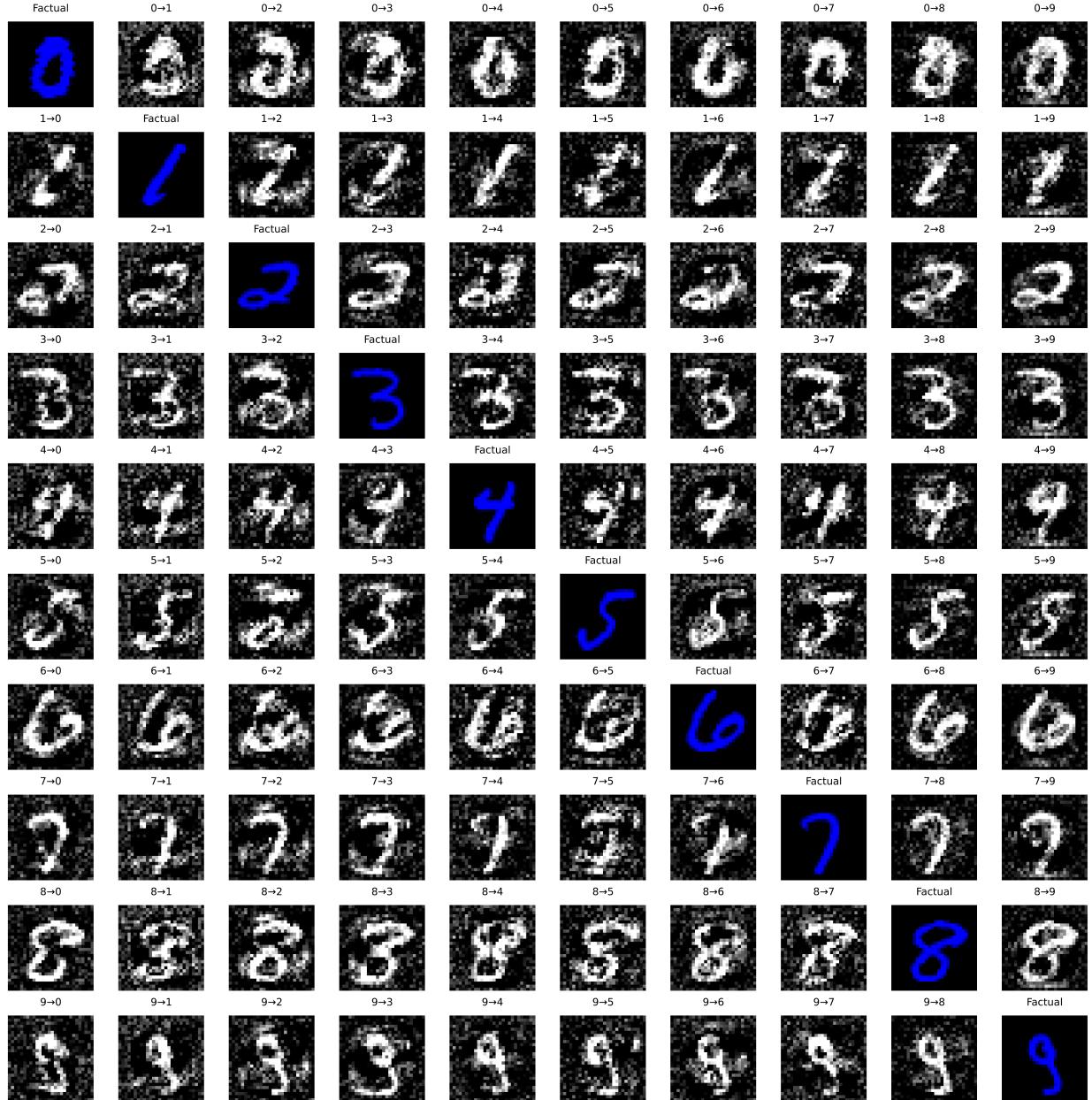


Figure A2: Counterfactual images for *MLP* with conventional training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

- 399     – Convergence: `max_iter`  
 400     – Maximum Iterations: 100  
 401     – No. Individuals: 100  
 402     – No. Runs: 5  
 403     • Generator Parameters:  
 404         –  $\lambda_{\text{cost}}$ : 0.0  
 405         –  $\lambda_{\text{div}}$ : 0.1, 0.5, 1.0, 5.0, 10.0, 20.0  
 406         – Learning Rate: 1.0  
 407         – Maximum Iterations: 50  
 408         – Optimizerimizer: `sgd`

409 **C.2.1.1 Linearly Separable**

- 410     • **Energy Penalty** (Table A1): *ECCo* generally does yield better results than *Vanilla* for higher choices of the  
 411     energy penalty (10,15) during training. *Generic* performs poorly accross the board. *Omni* seems to have an  
 412     anchoring effect, in that it never performs terribly but also never as good as the best *ECCo* results. *REVISE*  
 413     performs poorly across the board.  
 414     • **Cost** (Table A2): Results for all generators (except *Omni*) are quite bad, which can likely be attributed to  
 415     extremely bad results for some choices of the **Energy Penalty** (results here are averaged). For *ECCo* and  
 416     *Generic*, higher cost values generally lead to worse results.  
 417     • **Maximum Iterations**: No clear patterns recognizable, so it seems that smaller choices are ok.  
 418     • **Validity**: *ECCo* almost always valid except for very low values during training and high values at evaluation  
 419     time. *Generic* often has poor validity.  
 420     • **Accuracy**: Seems largely unaffected.

Table A1: Results for Linearly Separable data by energy penalty.

Objective	$\lambda_{\text{div}}$ (train)	Generator	Value	Std
full	0.01	<i>ECCo</i>	$-9.91 \cdot 10^{11}$	$2.25 \cdot 10^{12}$
full	0.01	<i>Generic</i>	$-5.71 \cdot 10^{17}$	$1.3 \cdot 10^{18}$
<b>full</b>	<b>0.01</b>	<b>Omniscient</b>	<b>-2.54</b>	<b>0.116</b>
full	0.01	<i>REVISE</i>	-15.6	13.2
vanilla	0.01	<i>ECCo</i>	-4.28	3.52
vanilla	0.01	<i>Generic</i>	-4.45	3.47
vanilla	0.01	<i>Omniscient</i>	-5.12	4.46
vanilla	0.01	<i>REVISE</i>	-4.91	4.24
full	0.05	<i>ECCo</i>	$-5.63 \cdot 10^5$	$1.28 \cdot 10^6$
full	0.05	<i>Generic</i>	$-8.35 \cdot 10^{17}$	$1.9 \cdot 10^{18}$
<b>full</b>	<b>0.05</b>	<b>Omniscient</b>	<b>-2.53</b>	<b>0.114</b>
full	0.05	<i>REVISE</i>	-15	12.6
vanilla	0.05	<i>ECCo</i>	-4.4	3.66
vanilla	0.05	<i>Generic</i>	-4.38	3.48
vanilla	0.05	<i>Omniscient</i>	-5.25	4.62
vanilla	0.05	<i>REVISE</i>	-4.94	4.22
full	0.1	<i>ECCo</i>	$-6.74 \cdot 10^5$	$1.53 \cdot 10^6$
full	0.1	<i>Generic</i>	$-1.71 \cdot 10^{11}$	$3.9 \cdot 10^{11}$
<b>full</b>	<b>0.1</b>	<b>Omniscient</b>	<b>-2.56</b>	<b>0.124</b>
full	0.1	<i>REVISE</i>	-15.6	13.2
vanilla	0.1	<i>ECCo</i>	-4.28	3.52
vanilla	0.1	<i>Generic</i>	-4.45	3.48
vanilla	0.1	<i>Omniscient</i>	-5.12	4.46
vanilla	0.1	<i>REVISE</i>	-4.91	4.25
full	0.5	<i>ECCo</i>	-11.8	9.83
full	0.5	<i>Generic</i>	$-1.06 \cdot 10^{18}$	$2.42 \cdot 10^{18}$
<b>full</b>	<b>0.5</b>	<b>Omniscient</b>	<b>-2.54</b>	<b>0.123</b>
full	0.5	<i>REVISE</i>	-15	12.6

Continuing table below.

<b>Objective</b>	$\lambda_{\text{div}}(\text{train})$	<b>Generator</b>	<b>Value</b>	<b>Std</b>
vanilla	0.5	<i>ECCo</i>	-4.4	3.65
vanilla	0.5	<i>Generic</i>	-4.38	3.48
vanilla	0.5	<i>Omniscient</i>	-5.25	4.61
vanilla	0.5	<i>REVISE</i>	-4.95	4.22
full	1	<i>ECCo</i>	-11.5	11.1
full	1	<i>Generic</i>	$-1.71 \cdot 10^{11}$	$3.88 \cdot 10^{11}$
<b>full</b>	<b>1</b>	<b>Omniscient</b>	<b>-2.59</b>	<b>0.117</b>
full	1	<i>REVISE</i>	-15.7	13.3
vanilla	1	<i>ECCo</i>	-4.28	3.51
vanilla	1	<i>Generic</i>	-4.44	3.47
vanilla	1	<i>Omniscient</i>	-5.11	4.46
vanilla	1	<i>REVISE</i>	-4.91	4.25
full	5	<i>ECCo</i>	-3.99	3.12
full	5	<i>Generic</i>	$-4.88 \cdot 10^{17}$	$1.11 \cdot 10^{18}$
<b>full</b>	<b>5</b>	<b>Omniscient</b>	<b>-2.53</b>	<b>0.117</b>
full	5	<i>REVISE</i>	-14.6	12.1
vanilla	5	<i>ECCo</i>	-4.4	3.65
vanilla	5	<i>Generic</i>	-4.38	3.48
vanilla	5	<i>Omniscient</i>	-5.25	4.61
vanilla	5	<i>REVISE</i>	-4.95	4.22
<b>full</b>	<b>10</b>	<b>ECCo</b>	<b>-2.31</b>	<b>0.735</b>
full	10	<i>Generic</i>	$-1.7 \cdot 10^{11}$	$3.86 \cdot 10^{11}$
full	10	<i>Omniscient</i>	-2.53	0.117
full	10	<i>REVISE</i>	-15.5	13
vanilla	10	<i>ECCo</i>	-4.28	3.51
vanilla	10	<i>Generic</i>	-4.44	3.47
vanilla	10	<i>Omniscient</i>	-5.12	4.46
vanilla	10	<i>REVISE</i>	-4.91	4.24
<b>full</b>	<b>15</b>	<b>ECCo</b>	<b>-2.01</b>	<b>0.488</b>
full	15	<i>Generic</i>	$-4.91 \cdot 10^{17}$	$1.12 \cdot 10^{18}$
full	15	<i>Omniscient</i>	-2.53	0.116
full	15	<i>REVISE</i>	-14.4	11.7
vanilla	15	<i>ECCo</i>	-4.4	3.65
vanilla	15	<i>Generic</i>	-4.38	3.48
vanilla	15	<i>Omniscient</i>	-5.25	4.6
vanilla	15	<i>REVISE</i>	-4.95	4.23

Table A2: Results for Linearly Separable data by cost penalty.

<b>Objective</b>	$\lambda_{\text{cost}}(\text{train})$	<b>Generator</b>	<b>Value</b>	<b>Std</b>
full	0	<i>ECCo</i>	$-5.32 \cdot 10^3$	$1.21 \cdot 10^4$
full	0	<i>Generic</i>	$-1.03 \cdot 10^{18}$	$2.34 \cdot 10^{18}$
<b>full</b>	<b>0</b>	<b>Omniscient</b>	<b>-2.64</b>	<b>0.125</b>
full	0	<i>REVISE</i>	-15.4	12.9
vanilla	0	<i>ECCo</i>	-4.34	3.58
vanilla	0	<i>Generic</i>	-4.41	3.48
vanilla	0	<i>Omniscient</i>	-5.18	4.54
vanilla	0	<i>REVISE</i>	-4.93	4.23
full	0.001	<i>ECCo</i>	-362	811
full	0.001	<i>Generic</i>	$-2.65 \cdot 10^{17}$	$6.04 \cdot 10^{17}$
<b>full</b>	<b>0.001</b>	<b>Omniscient</b>	<b>-2.49</b>	<b>0.115</b>
full	0.001	<i>REVISE</i>	-15.5	13
vanilla	0.001	<i>ECCo</i>	-4.34	3.58
vanilla	0.001	<i>Generic</i>	-4.41	3.48

Continuing table below.

Objective	$\lambda_{\text{cost}}(\text{train})$	Generator	Value	Std
vanilla	0.001	<i>Omniscient</i>	-5.18	4.53
vanilla	0.001	<i>REVISE</i>	-4.93	4.23
full	0.1	<i>ECCo</i>	$-3.72 \cdot 10^{11}$	$8.46 \cdot 10^{11}$
full	0.1	<i>Generic</i>	$-4.48 \cdot 10^{14}$	$1.02 \cdot 10^{15}$
<b>full</b>	<b>0.1</b>	<b>Omniscient</b>	<b>-2.5</b>	<b>0.112</b>
full	0.1	<i>REVISE</i>	-14.6	12.2
vanilla	0.1	<i>ECCo</i>	-4.34	3.58
vanilla	0.1	<i>Generic</i>	-4.41	3.48
vanilla	0.1	<i>Omniscient</i>	-5.18	4.54
vanilla	0.1	<i>REVISE</i>	-4.93	4.24

421 **C.2.1.2 Moons**

- 422 • **Energy Penalty** (Table A3): *ECCo* consistently yields better results than *Vanilla*, except for very low choices  
423 of the energy penalty during training for which it performs abysmal. *Generic* performs quite badly across  
424 the board for high enough choices of the energy penalty at evaluation time. *Omni* has small positive effect.  
425 *REVISE* performs poorly across the board.
- 426 • **Cost (distance penalty)**: *Generic* generally does better for higher values, while *ECCo* does better for lower  
427 values.
- 428 • **Maximum Iterations**: No clear patterns recognizable, so it seems that smaller choices are ok.
- 429 • **Validity**: *ECCo* generally achieves full validity except for very low choices the energy penalty during training  
430 and high choices at evaluation time. *Generic* performs poorly for high choices of the energy penalty during  
431 evaluation.
- 432 • **Accuracy**: Largely unaffected although *ECCo* suffers a bit for very low choices the energy penalty during  
433 training. *REVISE* suffers a lot in general (around 10 percentage points).

Table A3: Results for Moons data by energy penalty.

Objective	$\lambda_{\text{div}}(\text{train})$	Generator	Value	Std
full	0.01	<i>ECCo</i>	$-2.8 \cdot 10^{22}$	$6.39 \cdot 10^{22}$
full	0.01	<i>Generic</i>	$-4.89 \cdot 10^{30}$	$1.11 \cdot 10^{31}$
<b>full</b>	<b>0.01</b>	<b>Omniscient</b>	<b>-4.74</b>	<b>5.08</b>
full	0.01	<i>REVISE</i>	-572	$1.25 \cdot 10^3$
vanilla	0.01	<i>ECCo</i>	-15.5	17.3
vanilla	0.01	<i>Generic</i>	-10.9	11.9
vanilla	0.01	<i>Omniscient</i>	-12.7	14.4
vanilla	0.01	<i>REVISE</i>	-11.2	13
full	0.05	<i>ECCo</i>	$-1.55 \cdot 10^{16}$	$3.52 \cdot 10^{16}$
full	0.05	<i>Generic</i>	$-2.22 \cdot 10^{20}$	$5 \cdot 10^{20}$
<b>full</b>	<b>0.05</b>	<b>Omniscient</b>	<b>-4.41</b>	<b>4.48</b>
full	0.05	<i>REVISE</i>	$-1.04 \cdot 10^3$	$2.3 \cdot 10^3$
vanilla	0.05	<i>ECCo</i>	-15.5	17.2
vanilla	0.05	<i>Generic</i>	-11.7	12.8
vanilla	0.05	<i>Omniscient</i>	-12.4	14.1
vanilla	0.05	<i>REVISE</i>	-11.3	13.1
full	0.1	<i>ECCo</i>	$-3.41 \cdot 10^3$	$7.73 \cdot 10^3$
full	0.1	<i>Generic</i>	$-5.22 \cdot 10^{30}$	$1.19 \cdot 10^{31}$
<b>full</b>	<b>0.1</b>	<b>Omniscient</b>	<b>-4.78</b>	<b>5.12</b>
full	0.1	<i>REVISE</i>	-288	594
vanilla	0.1	<i>ECCo</i>	-15.5	17.2
vanilla	0.1	<i>Generic</i>	-10.9	11.9
vanilla	0.1	<i>Omniscient</i>	-12.7	14.4
vanilla	0.1	<i>REVISE</i>	-11.3	13.1
full	0.5	<i>ECCo</i>	-7.09	7.51

Continuing table below.

Objective	$\lambda_{\text{div}}(\text{train})$	Generator	Value	Std
full	0.5	<i>Generic</i>	$-1.11 \cdot 10^{31}$	$2.53 \cdot 10^{31}$
<b>full</b>	<b>0.5</b>	<b>Omniscient</b>	<b>-4.58</b>	<b>4.83</b>
full	0.5	<i>REVISE</i>	$-1.19 \cdot 10^3$	$2.64 \cdot 10^3$
vanilla	0.5	<i>ECCo</i>	-15.5	17.2
vanilla	0.5	<i>Generic</i>	-11.7	12.8
vanilla	0.5	<i>Omniscient</i>	-12.4	14.1
vanilla	0.5	<i>REVISE</i>	-11.3	13.1
full	1	<i>ECCo</i>	-6.06	6.33
full	1	<i>Generic</i>	$-1.58 \cdot 10^{33}$	$3.59 \cdot 10^{33}$
<b>full</b>	<b>1</b>	<b>Omniscient</b>	<b>-4.66</b>	<b>4.89</b>
full	1	<i>REVISE</i>	$-1.16 \cdot 10^3$	$2.59 \cdot 10^3$
vanilla	1	<i>ECCo</i>	-15.5	17.3
vanilla	1	<i>Generic</i>	-10.9	11.9
vanilla	1	<i>Omniscient</i>	-12.7	14.4
vanilla	1	<i>REVISE</i>	-11.3	13.1
<b>full</b>	<b>5</b>	<b>ECCo</b>	<b>-2.57</b>	<b>2.07</b>
full	5	<i>Generic</i>	$-1.17 \cdot 10^{28}$	$2.66 \cdot 10^{28}$
full	5	<i>Omniscient</i>	-4.29	4.31
full	5	<i>REVISE</i>	-530	$1.16 \cdot 10^3$
vanilla	5	<i>ECCo</i>	-15.5	17.2
vanilla	5	<i>Generic</i>	-11.7	12.7
vanilla	5	<i>Omniscient</i>	-12.4	14.1
vanilla	5	<i>REVISE</i>	-11.3	13.1
<b>full</b>	<b>10</b>	<b>ECCo</b>	<b>-1.76</b>	<b>0.974</b>
full	10	<i>Generic</i>	$-1.54 \cdot 10^{33}$	$3.51 \cdot 10^{33}$
full	10	<i>Omniscient</i>	-4.44	4.56
full	10	<i>REVISE</i>	$-1.52 \cdot 10^3$	$3.4 \cdot 10^3$
vanilla	10	<i>ECCo</i>	-15.5	17.3
vanilla	10	<i>Generic</i>	-10.9	11.9
vanilla	10	<i>Omniscient</i>	-12.7	14.4
vanilla	10	<i>REVISE</i>	-11.3	13.1
<b>full</b>	<b>15</b>	<b>ECCo</b>	<b>-1.37</b>	<b>0.365</b>
full	15	<i>Generic</i>	$-5.32 \cdot 10^{28}$	$1.21 \cdot 10^{29}$
full	15	<i>Omniscient</i>	-4.34	4.38
full	15	<i>REVISE</i>	-473	$1.03 \cdot 10^3$
vanilla	15	<i>ECCo</i>	-15.5	17.2
vanilla	15	<i>Generic</i>	-11.7	12.8
vanilla	15	<i>Omniscient</i>	-12.4	14.1
vanilla	15	<i>REVISE</i>	-11.3	13.1

434 **C.2.1.3 Circles**

- 435 • **Energy Penalty** (Table A4): *ECCo* consistently yields better results than *Vanilla*, though primarily for low to  
436 medium choices of the energy penalty ( $<=5$ ) during training. The same goes for *Generic*, which sometimes  
437 outperforms *ECCo* (for small energy penalty at evaluation time). *Omni* does alright for lower energy penalty  
438 at evaluation time, but loses out for higher choices. *REVISE* performs poorly across the board (except very  
439 low choices at evaluation time).
- 440 • **Cost (distance penalty)**: *ECCo* and *Generic* generally achieve the best results when no cost penalty is used  
441 during training. Both *Omni* and *REVISE* are largely unaffected.
- 442 • **Maximum Iterations**: *ECCo* consistently yields better results for higher numbers of iterations. *Generic*  
443 generally does best for a medium number (50). *Omni* is sometimes invalid (???).
- 444 • **Validity**: *ECCo* tends to outperform its *Vanilla* counterpart, though primarily for low to medium choices of  
445 the energy penalty ( $<=5$ ) during training and evaluation. *Vanilla* typically worse across the board.
- 446 • **Accuracy**: Mostly unaffected, but *REVISE* again consistently some deterioration and *ECCo* deteriorates for  
447 high choices of energy penalty during training, reflecting other outcomes above.

Table A4: Results for Circles data by energy penalty.

Objective	$\lambda_{\text{div}}(\text{train})$	Generator	Value	Std
<b>full</b>	<b>0.01</b>	<b>ECCo</b>	<b>-1.26</b>	<b>0.423</b>
full	0.01	<i>Generic</i>	-1.49	0.71
full	0.01	<i>Omniscient</i>	-5.21	5.25
full	0.01	<i>REVISE</i>	$-2.71 \cdot 10^{26}$	$6.37 \cdot 10^{26}$
vanilla	0.01	<i>ECCo</i>	-9.33	7.34
vanilla	0.01	<i>Generic</i>	-8.89	6.88
vanilla	0.01	<i>Omniscient</i>	-8.67	6.87
vanilla	0.01	<i>REVISE</i>	-8.65	6.8
full	0.05	<i>ECCo</i>	-1.29	0.397
<b>full</b>	<b>0.05</b>	<b>Generic</b>	<b>-1.21</b>	<b>0.356</b>
full	0.05	<i>Omniscient</i>	-5.08	5.09
full	0.05	<i>REVISE</i>	$-5.91 \cdot 10^{27}$	$1.36 \cdot 10^{28}$
vanilla	0.05	<i>ECCo</i>	-9.35	7.32
vanilla	0.05	<i>Generic</i>	-8.85	6.87
vanilla	0.05	<i>Omniscient</i>	-8.7	6.96
vanilla	0.05	<i>REVISE</i>	-8.52	6.76
<b>full</b>	<b>0.1</b>	<b>ECCo</b>	<b>-1.2</b>	<b>0.383</b>
full	0.1	<i>Generic</i>	-1.5	0.735
full	0.1	<i>Omniscient</i>	-5.17	5.23
full	0.1	<i>REVISE</i>	$-3.06 \cdot 10^{26}$	$7.7 \cdot 10^{26}$
vanilla	0.1	<i>ECCo</i>	-9.33	7.32
vanilla	0.1	<i>Generic</i>	-8.88	6.86
vanilla	0.1	<i>Omniscient</i>	-8.69	6.9
vanilla	0.1	<i>REVISE</i>	-8.68	6.81
<b>full</b>	<b>0.5</b>	<b>ECCo</b>	<b>-1.12</b>	<b>0.217</b>
full	0.5	<i>Generic</i>	-1.21	0.352
full	0.5	<i>Omniscient</i>	-5.09	5.12
full	0.5	<i>REVISE</i>	$-5.97 \cdot 10^{27}$	$1.37 \cdot 10^{28}$
vanilla	0.5	<i>ECCo</i>	-9.35	7.3
vanilla	0.5	<i>Generic</i>	-8.89	6.92
vanilla	0.5	<i>Omniscient</i>	-8.68	6.93
vanilla	0.5	<i>REVISE</i>	-8.53	6.75
<b>full</b>	<b>1</b>	<b>ECCo</b>	<b>-1.1</b>	<b>0.163</b>
full	1	<i>Generic</i>	-1.49	0.726
full	1	<i>Omniscient</i>	-5.16	5.2
full	1	<i>REVISE</i>	$-3.09 \cdot 10^{26}$	$7.22 \cdot 10^{26}$
vanilla	1	<i>ECCo</i>	-9.34	7.36
vanilla	1	<i>Generic</i>	-8.86	6.85
vanilla	1	<i>Omniscient</i>	-8.7	6.9
vanilla	1	<i>REVISE</i>	-8.69	6.85
full	5	<i>ECCo</i>	-1.75	0.154
<b>full</b>	<b>5</b>	<b>Generic</b>	<b>-1.21</b>	<b>0.363</b>
full	5	<i>Omniscient</i>	-5.14	5.16
full	5	<i>REVISE</i>	$-1.1 \cdot 10^{28}$	$2.5 \cdot 10^{28}$
vanilla	5	<i>ECCo</i>	-9.36	7.32
vanilla	5	<i>Generic</i>	-8.88	6.91
vanilla	5	<i>Omniscient</i>	-8.7	6.93
vanilla	5	<i>REVISE</i>	-8.52	6.73
full	10	<i>ECCo</i>	$-1.02 \cdot 10^6$	$2.32 \cdot 10^6$
<b>full</b>	<b>10</b>	<b>Generic</b>	<b>-1.49</b>	<b>0.702</b>
full	10	<i>Omniscient</i>	-5.13	5.16
full	10	<i>REVISE</i>	$-3.74 \cdot 10^{26}$	$9.09 \cdot 10^{26}$
vanilla	10	<i>ECCo</i>	-9.31	7.33
vanilla	10	<i>Generic</i>	-8.87	6.86

Continuing table below.

<b>Objective</b>	$\lambda_{\text{div}}(\text{train})$	<b>Generator</b>	<b>Value</b>	<b>Std</b>
vanilla	10	<i>Omniscient</i>	-8.7	6.89
vanilla	10	<i>REVISE</i>	-8.69	6.83
full	15	<i>ECCo</i>	$-3.31 \cdot 10^{13}$	$7.54 \cdot 10^{13}$
<b>full</b>	<b>15</b>	<b>Generic</b>	<b>-1.22</b>	<b>0.37</b>
full	15	<i>Omniscient</i>	-5.2	5.23
full	15	<i>REVISE</i>	$-9.01 \cdot 10^{27}$	$2.06 \cdot 10^{28}$
vanilla	15	<i>ECCo</i>	-9.38	7.34
vanilla	15	<i>Generic</i>	-8.86	6.87
vanilla	15	<i>Omniscient</i>	-8.69	6.96
vanilla	15	<i>REVISE</i>	-8.51	6.73