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# COUNTERFACTUAL TRAINING: TEACHING MODELS PLAUSIBLE AND ACTIONABLE EXPLANATIONS

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## ABSTRACT

We propose a novel training regime called Counterfactual Training that leverages counterfactual explanations to increase the explanatory capacity of models. Counterfactual explanations have emerged as a popular post-hoc explanation method for opaque machine learning models: they inform how factual inputs would need to change in order for a model to produce some desired output. To be useful in real-word decision-making systems, counterfactuals should be plausible with respect to the underlying data and actionable with respect to stakeholder requirements. Much existing research has therefore focused on developing post-hoc methods to generate counterfactuals that meet these desiderata. In this work, we instead hold models directly accountable for this desired end goal: Counterfactual Training employs counterfactuals ad-hoc during the training phase to minimize the divergence between learned representations and plausible, actionable explanations. We demonstrate empirically and theoretically that our proposed method facilitates training models that deliver inherently desirable explanations while maintaining high predictive performance.

**Keywords** Counterfactual Training • Counterfactual Explanations • Algorithmic Recourse • 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)

18 models are tasked with learning these representations from scratch, guided by narrow objectives such as predictive  
 19 accuracy ([I. Goodfellow, Bengio, and Courville 2016](#)). Modern advances in computing have made it possible to  
 20 provide such models with ever greater degrees of freedom to achieve that task, which has often led them to outperform  
 21 traditionally more parsimonious models. Unfortunately, in doing so they also learn increasingly complex and highly  
 22 sensitive representations that we can no longer easily interpret.

23 This trend towards complexity for the sake of performance has come under serious scrutiny in recent years. At the very  
 24 cusp of the deep learning revolution, Szegedy et al. ([2013](#)) showed that artificial neural networks (ANN) are sensitive  
 25 to adversarial examples: counterfactuals of model inputs that yield vastly different model predictions despite being  
 26 “imperceptible” in that they are semantically indifferent from their factual counterparts. Despite partially effective  
 27 mitigation strategies such as **adversarial training** ([I. J. Goodfellow, Shlens, and Szegedy 2014](#)), truly robust deep  
 28 learning (DL) remains unattainable even for models that are considered shallow by today’s standards ([Kolter 2023](#)).

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

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

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

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

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

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

## 66 2 Related Literature

67 To the best of our knowledge, our proposed framework for counterfactual training represents the first attempt to use  
 68 counterfactual explanations during training to improve model explainability. In high-level terms, we define model

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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.

69 explainability as the extent to which valid explanations derived for an opaque model are also deemed plausible with  
 70 respect to the underlying data and stakeholder requirements. To make this more concrete, we follow Augustin, Meinke,  
 71 and Hein (2020) in tying the concept of explainability to the quality of counterfactual explanations that we can  
 72 generate for a given model. The authors show that counterfactual explanations—understood here as minimal input  
 73 perturbations that yield some desired model prediction—are generally more meaningful if the underlying model is  
 74 more robust to adversarial examples. We can make intuitive sense of this finding when looking at adversarial training  
 75 (AT) through the lens of representation learning with high degrees of freedom: by inducing models to “unlearn”  
 76 representations that are susceptible to worst-case counterfactuals (i.e. adversarial examples), AT effectively removes  
 77 some implausible explanations from the solution space.

## 78 2.1 Adversarial Examples are Counterfactual Explanations

79 This interpretation of the link between explainability through counterfactuals on one side, and robustness to adversarial  
 80 examples on the other, is backed by empirical evidence. Sauer and Geiger (2021) demonstrate that using counterfactual  
 81 images during classifier training improves model robustness. Similarly, Abbasnejad et al. (2020) argue that counter-  
 82 factuals represent potentially useful training data in machine learning, especially in supervised settings where inputs  
 83 may be reasonably mapped to multiple outputs. They, too, demonstrate the augmenting the training data of image  
 84 classifiers can improve generalization. Teney, Abbasnejad, and Hengel (2020) propose an approach using counterfac-  
 85 tuals in training that does not rely on data augmentation: they argue that counterfactual pairs typically already exist in  
 86 training datasets. Specifically, their approach relies on, firstly, identifying similar input samples with different annota-  
 87 tions and, secondly, ensuring that the gradient of the classifier aligns with the vector between pairs of counterfactual  
 88 inputs using the cosine distance as a loss function.

89 In the natural language processing (NLP) domain, counterfactuals have similarly been used to improve models through  
 90 data augmentation: Wu et al. (2021), propose *Polyjuice*, a general-purpose counterfactual generator for language mod-  
 91 els. They demonstrate empirically that augmenting training data through *Polyjuice* counterfactuals improves robust-  
 92 ness in a number of NLP tasks. Balashankar et al. (2023) also use *Polyjuice* to augment NLP datasets through diverse  
 93 counterfactuals and show that classifier robustness improves up to 20%. Finally, Luu and Inoue (2023) introduce  
 94 Counterfactual Adversarial Training (CAT), which also aims at improving generalization and robustness of language  
 95 models. Specifically, they propose to proceed as follows: firstly, they identify training samples that are subject to  
 96 high predictive uncertainty; secondly, they generate counterfactual explanations for those samples; and, finally, they  
 97 fine-tune the given language model on the augmented dataset that includes the generated counterfactuals.

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

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

## 116 2.2 Beyond Robustness

117 Improving the adversarial robustness of models is not the only path towards aligning representations with plausible  
 118 explanations. In a work closely related to this one, Altmeyer et al. (2024) show that explainability can be improved  
 119 through model averaging and refined model objectives. The authors propose a way to generate counterfactuals that  
 120 are maximally **faithful** to the model in that they are consistent with what the model has learned about the underlying  
 121 data. Formally, they rely on tools from energy-based modelling to minimize the divergence between the distribution  
 122 of counterfactuals and the conditional posterior over inputs learned by the model. Their proposed counterfactual  
 123 explainer, *ECCCo*, yields plausible explanations if and only if the underlying model has learned representations that

124 align with them. They find that both deep ensembles (Lakshminarayanan, Pritzel, and Blundell 2017) and joint energy-based models (JEMs) (Grathwohl et al. 2020) tend to do well in this regard.

125 Once again it helps to look at these findings through the lens of representation learning with high degrees of freedom.  
 126 Deep ensembles are approximate Bayesian model averages, which are most called for when models are underspecified  
 127 by the available data (Wilson 2020). Averaging across solutions mitigates the aforementioned risk of relying on a  
 128 single locally optimal representations that corresponds to semantically meaningless explanations for the data. Previous  
 129 work by Schut et al. (2021) similarly found that generating plausible (“interpretable”) counterfactual explanations is  
 130 almost trivial for deep ensembles that have also undergone adversarial training. The case for JEMs is even clearer:  
 131 they involve a hybrid objective that induces both high predictive performance and generative capacity (Grathwohl et al.  
 132 2020). This is closely related to the idea of aligning models with plausible explanations and has inspired our proposed  
 133 counterfactual training objective, as we explain in Section 3.

### 135 3 Counterfactual Training

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

149 **Definition 3.1** (Model Explainability). Let  $M_\theta : \mathcal{X} \mapsto \mathcal{Y}$  denote a supervised classification model that maps from the  
 150  $D$ -dimensional input space  $\mathcal{X}$  to representations  $\phi(\mathbf{x}; \theta)$  and finally to the  $K$ -dimensional output space  $\mathcal{Y}$ . Assume  
 151 that for any given input-output pair  $\{\mathbf{x}, \mathbf{y}\}_i$  there exists a counterfactual  $\mathbf{x}' = \mathbf{x} + \Delta : M_\theta(\mathbf{x}') = \mathbf{y}^+ \neq \mathbf{y} = M_\theta(\mathbf{x})$   
 152 where  $\arg \max_y \mathbf{y}^+ = y^+$  and  $y^+$  denotes the index of the target class.

153 We say that  $M_\theta$  is **explainable** to the extent that faithfully generated counterfactuals are plausible (i.e. consistent with  
 154 the data) and actionable. Formally, we define these properties as follows:

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

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

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

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

#### 164 3.1 Our Proposed Objective

165 Let  $\mathbf{x}'_t$  for  $t = 0, \dots, T$  denote a counterfactual explanation generated through gradient descent over  $T$  iterations  
 166 as initially proposed by Wachter, Mittelstadt, and Russell (2017). For our purposes, we let  $T$  vary and consider the  
 167 counterfactual search as converged as soon as the predicted probability for the target class has reached a pre-determined  
 168 threshold,  $\tau$ :  $S(M_\theta(\mathbf{x}'))[y^+] \geq \tau^2$ .

169 To train models with high explainability as defined in Definition 3.1, we propose to leverage counterfactuals in the  
 170 following objective,

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<sup>2</sup>For detailed background information on gradient-based counterfactual search and convergence see Section H.1.

$$\min_{\theta} \text{yloss}(\mathbf{M}_{\theta}(\mathbf{x}), \mathbf{y}) + \lambda_{\text{div}} \text{div}(\mathbf{x}, \mathbf{x}'_T, y; \theta) + \lambda_{\text{adv}} \text{advloss}(\mathbf{M}_{\theta}(\mathbf{x}'_{t \leq T}), \mathbf{y}) \quad (1)$$

171 where  $\text{yloss}(\cdot)$  is any conventional classification loss that induces discriminative performance (e.g. cross-entropy).  
 172 The two additional components in Equation 1 are explained in more detail below. For now, they can be sufficiently de-  
 173 scribed as inducing explainability directly and indirectly by penalizing: 1) the contrastive divergence,  $\text{div}(\cdot)$ , between  
 174 mature counterfactuals  $\mathbf{x}'_T$  and observed samples  $\mathbf{x}$  and, 2) the adversarial loss,  $\text{advloss}(\cdot)$ , with respect to nascent  
 175 counterfactuals  $\mathbf{x}'_{t \leq T}$ . The tradeoff between the different components can be governed by adjusting the strengths of  
 176 the penalties  $\lambda_{\text{div}}$  and  $\lambda_{\text{adv}}$ .

### 177 3.1.1 Directly Inducing Explainability through Contrastive Divergence

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

184 A key empirical finding in Altmeyer et al. (2024) was that JEMs tend to do well with respect to the plausibility objec-  
 185 tive in Definition 3.1. If we consider samples drawn from  $p_{\theta}(\mathbf{x})$  as counterfactuals, this is an expected finding, because  
 186 the JEM objective effectively minimizes the divergence between the conditional posterior and  $p(\mathbf{x}|y^+)$ . To generate  
 187 samples, Grathwohl et al. (2020) rely on Stochastic Gradient Langevin Dynamics (SGLD) using an uninformative  
 188 prior for initialization. This is where we depart from their methodology: instead of generating samples through SGLD,  
 189 we propose using counterfactual explainers to generate counterfactuals for observed training samples. Specifically, we  
 190 have

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

191 where  $\mathcal{E}_{\theta}(\cdot)$  denotes the energy function. In particular, we set  $\mathcal{E}_{\theta}(\mathbf{x}, y) = -\mathbf{M}_{\theta}(\mathbf{x}^+)[y^+]$  where  $y^+$  denotes the index  
 192 of the randomly drawn target class,  $y^+ \sim p(y)$ , and  $\mathbf{x}^+$  denotes an observed data point sampled from target domain:  
 193  $\mathbf{X}^+ = \{\mathbf{x} : y = y^+\}$ . Conditional on the target class  $y^+$ ,  $\mathbf{x}'_T$  denotes a mature counterfactual for a randomly sampled  
 194 factual from a non-target class generated through a gradient-based counterfactual generator for at most  $T$  iterations.  
 195 We define mature counterfactuals as those that have either exhausted  $T$  or reached convergence in terms of the pre-  
 196 determined decision threshold earlier.

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

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

### 206 3.1.2 Indirectly Inducing Explainability through Adversarial Robustness

207 Based on our analysis in Section 2, counterfactuals  $\mathbf{x}'$  can be repurposed as additional training samples (Luu and Inoue  
 208 2023; Balashankar et al. 2023) or adversarial examples (Freiesleben 2022; Pawelczyk et al. 2022). This leaves some  
 209 flexibility with respect to the exact choice for  $\text{advloss}(\cdot)$  in Equation 1. An intuitive functional form to use, though  
 210 likely not the only reasonable choice, is inspired by adversarial training:

$$\begin{aligned} \text{advloss}(\mathbf{M}_{\theta}(\mathbf{x}'_{t \leq T}), \mathbf{y}; \varepsilon) &= \text{yloss}(\mathbf{M}_{\theta}(\mathbf{x}'_{t_{\varepsilon}}), \mathbf{y}) \\ t_{\varepsilon} &= \max_t \{t : \|\Delta_t\|_{\infty} < \varepsilon\} \end{aligned} \quad (3)$$

211 Under this choice, we consider nascent counterfactuals  $\mathbf{x}'_{t \leq T}$  as adversarial examples as long as the magnitude of the  
 212 perturbation to any individual feature is at most  $\varepsilon$ . This is closely aligned with Szegedy et al. (2013), who define an  
 213 adversarial attack as an “imperceptible non-random perturbation”. Thus, we choose to work with a different distinction  
 214 between CE and AE than Freiesleben (2022), who considers misclassification as the key distinguishing feature of AE.

215 One of the key observations in this work is that we can leverage counterfactual explanations during training and get  
 216 adversarial examples, essentially for free.

217 **3.2 Encoding Actionability Constraints**

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

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

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

233 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  
 234 respect to feature  $d$ . Intuitively, we think of this simply in terms ignoring implausibility costs with respect to immutable  
 235 features, which effectively forces the model to instead seek plausibility with respect to the remaining features. This  
 236 in turn results in lower overall sensitivity to immutable features, which we demonstrate empirically for different  
 237 classifiers in Section 4. Under certain conditions, this results holds theoretically[For the proof, see the supplementary  
 238 appendix.]:

239 **Proposition 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  
 240 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  
 241 multivariate Gaussian class densities with common diagonal covariance matrix  $\Sigma_k = \Sigma$  for all  $k \in \mathcal{K}$ , then protecting  
 242 an immutable feature from the contrastive divergence penalty (Equation 2) will result in lower classifier sensitivity to  
 243 that feature relative to the remaining features, provided that at least one of those is mutable and discriminative.*

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

247 **3.3 Illustration**

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

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

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

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

263 In panel (c), we have used conventional training again, this time imposing the mutability constraint on *age* at test  
 264 time. Counterfactuals are valid but involve some substantial reductions in *debt* for some individuals, in particular  
 265 very young applicants. By comparison, counterfactual paths are shorter on average in panel (d), where we have used

266 counterfactual training and protected immutable features as described in Section 3.2. In particular, we observe that due  
 267 to the classifier's lower sensitivity to *age*, recourse recommendations with respect to *debt* are much more homogenous,  
 268 in that they do not disproportionately punish younger individuals. The counterfactuals are also plausible with respect  
 269 to the mutable feature. Thus, we consider the model in panel (d) as the most explainable according to Definition 3.1.

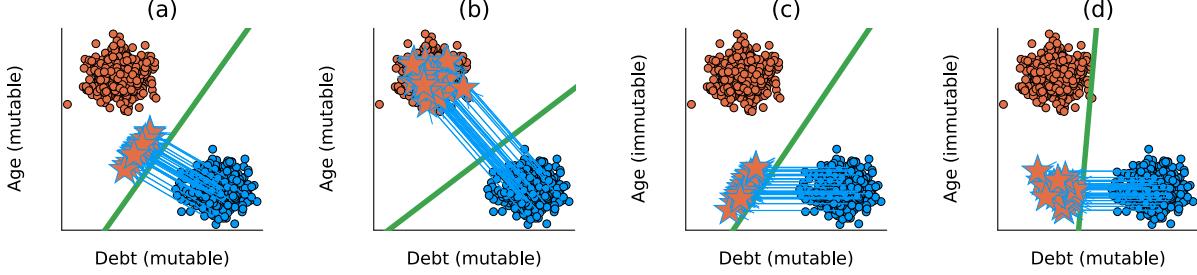


Figure 1: Visual illustration of how counterfactual training improves explainability. See Example 3.1 for details.

## 270 4 Experiments

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

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

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

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

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

### 279 4.1 Experimental Setup

#### 280 4.1.1 Evaluation

281 Our key outcome of interest is how well models perform with respect to explainability (Definition 3.1): to this end, we  
 282 focus primarily on the plausibility and cost of faithfully generated counterfactuals at test time. To measure the cost of  
 283 counterfactuals, we follow the standard convention of using distances ( $\ell_1$ -norm) between factuals and counterfactuals  
 284 as a proxy. For plausibility, we assess how similar counterfactuals are to observed samples in the target domain. We  
 285 rely on the distance-based metric used by Altmeyer et al. (2024),

$$\text{implaus}_{\text{dist}}(\mathbf{x}', \mathbf{X}^+) = \frac{1}{|\mathbf{X}^+|} \sum_{\mathbf{x} \in \mathbf{X}^+} \text{dist}(\mathbf{x}', \mathbf{x}) \quad (4)$$

286 and introduce a novel divergence metric,

$$\text{implaus}_{\text{div}}(\mathbf{X}', \mathbf{X}^+) = \text{MMD}(\mathbf{X}', \mathbf{X}^+) \quad (5)$$

287 where  $\mathbf{X}'$  denotes a set of multiple counterfactuals and  $\text{MMD}(\cdot)$  is an unbiased estimate of the squared population  
 288 maximum mean discrepancy (Gretton et al. 2012). The metric in Equation 5 is equal to zero iff  $\mathbf{X}' = \mathbf{X}^+$ .

289 In addition to cost and plausibility, we also compute other standard metrics to evaluate counterfactuals at test time in-  
 290 cluding validity and redundancy. Finally, we also assess the predictive performance of models using standard metrics.

### 291 4.2 Experimental Results

## 292 5 Discussion

### 293 5.1 Approach/Future Directions

- 294 1. Limited to classification models.
- 295 2. Training instabilities.
- 296 3. Hyperparameter sensitivity -> can we do better than grid search? (Bayes opt, ...)

297 **5.2 Limitations**

- 298     3. Proxy attributes of immutable features.  
 299     4. Increased training time.  
 300     5. Fairness and caveats (aware it's not a classical approach in this context, but there is a clear link).

301 **6 Conclusion**302 **References**

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396 **G Notation**

- 397 •  $y^+$ : The target class and also the index of the target class.  
 398 •  $y^-$ : The non-target class and also the index of non-the target class.  
 399 •  $\mathbf{y}^+$ : The one-hot encoded output vector for the target class.  
 400 •  $\theta$ : Model parameters (unspecified).  
 401 •  $\Theta$ : Matrix of parameters.

402 **G.1 Other Technical Details**

$$\begin{aligned} MMD(X', \tilde{X}') &= \frac{1}{m(m-1)} \sum_{i=1}^m \sum_{j \neq i}^m k(x_i, x_j) \\ &\quad + \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i}^n k(\tilde{x}_i, \tilde{x}_j) \\ &\quad - \frac{2}{mn} \sum_{i=1}^m \sum_{j=1}^n k(x_i, \tilde{x}_j) \end{aligned} \tag{6}$$

403 **H Technical Details of Our Approach**

404 **H.1 Generating Counterfactuals through Gradient Descent**

405 In this section, we provide some background on gradient-based counterfactual generators (Section H.1.1) and discuss  
 406 how we define convergence in this context (Section H.1.2).

407 **H.1.1 Background**

408 Gradient-based counterfactual search was originally proposed by Wachter, Mittelstadt, and Russell (2017). It generally  
 409 solves the following unconstrained objective,

$$\min_{\mathbf{z}' \in \mathcal{Z}^L} \{ \text{yloss}(\mathbf{M}_\theta(g(\mathbf{z}')), \mathbf{y}^+) + \lambda \text{cost}(g(\mathbf{z}')) \}$$

410 where  $g : \mathcal{Z} \mapsto \mathcal{X}$  is an invertible function that maps from the  $L$ -dimensional counterfactual state space to the  
 411 feature space and  $\text{cost}(\cdot)$  denotes one or more penalties that are used to induce certain properties of the counterfactual  
 412 outcome. As above,  $\mathbf{y}^+$  denotes the target output and  $\mathbf{M}_\theta(\mathbf{x})$  returns the logit predictions of the underlying classifier  
 413 for  $\mathbf{x} = g(\mathbf{z})$ .

414 For all generators used in this work we use standard logit crossentropy loss for  $\text{ylloss}(\cdot)$ . All generators also penalize  
 415 the distance ( $\ell_1$ -norm) of counterfactuals from their original factual state. For *Generic* and *ECCo*, we have  $\mathcal{Z} := \mathcal{X}$   
 416 and  $g(\mathbf{z}) = g(\mathbf{z})^{-1} = \mathbf{z}$ , that is counterfactual are searched directly in the feature space. Conversely, *REVISE* traverses  
 417 the latent space of a variational autoencoder (VAE) fitted to the training data, where  $g(\cdot)$  corresponds to the decoder  
 418 (Joshi et al. 2019). In addition to the distance penalty, *ECCo* uses an additional penalty component that regularizes  
 419 the energy associated with the counterfactual,  $\mathbf{x}'$  (Altmeyer et al. 2024).

420 **H.1.2 Convergence**

421 An important consideration when generating counterfactual explanations using gradient-based methods is how to  
 422 define convergence. Two common choices are to 1) perform gradient descent over a fixed number of iterations  $T$ , or  
 423 2) conclude the search as soon as the predicted probability for the target class has reached a pre-determined threshold,  
 424  $\tau$ :  $\mathcal{S}(\mathbf{M}_\theta(\mathbf{x}'))[y^+] \geq \tau$ . We prefer the latter for our purposes, because it explicitly defines convergence in terms of the  
 425 black-box model,  $\mathbf{M}(\mathbf{x})$ .

426 Defining convergence in this way allows for a more intuitive interpretation of the resulting counterfactual outcomes  
 427 than with fixed  $T$ . Specifically, it allows us to think of counterfactuals as explaining ‘high-confidence’ predictions by  
 428 the model for the target class  $y^+$ . Depending on the context and application, different choices of  $\tau$  can be considered  
 429 as representing ‘high-confidence’ predictions.

430 **H.2 Protecting Mutability Constraints with Linear Classifiers**

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

435 *Proof.* Let  $d_{\text{mtbl}}$  and  $d_{\text{immtbl}}$  denote some mutable and immutable feature, respectively. Suppose that  $\mu_{y^-, d_{\text{immtbl}}} <$   
 436  $\mu_{y^+, d_{\text{immtbl}}}$  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,  
 437 we assume that the immutable feature tends to take lower values for samples in the non-target class  $y^-$  than in the  
 438 target class  $y^+$ . We assume the opposite to hold for the mutable feature.

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

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \mathbf{x}^\top \Sigma^{-1} (\mu_k - \mu_m) + \text{const} \quad (7)$$

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

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \sum_{d=1}^D \frac{\mu_{k,d} - \mu_{m,d}}{\sigma_d^2} x_d + \text{const} \quad (8)$$

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

$$\log \frac{p(k|\mathbf{x})}{p(m|\mathbf{x})} = \sum_{d=1}^D (\theta_{k,d} - \theta_{m,d}) x_d + \text{const} \quad (9)$$

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

444 Based on Equation 8 and Equation 9 we can identify that  $(\mu_{k,d} - \mu_{m,d}) \propto (\theta_{k,d} - \theta_{m,d})$  under the assumptions we  
 445 made above. Hence, we have that  $(\theta_{y^-, d_{\text{immtbl}}} - \theta_{y^+, d_{\text{immtbl}}}) < 0$  and  $(\theta_{y^-, d_{\text{mtbl}}} - \theta_{y^+, d_{\text{mtbl}}}) > 0$

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

$$\frac{\partial}{\partial \theta_{y^+, d}} (\text{div}(\mathbf{x}, \mathbf{x}', \mathbf{y}; \theta)) = \frac{\partial}{\partial \theta_{y^+, d}} ((-\mathbf{M}_\theta(\mathbf{x})[y^+]) - (-\mathbf{M}_\theta(\mathbf{x}')[y^+])) = x'_d - x_d \quad (10)$$

449 and equal to zero everywhere else.

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

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

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

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

### 462 H.3 Domain Constraints

463 We apply domain constraints on counterfactuals during training and evaluation. There are at least two good reasons for  
 464 doing so. Firstly, within the context of explainability and algorithmic recourse, real-world attributes are often domain  
 465 constrained: the *age* feature, for example, is lower bounded by zero and upper bounded by the maximum human  
 466 lifespan. Secondly, domain constraints help mitigate training instabilities commonly associated with energy-based  
 467 modelling (Grathwohl et al. 2020; Altmeyer et al. 2024).

468 For our image datasets, features are pixel values and hence the domain is constrained by the lower and upper bound  
 469 of values that pixels can take depending on how they are scaled (in our case  $[-1, 1]$ ). For all other features  $d$  in our  
 470 synthetic and tabular datasets, we automatically infer domain constraints  $[x_d^{\text{LB}}, x_d^{\text{UB}}]$  as follows,

$$\begin{aligned} x_d^{\text{LB}} &= \arg \min_{x_d} \{\mu_d - n_{\sigma_d} \sigma_d, \arg \min_{x_d} x_d\} \\ x_d^{\text{UB}} &= \arg \max_{x_d} \{\mu_d + n_{\sigma_d} \sigma_d, \arg \max_{x_d} x_d\} \end{aligned} \quad (11)$$

471 where  $\mu_d$  and  $\sigma_d$  denote the sample mean and standard deviation of feature  $d$ . We set  $n_{\sigma_d} = 3$  across the board but  
 472 higher values and hence wider bounds may be appropriate depending on the application.

#### 473 H.4 Training Details

474 In this section, we describe the training procedure in detail. While the details laid out here are not crucial for under-  
 475 standing our proposed approach, they are of importance to anyone looking to implement counterfactual training.

## 476 I Detailed Results

### 477 I.1 Qualitative Findings for Image Data

Note

Figure A2 shows much more plausible (faithful) counterfactuals for a model with CT than the model with conventional training (Figure A3). 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.

478

### 479 I.2 Grid Searches

480 To assess the hyperparameter sensitivity of our proposed training regime we ran multiple large grid searches for all of  
 481 our synthetic datasets. We have grouped these grid searches into multiple categories:

- 482 1. **Generator Parameters** (Section I.2.2): Investigates the effect of changing hyperparameters that affect the  
 483 counterfactual outcomes during the training phase.
- 484 2. **Penalty Strengths** (Section I.2.3): Investigates the effect of changing the penalty strengths in our proposed  
 485 objective (Equation 1).
- 486 3. **Other Parameters** (Section I.2.4): Investigates the effect of changing other training parameters, including  
 487 the total number of generated counterfactuals in each epoch.

488 We begin by summarizing the high-level findings in Section I.2.1.2. For each of the categories, Section I.2.2 to  
 489 Section I.2.4 then present all details including the exact parameter grids, average predictive performance outcomes  
 490 and key evaluation metrics for the generated counterfactuals.

#### 491 I.2.1 Evaluation Details

492 To measure predictive performance, we compute the accuracy and F1-score for all models on test data (Table A1,  
 493 Table A2, Table A3). With respect to explanatory performance, we report here our findings for the (im)plausibility  
 494 and cost of counterfactuals at test time. Since the computation of our proposed divergence metric (Equation 5) is  
 495 memory-intensive, we rely on the distance-based metric for the grid searches. For the counterfactual evaluation, we  
 496 draw factual samples from the training data for the grid searches to avoid data leakage with respect to our final results  
 497 reported in the body of the paper. Specifically, we want to avoid choosing our default hyperparameters based on results  
 498 on the test data. Since we are optimizing for explainability, not predictive performance, we still present test accuracy  
 499 and F1-scores.

500 **I.2.1.1 Predictive Performance** We find that CT is associated with little to no decrease in average predictive  
 501 performance for our synthetic datasets: test accuracy and F1-scores decrease by at most ~1 percentage point, but  
 502 generally much less (Table A1, Table A2, Table A3). Variation across hyperparameters is negligible as indicated by  
 503 small standard deviations for these metrics across the board.

504 **I.2.1.2 Counterfactual Outcomes** Overall, we find that Counterfactual Training (CT) achieves its key objectives  
 505 consistently across all hyperparameter settings and also broadly across datasets: plausibility is improved by up to  
 506 ~60 percentage points (ppts) for the *Circles* data (e.g. Figure A4), ~25-30ppts for the *Moons* data (e.g. Figure A6)  
 507 and ~10-20ppts for the *Linearly Separable* data (e.g. Figure A5). At the same time, the average costs of faithful

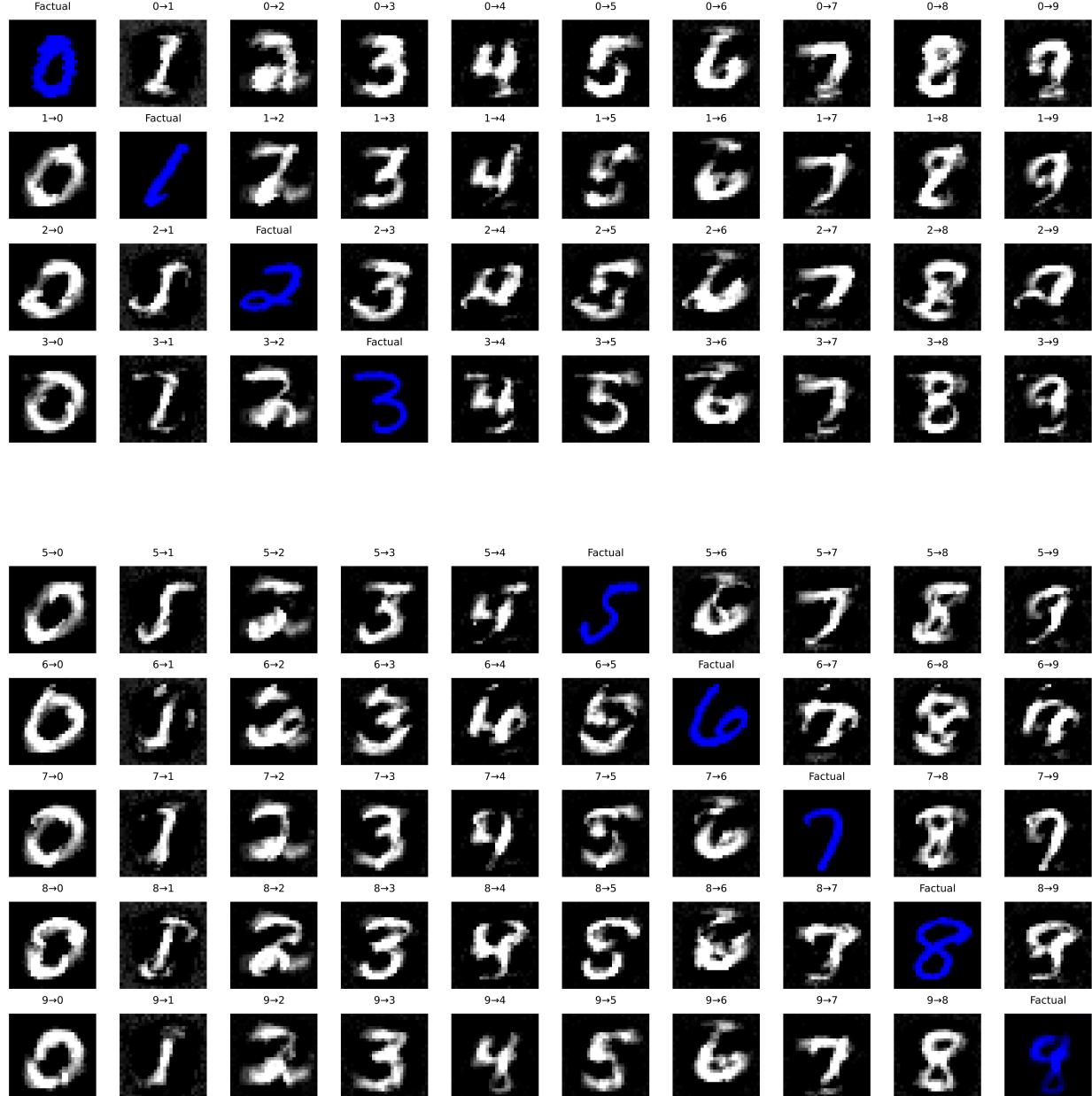


Figure A2: Counterfactual images for *MLP* with counterfactual training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

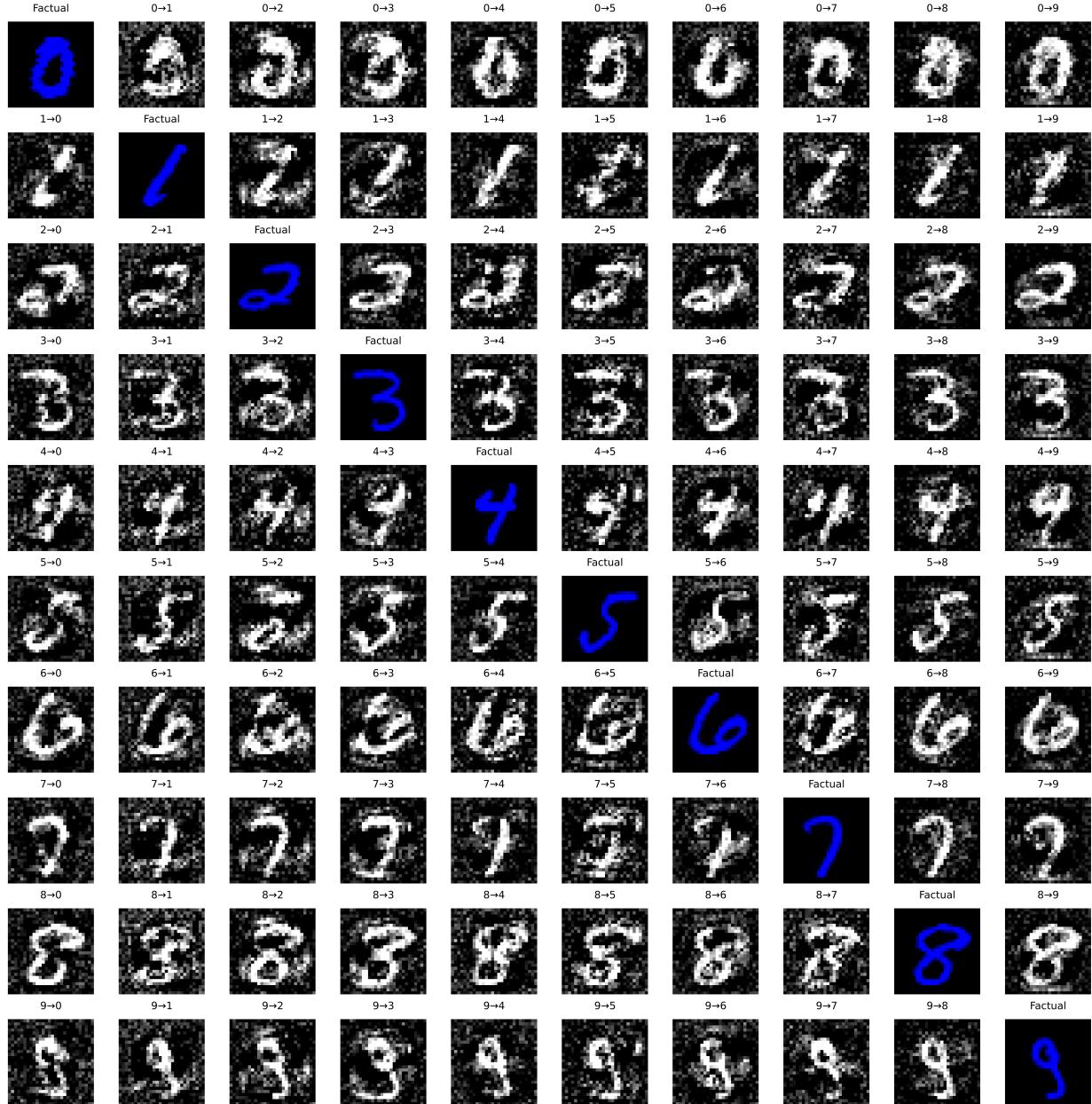


Figure A3: Counterfactual images for *MLP* with conventional training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

508 counterfactuals are reduced in many cases by around ~20-25ppts for *Circles* (e.g. Figure A8) and up to ~50ppts for  
 509 *Moons* (e.g. Figure A10). For the *Linearly Separable* data, costs are generally increased although typically by less  
 510 than 10ppts (e.g. Figure A9), which reflects a common tradeoff between costs and plausibility (Altmeyer et al. 2024).

511 We do observe strong sensitivity to certain hyperparameters, with clear and manageable patterns. Concerning generator  
 512 parameters, we firstly find that using *REVISE* to generate counterfactuals during training typically yields the worst  
 513 outcomes out of all generators, often leading to a substantial decrease in plausibility. This finding can be attributed to  
 514 the fact that *REVISE* effectively assigns the task of learning plausible explanations from the model itself to a surrogate  
 515 VAE. In other words, counterfactuals generated by *REVISE* are less faithful to the model than *ECCo* and *Generic*, and  
 516 hence we would expect them to be a less effective and, in fact, potentially detrimental role in our training regime.  
 517 Secondly, we observe that allowing for a higher number of maximum steps  $T$  for the counterfactual search generally  
 518 yields better outcomes. This is intuitive, because it allows more counterfactuals to reach maturity in any given iteration.  
 519 Looking in particular at the results for *Linearly Separable*, it seems that higher values for  $T$  in combination with higher  
 520 decision thresholds ( $\tau$ ) yields the best results when using *ECCo*. But depending on the degree of class separability  
 521 of the underlying data, a high decision-threshold can also affect results adversely, as evident from the results for  
 522 the *Overlapping* data (Figure A7): here we find that CT generally fails to achieve its objective because only a tiny  
 523 proportion of counterfactuals ever reaches maturity.

524 Regarding penalty strengths, we find that the strength of the energy regularization,  $\lambda_{\text{reg}}$  is a key hyperparameter, while  
 525 sensitivity with respect to  $\lambda_{\text{div}}$  and  $\lambda_{\text{adv}}$  is much less evident. In particular, we observe that not regularizing energy  
 526 enough or at all typically leads to poor performance in terms of decreased plausibility and increased costs, in particular  
 527 for *Circles* (Figure A12), *Linearly Separable* (Figure A13) and *Overlapping* (Figure A15). High values of  $\lambda_{\text{reg}}$  can  
 528 increase the variability in outcomes, in particular when combined with high values for  $\lambda_{\text{div}}$  and  $\lambda_{\text{adv}}$ , but this effect is  
 529 less pronounced.

530 Finally, concerning other hyperparameters we observe that the effectiveness and stability of CT is positively associated  
 531 with the number of counterfactuals generated during each training epoch, in particular for *Circles* (Figure A20) and  
 532 *Moons* (Figure A22). We further find that a higher number of training epochs is beneficial as expected, where we  
 533 tested training models for 50 and 100 epochs. Interestingly, we find that it is not necessary to employ CT during  
 534 the entire training phase to achieve the desired improvements in explainability: specifically, we have tested training  
 535 models conventionally during the first half of training before switching to CT after this initial burn-in period.

### 536 I.2.2 Generator Parameters

537 The hyperparameter grid with varying generator parameters during training is shown in Note 1. The corresponding  
 538 evaluation grid used for these experiments is shown in Note 2.

#### Note 1: Training Phase

- Generator Parameters:
  - Decision Threshold: 0.75, 0.9, 0.95
  - $\lambda_{\text{energy}}$ : 0.1, 0.5, 5.0, 10.0, 20.0
  - Maximum Iterations: 5, 25, 50
- Generator: *ecco*, *generic*, *revise*
- Model: *mlp*
- Training Parameters:
  - Objective: *full*, *vanilla*

539

#### Note 2: Evaluation Phase

- Generator Parameters:
  - $\lambda_{\text{energy}}$ : 0.1, 0.5, 1.0, 5.0, 10.0

540

### 541 I.2.2.1 Accuracy

Table A1: Predictive performance measures by dataset and objective averaged across training-phase parameters (Note 1) and evaluation-phase parameters (Note 2).

Dataset	Variable	Objective	Mean	Std
Circles	Accuracy	Full	0.997	0.00309
Circles	Accuracy	Vanilla	0.998	0.000557
Circles	F1-score	Full	0.997	0.00309
Circles	F1-score	Vanilla	0.998	0.000558
Lin Sep	Accuracy	Full	0.999	0.00201
Lin Sep	Accuracy	Vanilla	1	0
Lin Sep	F1-score	Full	0.999	0.00201
Lin Sep	F1-score	Vanilla	1	0
Moons	Accuracy	Full	0.999	0.000696
Moons	Accuracy	Vanilla	1	0.00111
Moons	F1-score	Full	0.999	0.000696
Moons	F1-score	Vanilla	1	0.00111
Over	Accuracy	Full	0.915	0.00477
Over	Accuracy	Vanilla	0.917	0.00123
Over	F1-score	Full	0.915	0.00478
Over	F1-score	Vanilla	0.917	0.00124

542 **I.2.2.2 Plausibility** The results with respect to the plausibility measure are shown in Figure A4 to Figure A7.

543 **I.2.2.3 Cost** The results with respect to the cost measure are shown in Figure A8 to Figure A11.

### 544 **I.2.3 Penalty Strengths**

545 The hyperparameter grid with varying penalty strengths during training is shown in Note 3. The corresponding eval-  
546 uation grid used for these experiments is shown in Note 4.

#### Note 3: Training Phase

- Generator: `ecco`, `generic`, `revise`
- Model: `mlp`
- Training Parameters:
  - $\lambda_{\text{adv}}$ : 0.1, 0.25, 1.0
  - $\lambda_{\text{div}}$ : 0.01, 0.1, 1.0
  - $\lambda_{\text{reg}}$ : 0.0, 0.01, 0.1, 0.25, 0.5
  - Objective: `full`, `vanilla`

547

#### Note 4: Evaluation Phase

- Generator Parameters:
  - $\lambda_{\text{energy}}$ : 0.1, 0.5, 1.0, 5.0, 10.0

548

### 549 **I.2.3.1 Accuracy**

Table A2: Predictive performance measures by dataset and objective averaged across training-phase parameters (Note 3) and evaluation-phase parameters (Note 4).

Dataset	Variable	Objective	Mean	Std
Circles	Accuracy	Full	0.994	0.0144
Circles	Accuracy	Vanilla	0.998	0.000875
Circles	F1-score	Full	0.994	0.0145
Circles	F1-score	Vanilla	0.998	0.000875
Lin Sep	Accuracy	Full	0.998	0.00772

Continuing table below.

<b>Dataset</b>	<b>Variable</b>	<b>Objective</b>	<b>Mean</b>	<b>Std</b>
Lin Sep	Accuracy	Vanilla	1	0
Lin Sep	F1-score	Full	0.998	0.00773
Lin Sep	F1-score	Vanilla	1	0
Moons	Accuracy	Full	0.987	0.0351
Moons	Accuracy	Vanilla	0.998	0.0101
Moons	F1-score	Full	0.987	0.0352
Moons	F1-score	Vanilla	0.998	0.0102
Over	Accuracy	Full	0.911	0.0217
Over	Accuracy	Vanilla	0.916	0.00236
Over	F1-score	Full	0.911	0.0219
Over	F1-score	Vanilla	0.916	0.00236

550 **I.2.3.2 Plausibility** The results with respect to the plausibility measure are shown in Figure A12 to Figure A15.

551 **I.2.3.3 Cost** The results with respect to the cost measure are shown in Figure A16 to Figure A19.

552 **I.2.4 Other Parameters**

553 The hyperparameter grid with other varying training parameters is shown in Note 5. The corresponding evaluation  
554 grid used for these experiments is shown in Note 6.

Note 5: Training Phase

- Generator: `ecco`, `generic`, `revise`
- Model: `mlp`
- Training Parameters:
  - Burnin: 0.0, 0.5
  - No. Counterfactuals: 100, 1000
  - No. Epochs: 50, 100
  - Objective: `full`, `vanilla`

555

Note 6: Evaluation Phase

- Generator Parameters:
  - $\lambda_{\text{energy}}$ : 0.1, 0.5, 1.0, 5.0, 10.0

556

557 **I.2.4.1 Accuracy**

Table A3: Predictive performance measures by dataset and objective averaged across training-phase parameters (Note 5) and evaluation-phase parameters (Note 6).

<b>Dataset</b>	<b>Variable</b>	<b>Objective</b>	<b>Mean</b>	<b>Std</b>
Circles	Accuracy	Full	0.995	0.00431
Circles	Accuracy	Vanilla	0.998	0.000566
Circles	F1-score	Full	0.995	0.00432
Circles	F1-score	Vanilla	0.998	0.000566
Lin Sep	Accuracy	Full	0.999	0.00231
Lin Sep	Accuracy	Vanilla	1	0
Lin Sep	F1-score	Full	0.999	0.00231
Lin Sep	F1-score	Vanilla	1	0
Moons	Accuracy	Full	0.996	0.0136
Moons	Accuracy	Vanilla	0.988	0.022
Moons	F1-score	Full	0.996	0.0136
Moons	F1-score	Vanilla	0.988	0.022

Continuing table below.

Dataset	Variable	Objective	Mean	Std
Over	Accuracy	Full	0.914	0.00563
Over	Accuracy	Vanilla	0.918	0.00116
Over	F1-score	Full	0.914	0.0057
Over	F1-score	Vanilla	0.918	0.00116

558 **I.2.4.2 Plausibility** The results with respect to the plausibility measure are shown in Figure A20 to Figure A23.

559 **I.2.4.3 Cost** The results with respect to the cost measure are shown in Figure A24 to Figure A27.

### 560 I.3 Hyperparameter Tuning

561 Based on the findings from our initial large grid searches (Section I.2), we tune selected hyperparameters for all  
 562 datasets: namely, the decision threshold  $\tau$  and the strength of the energy regularization  $\lambda_{\text{reg}}$ . The final hyperparameter  
 563 choices for each dataset are presented in **ADD TABLE**. Detailed results for each data set are shown in Figure A28  
 564 to Figure A45. From **ADD TABLE**, we notice that the same decision threshold of  $\tau = 0.5$  is optimal for all but one  
 565 dataset. We attribute this to the fact that a low decision threshold results in a higher share of mature counterfactuals  
 566 and hence more opportunities for the model to learn from examples (Figure A37 to Figure A45). This has played  
 567 a role in particular for our real-world tabular datasets and MNIST, which suffered from low levels of maturity for  
 568 higher decision thresholds. In cases where maturity is not an issue, as for *Moons*, higher decision thresholds lead to  
 569 better outcomes, which may have to do with the fact that the resulting counterfactuals are more faithful to the model.  
 570 Concerning the regularization strength, we find somewhat high variation across datasets. Most notably, we find that  
 571 relatively low levels of regularization are optimal for MNIST. We hypothesize that this finding may be attributed to  
 572 the uniform scaling of all input features (digits). Finally, to increase the proportion of mature counterfactuals for some  
 573 datasets, we have also investigated the effect on the learning rate  $\eta$  for the counterfactual search, but found little effect  
 574 on the results.

#### Package Version (Reproducibility)

Tuning was run using v1.1.3 of TaijaData. The follow-up version v1.1.4 introduced an option to split real-world tabular datasets into train and test set, ensuring that pre-processing steps like standardization is fit on the training set only. If you are rerunning the tuning experiments with a version of TaijaData that is higher than v1.1.3, than for the default parameters specified in the configuration files, you may end up with slightly different results, although we would not expect any changes in terms of qualitative findings. For exact reproducibility, please use v1.1.3.

575

#### 576 I.3.1 Key Parameters

577 The hyperparameter grid for tuning key parameters is shown in Note 7. The corresponding evaluation grid used for  
 578 these experiments is shown in Note 8.

#### Note 7: Training Phase

- Generator Parameters:
  - Decision Threshold: 0.5, 0.75, 0.9
- Model: mlp
- Training Parameters:
  - $\lambda_{\text{reg}}$ : 0.1, 0.25, 0.5
  - Objective: full, vanilla

579

#### Note 8: Evaluation Phase

- Generator Parameters:
  - $\lambda_{\text{energy}}$ : 0.1, 0.5, 1.0, 5.0, 10.0

580

581 **I.3.1.1 Plausibility** The results with respect to the plausibility measure are shown in Figure A28 to Figure A36.

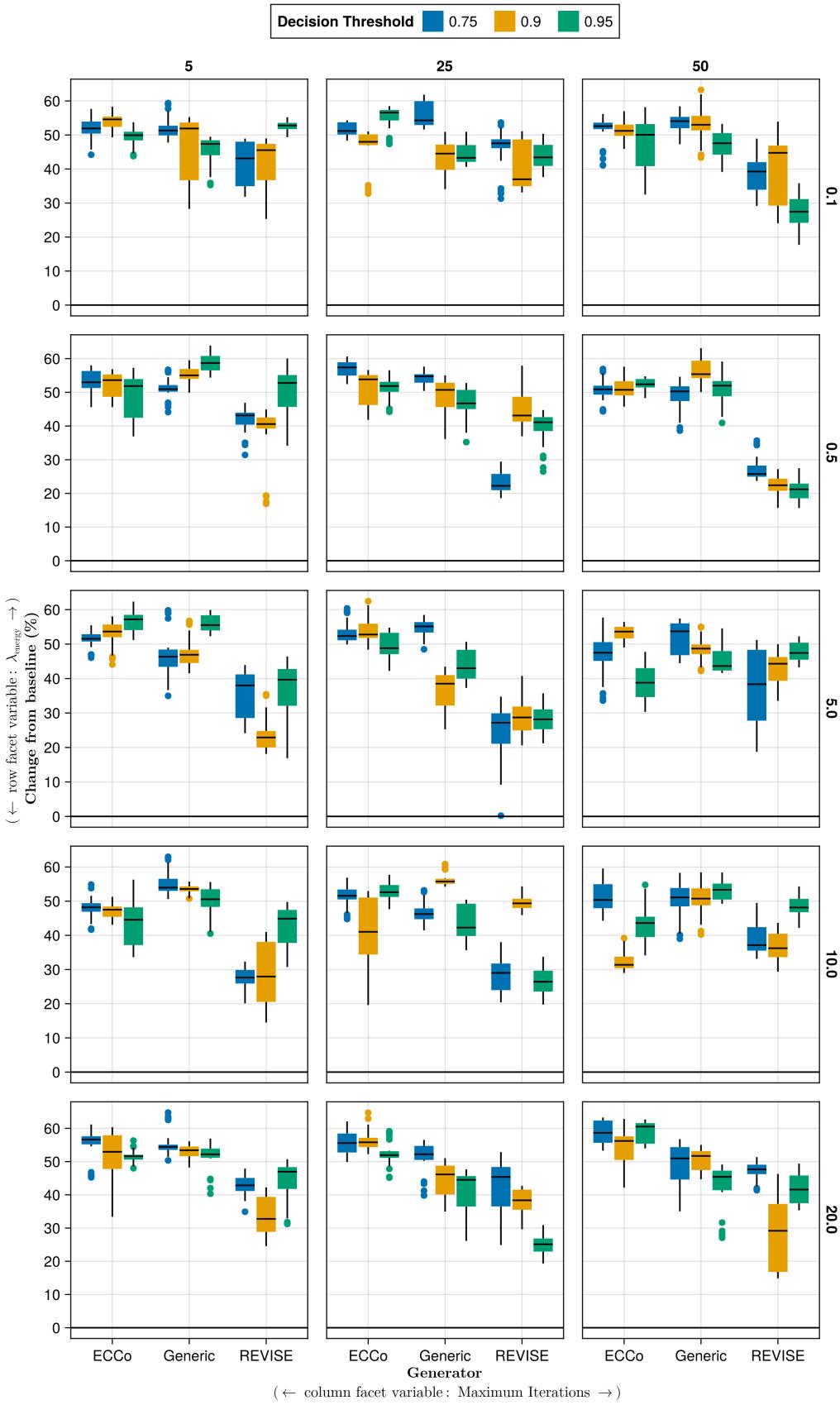


Figure A4: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

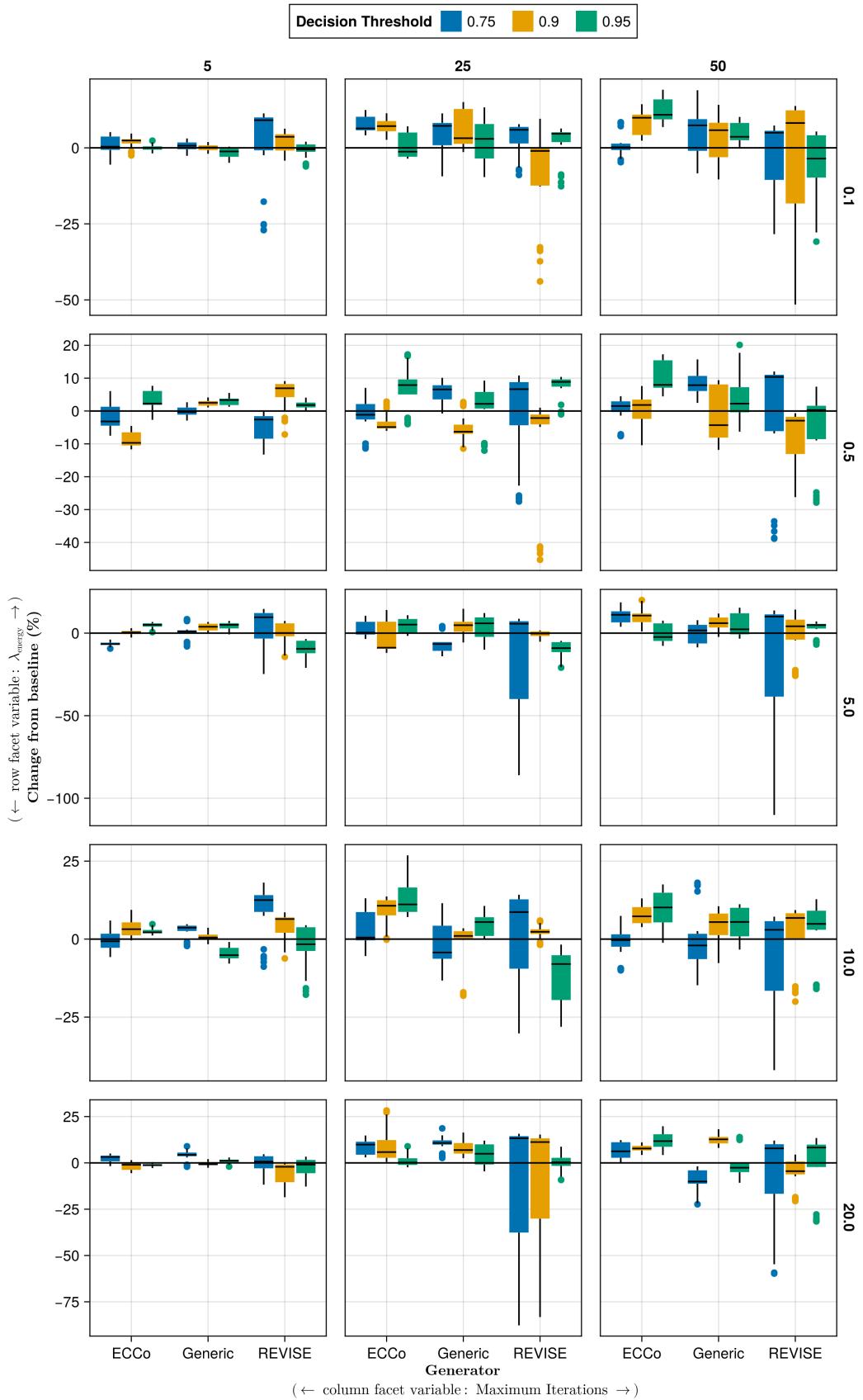


Figure A5: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

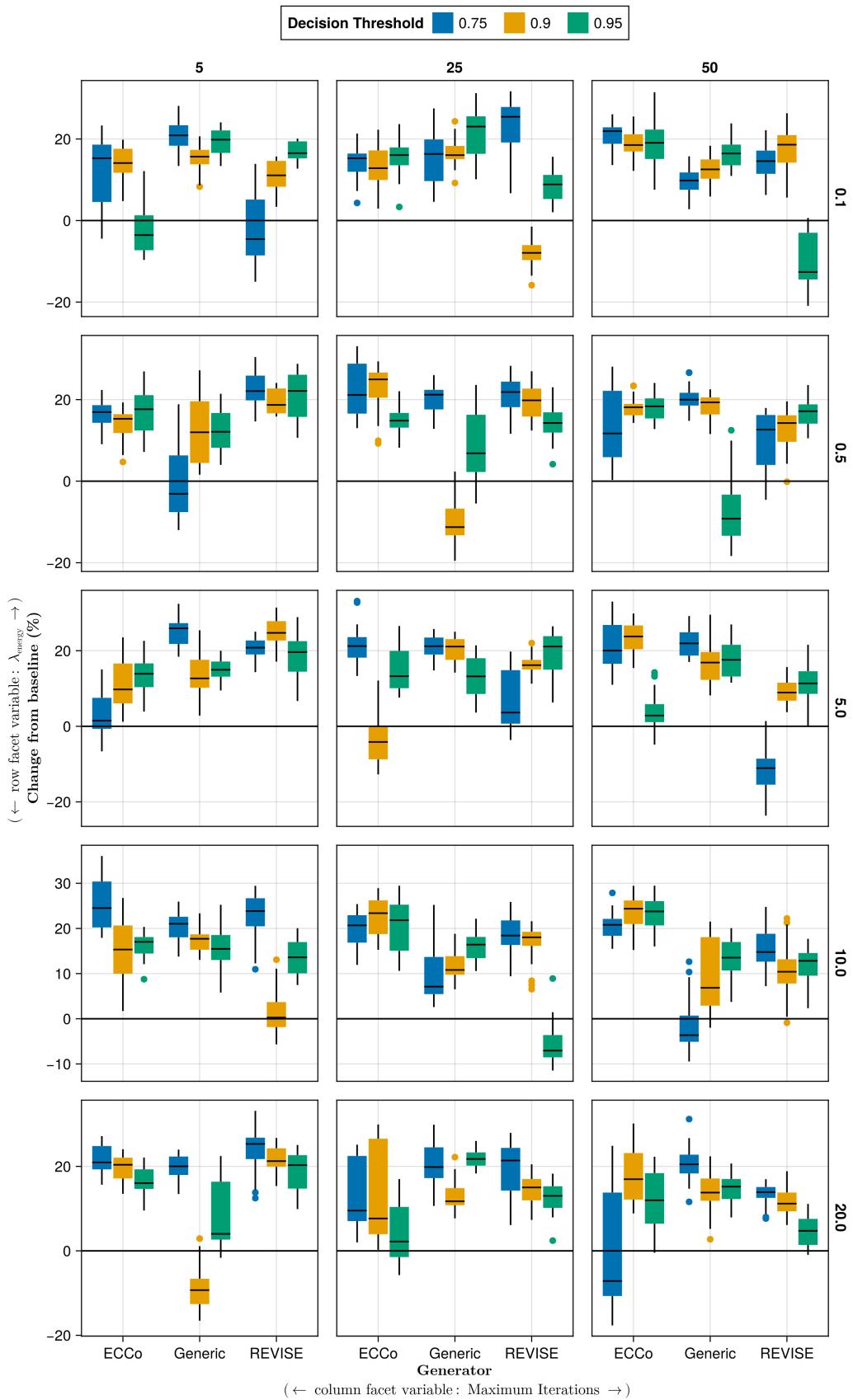


Figure A6: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

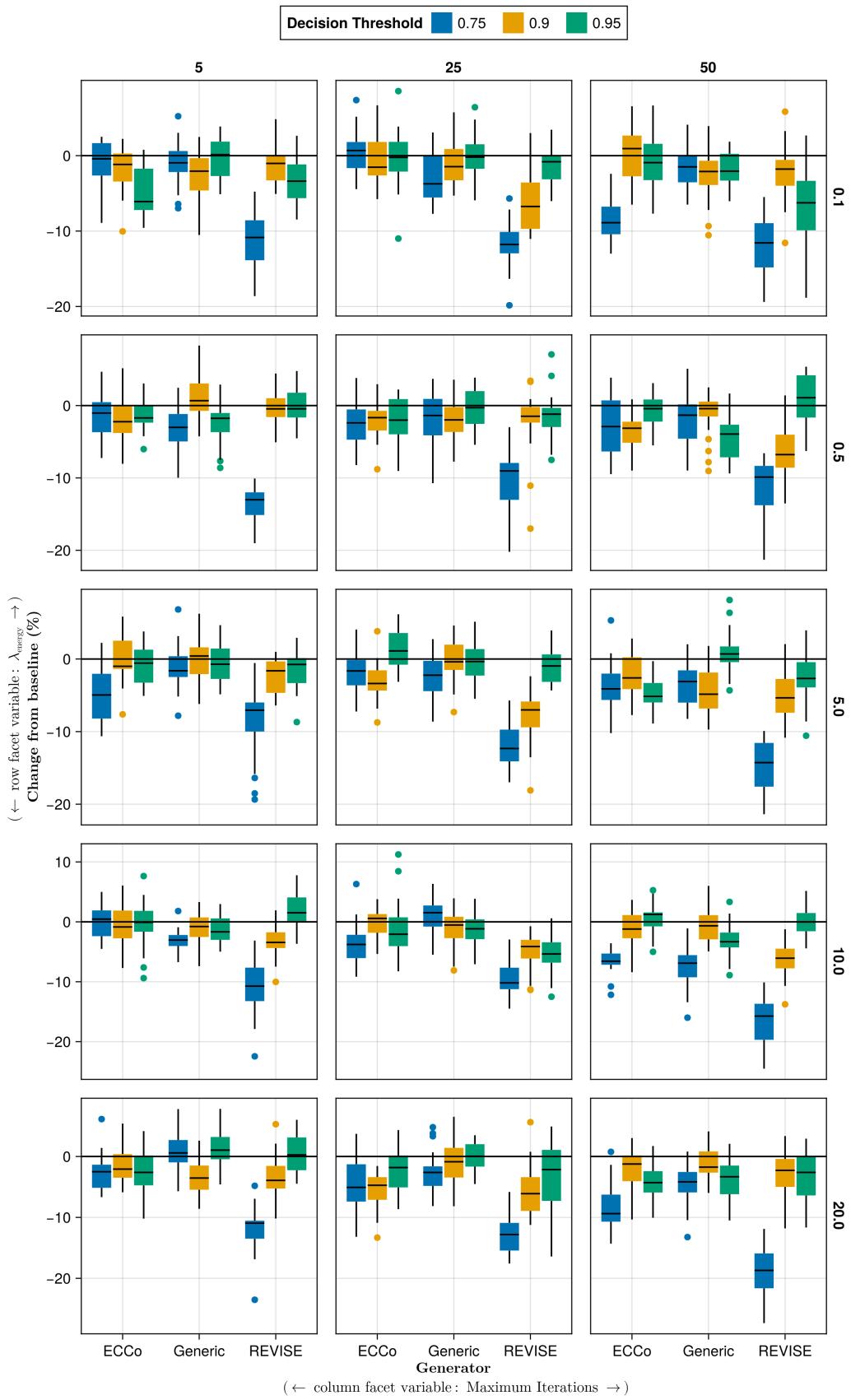


Figure A7: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

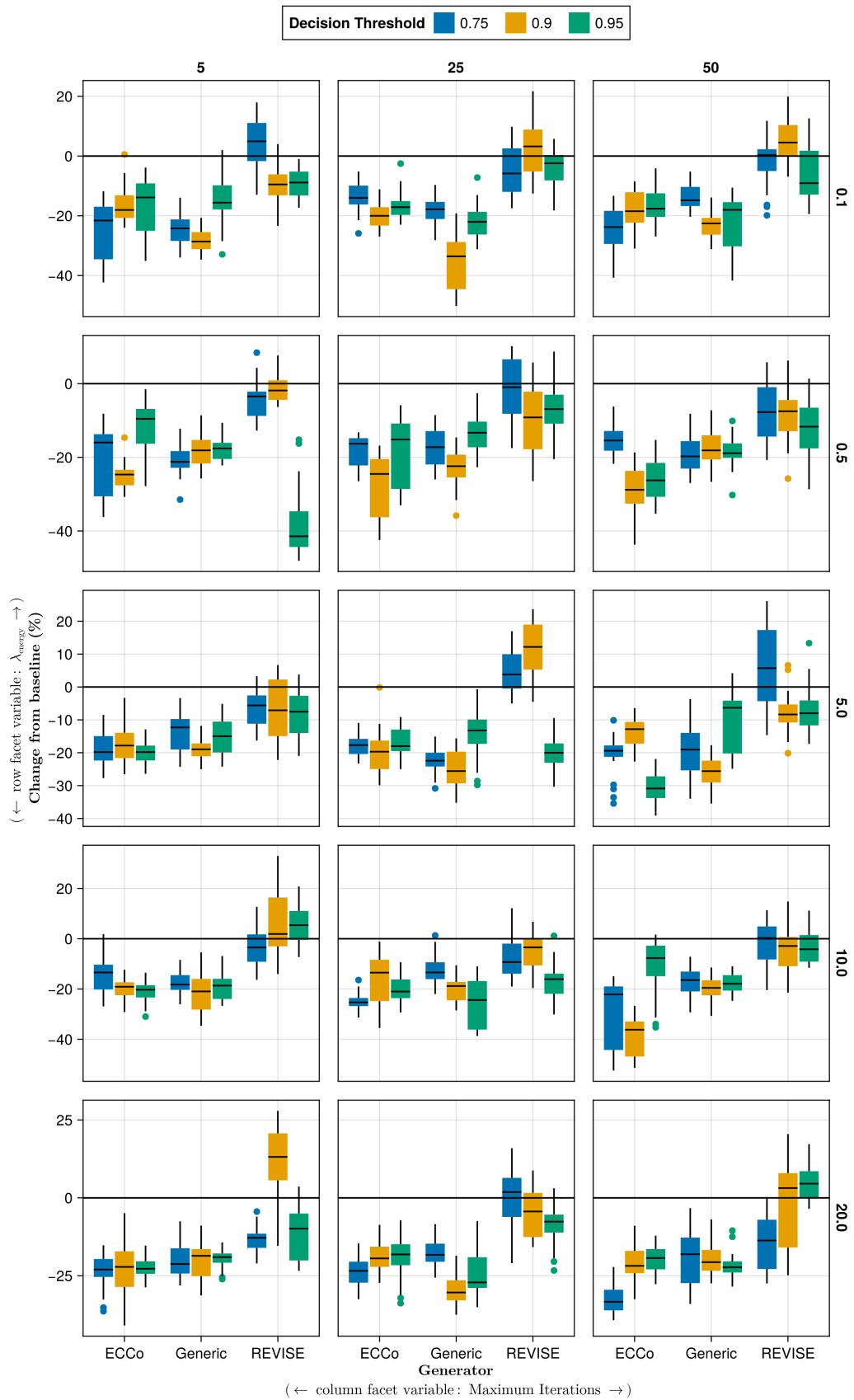


Figure A8: Average outcomes for the cost measure across hyperparameters. Data: Circles.

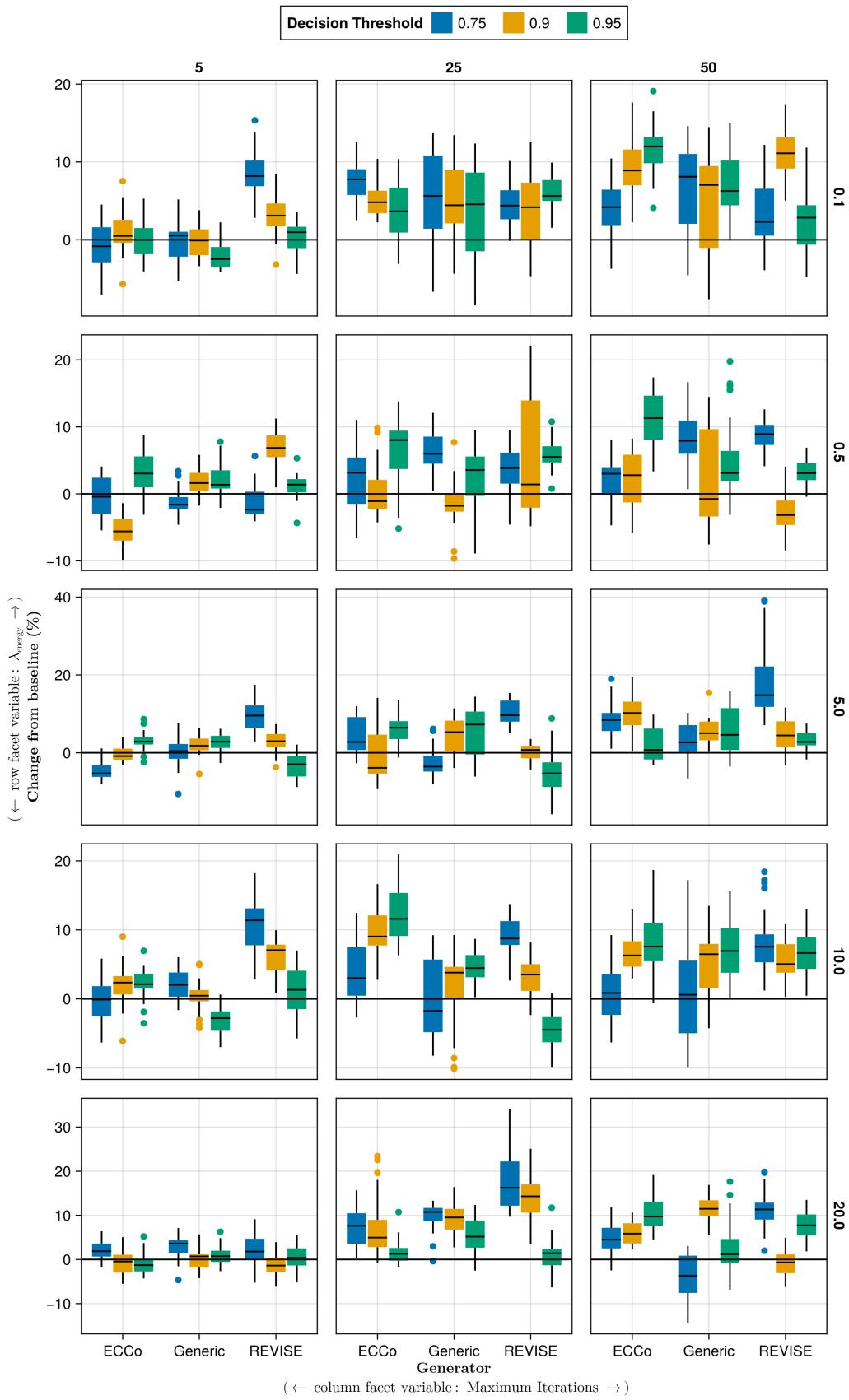


Figure A9: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

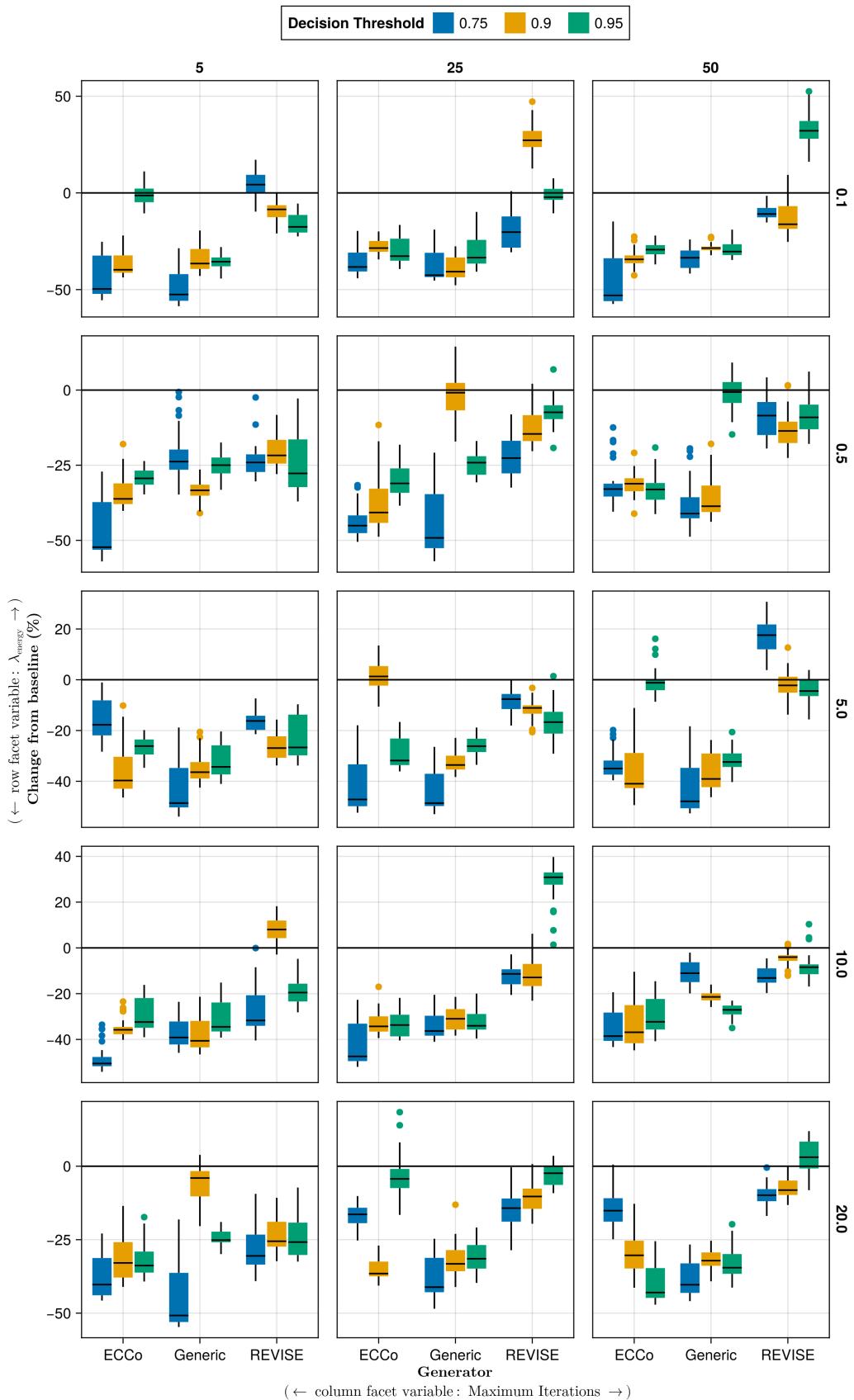


Figure A10: Average outcomes for the cost measure across hyperparameters. Data: Moons.

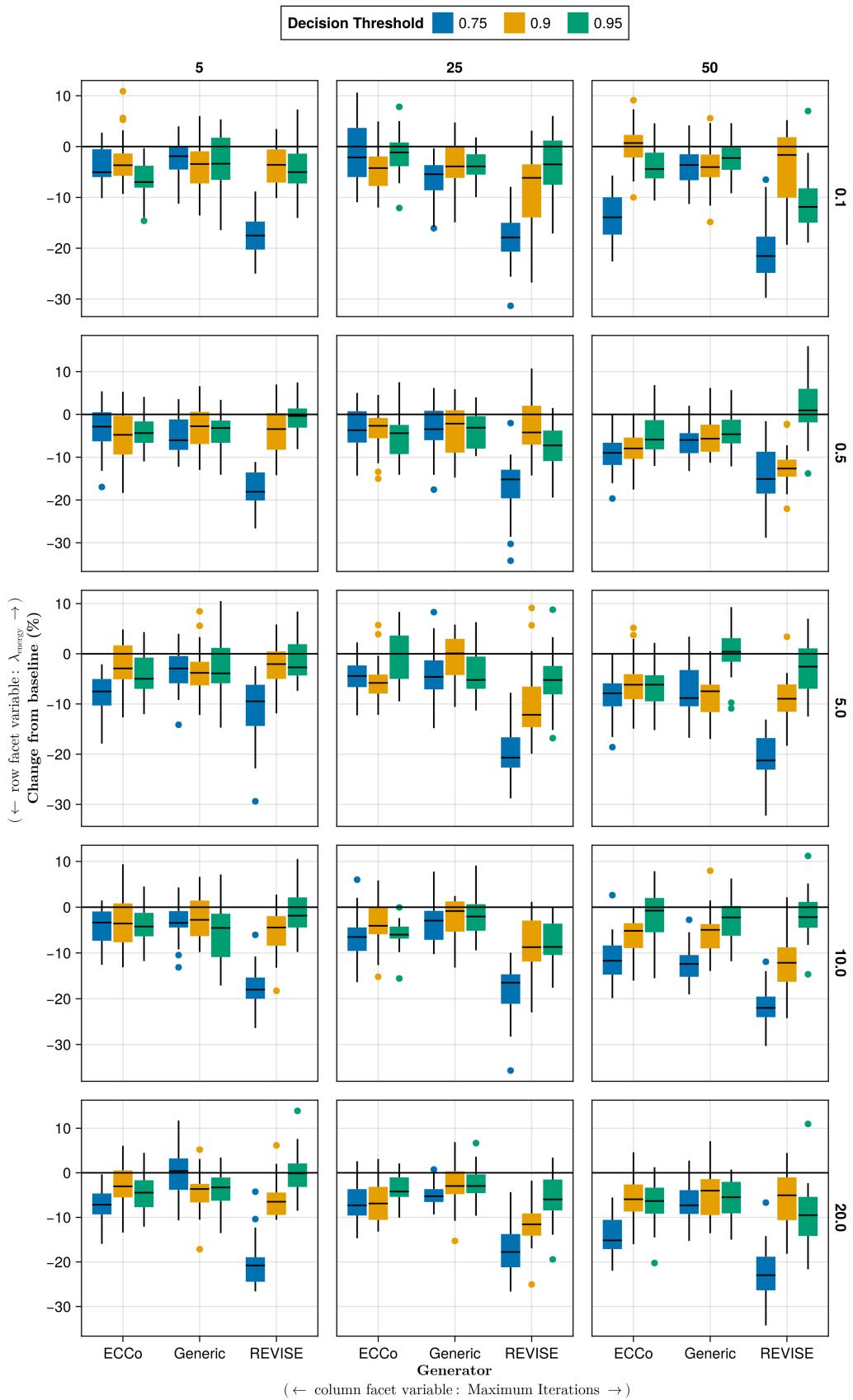


Figure A11: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

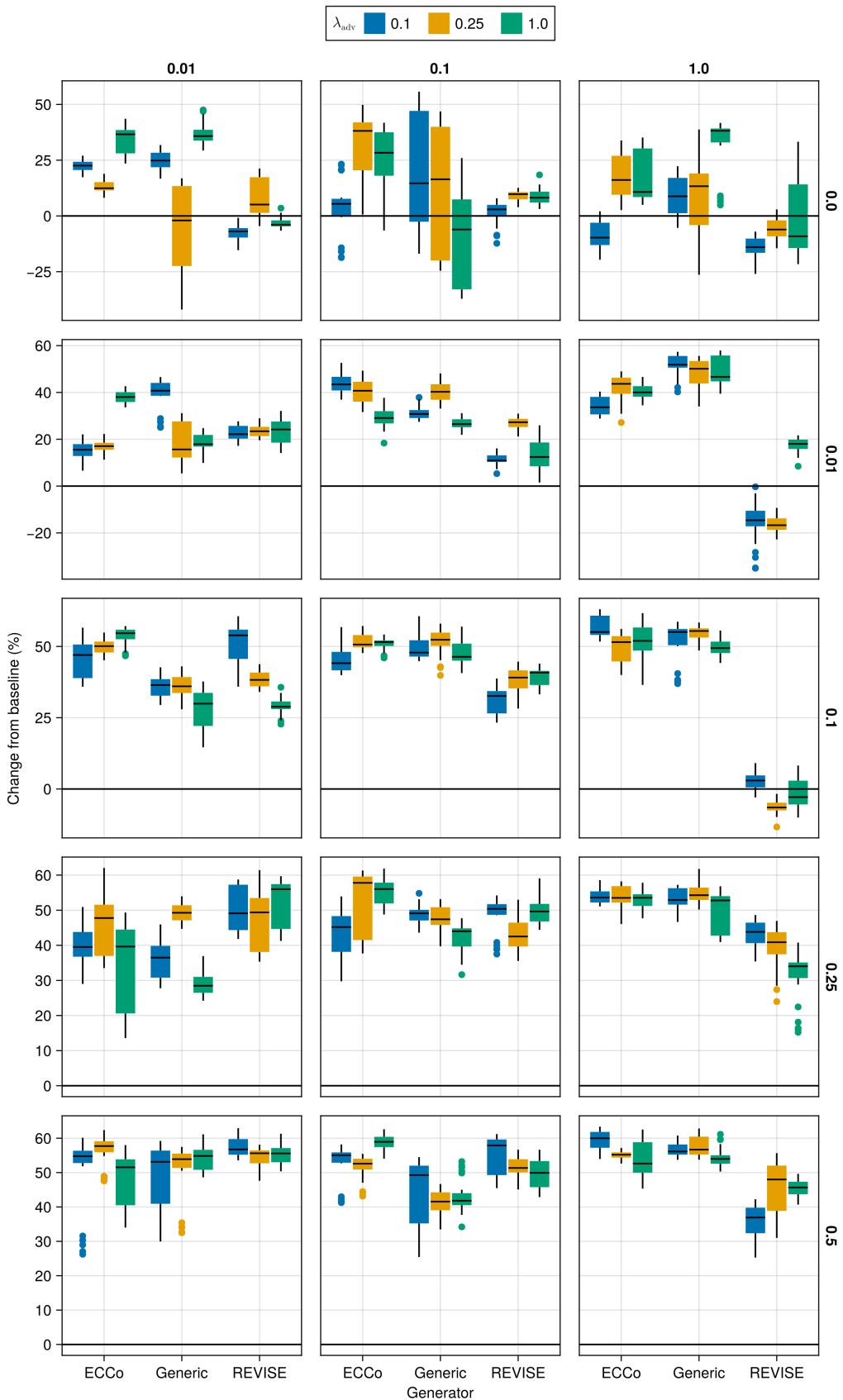


Figure A12: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

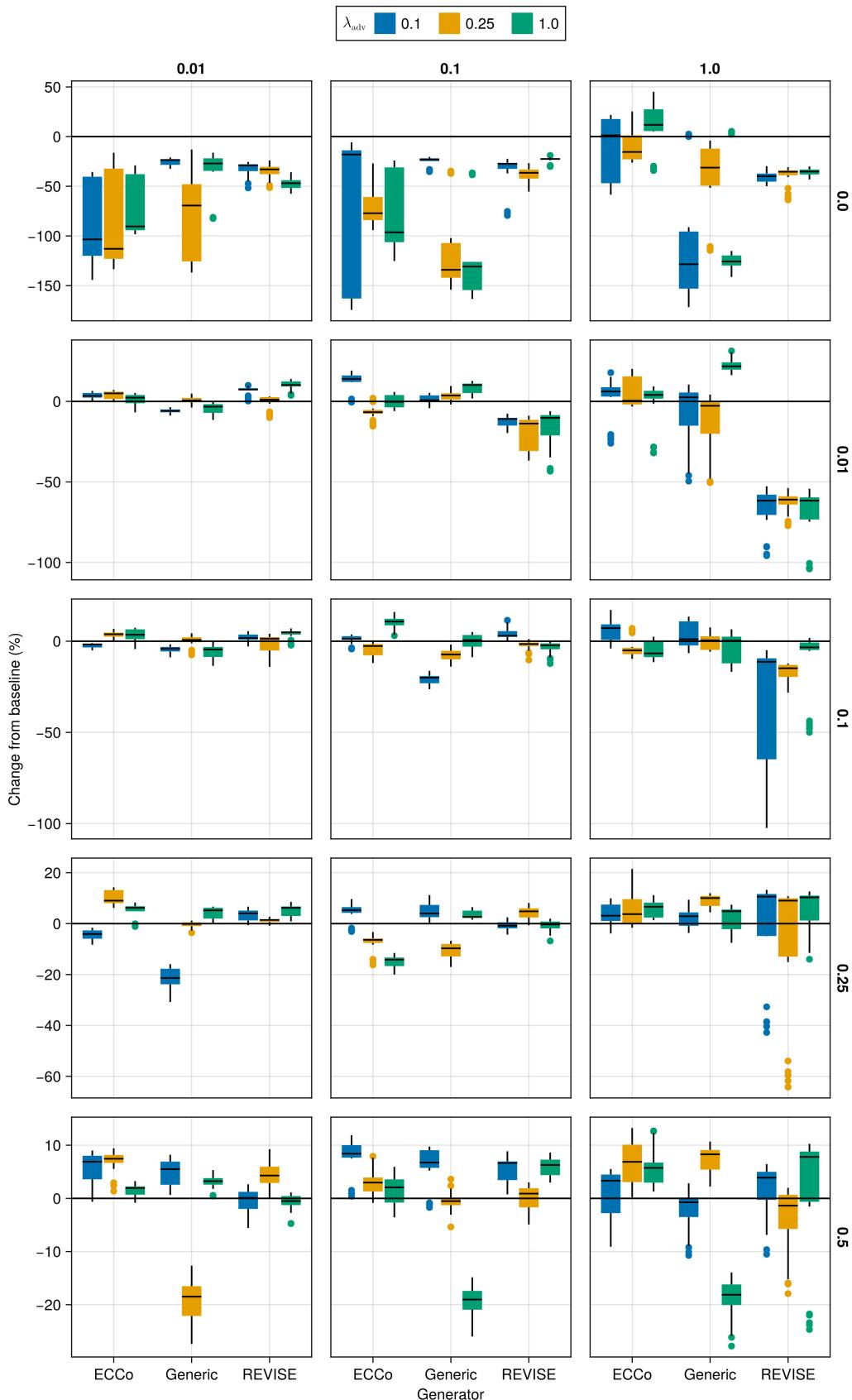


Figure A13: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

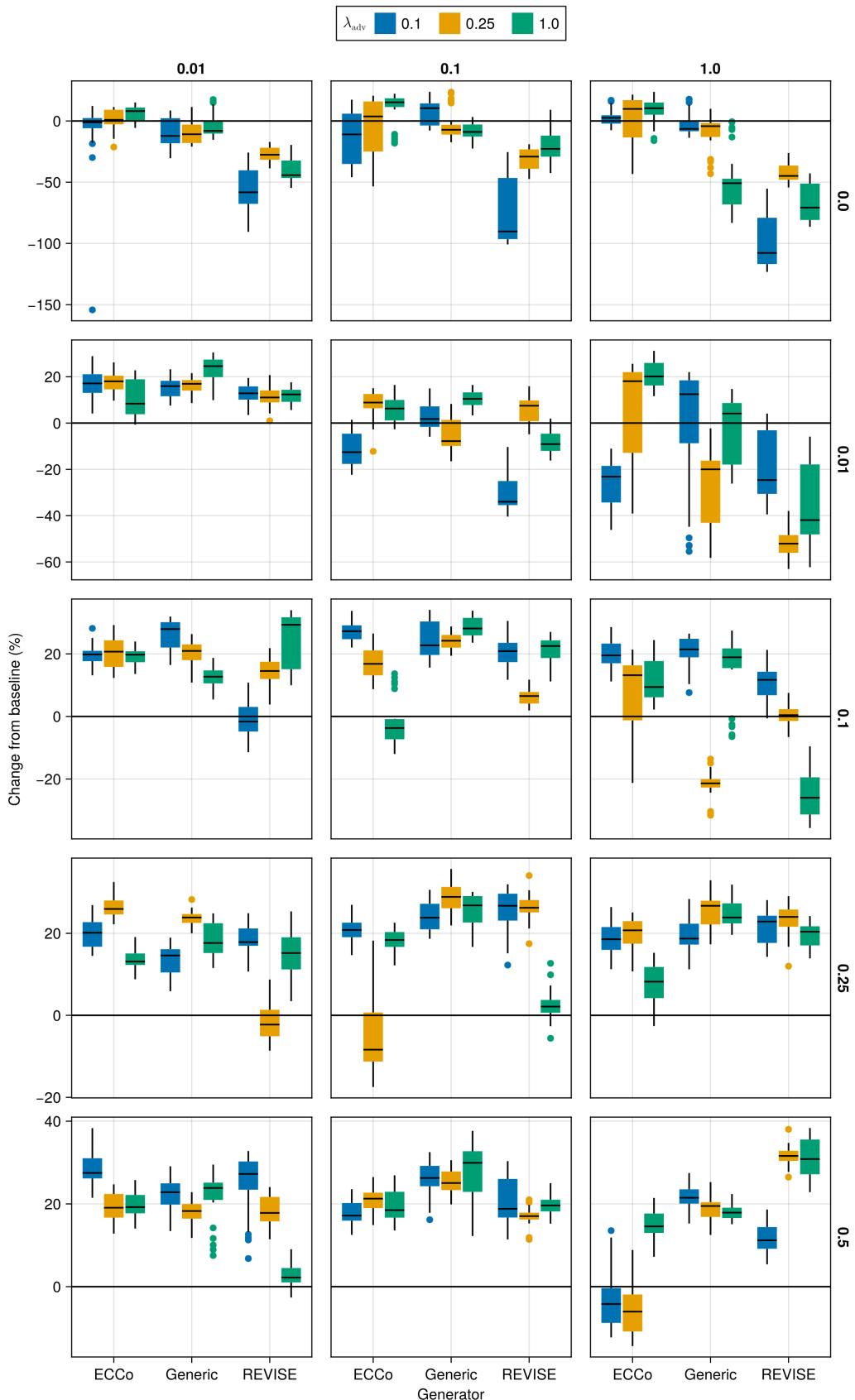


Figure A14: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

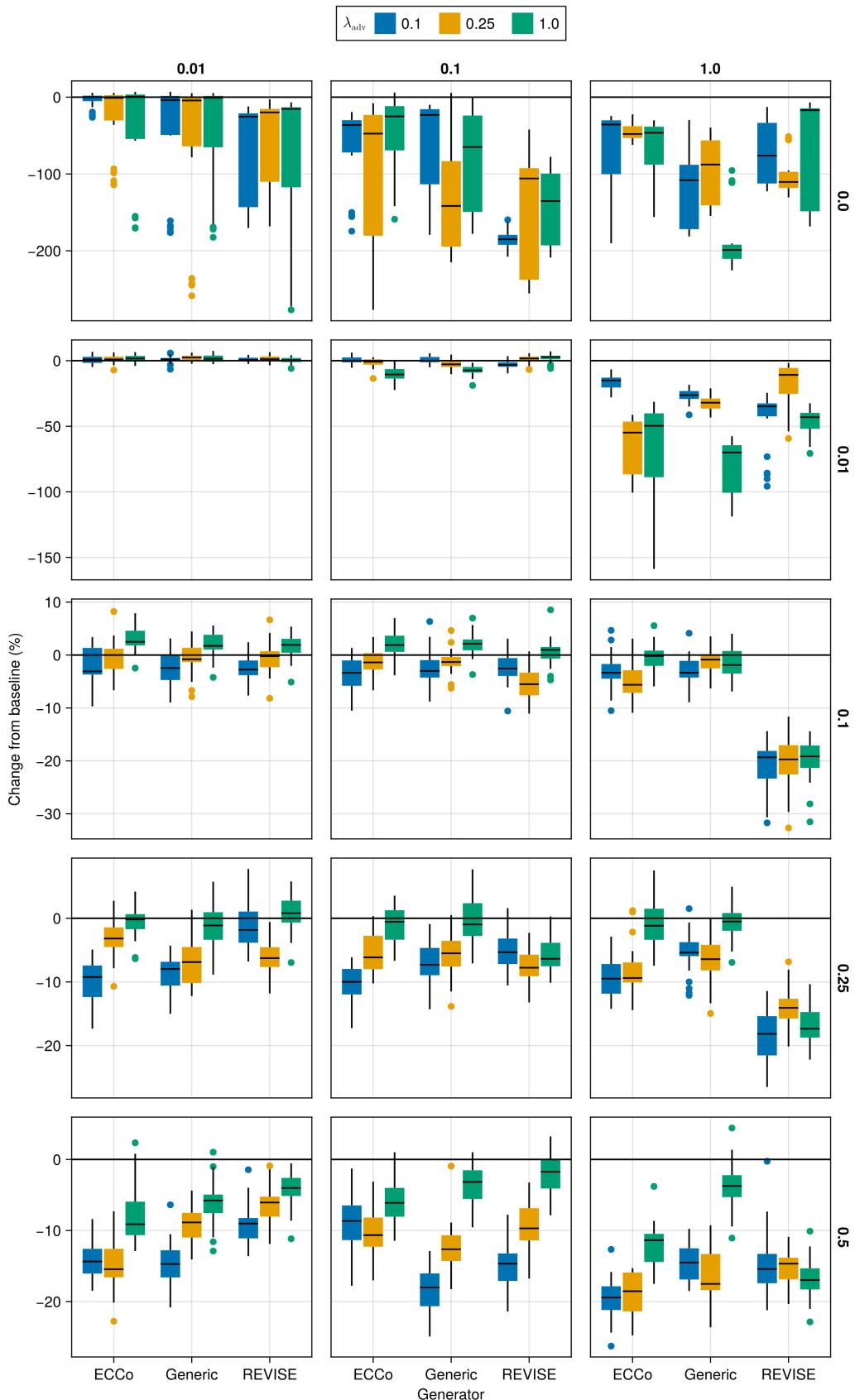


Figure A15: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

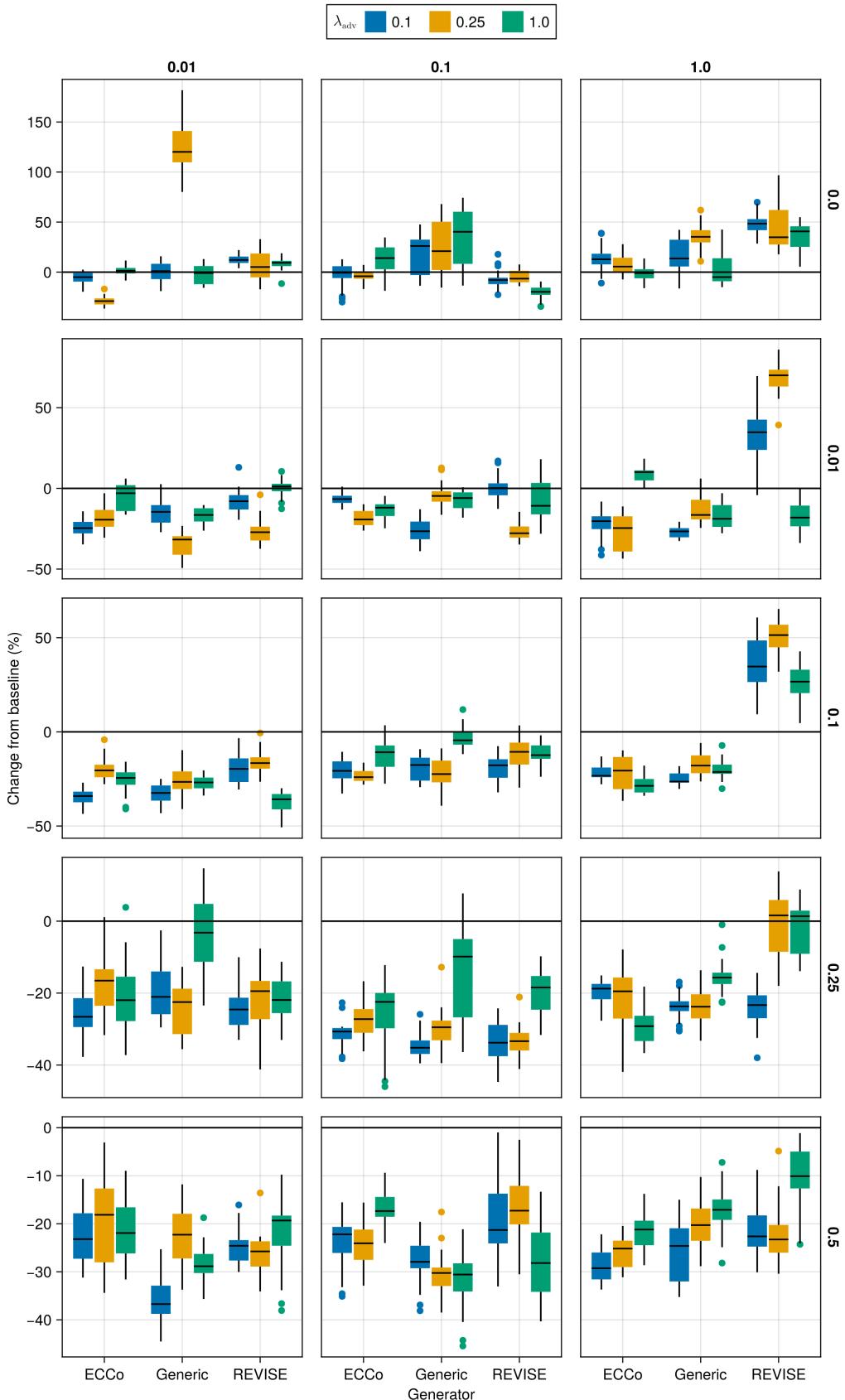


Figure A16: Average outcomes for the cost measure across hyperparameters. Data: Circles.

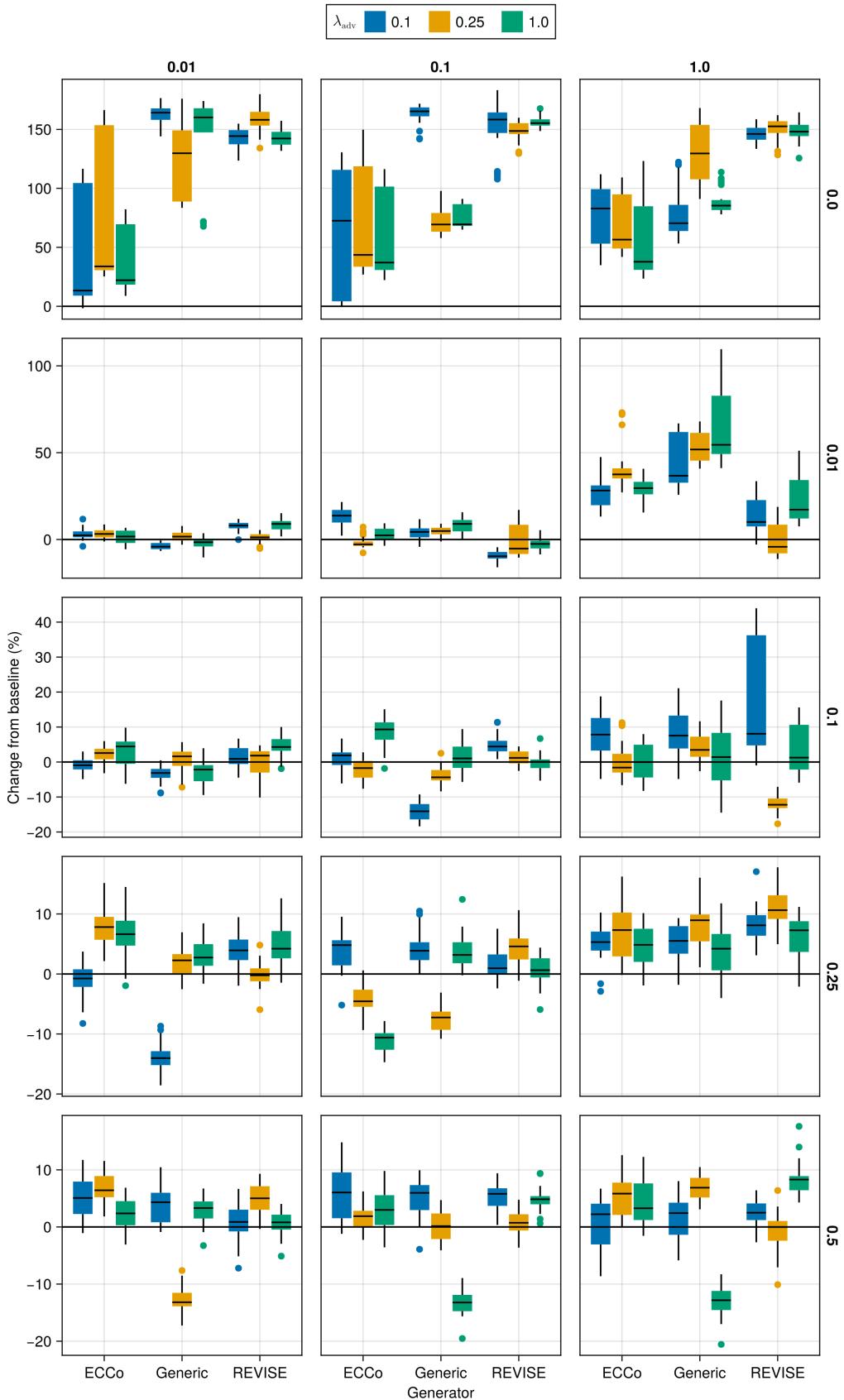


Figure A17: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

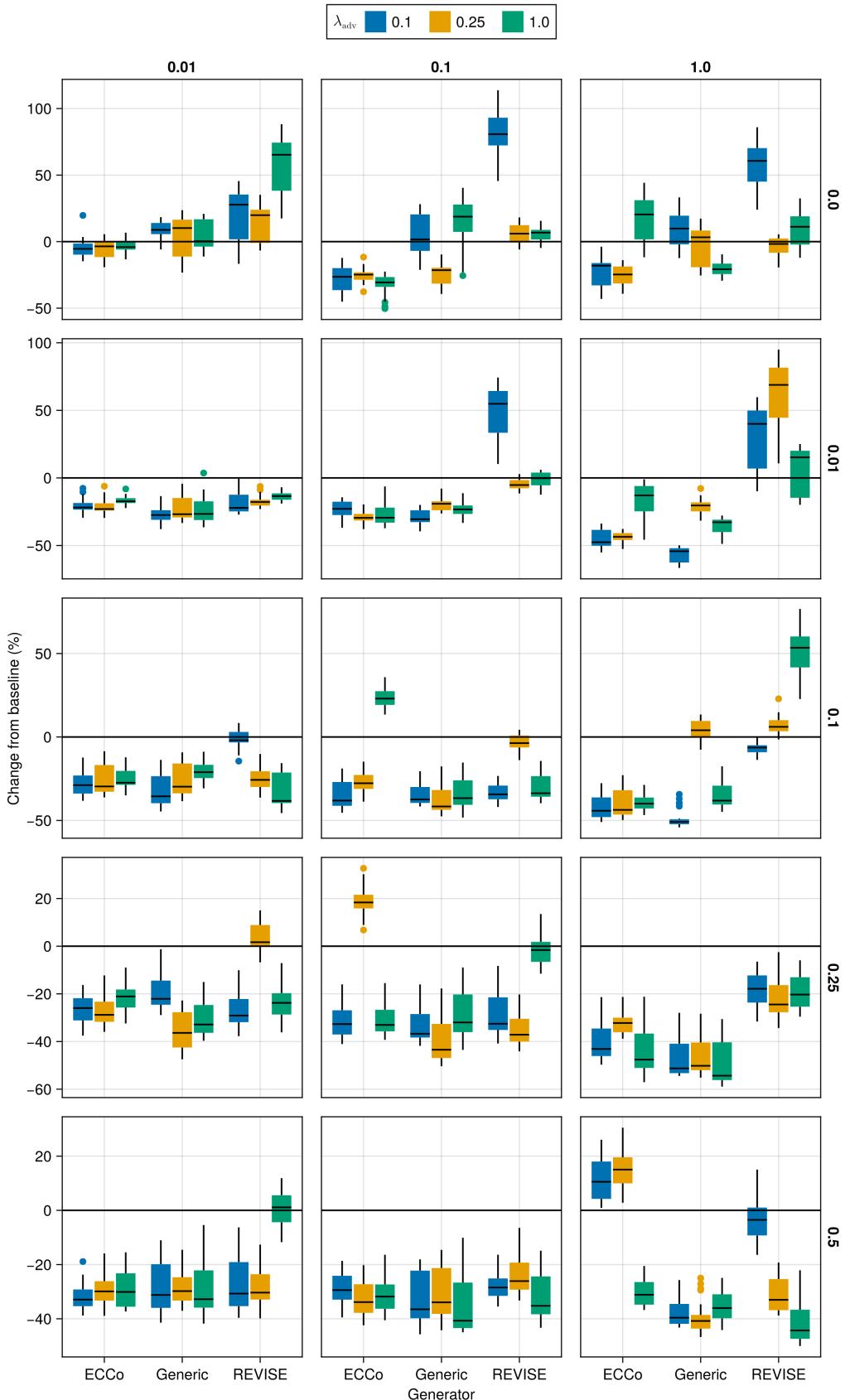


Figure A18: Average outcomes for the cost measure across hyperparameters. Data: Moons.

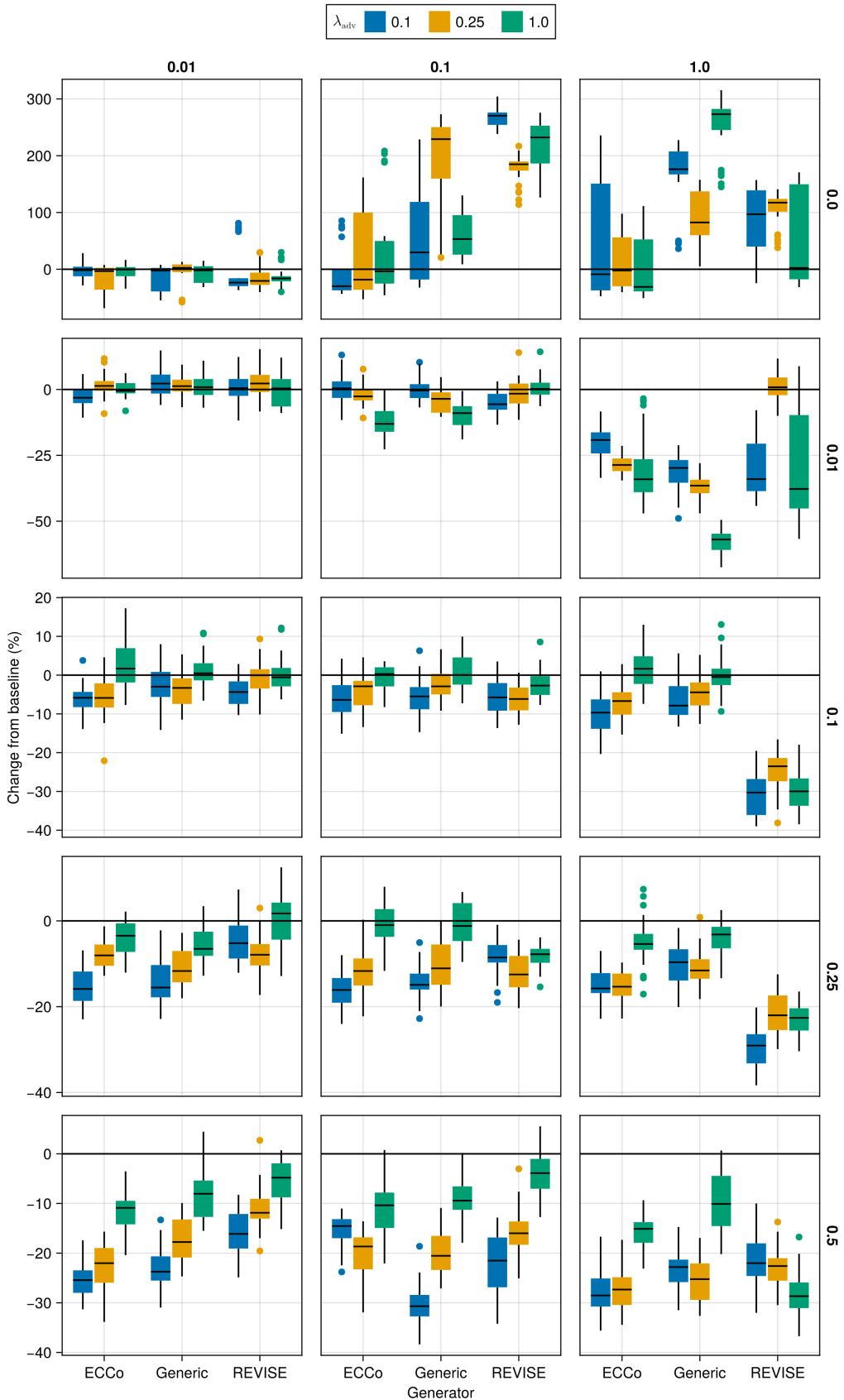


Figure A19: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

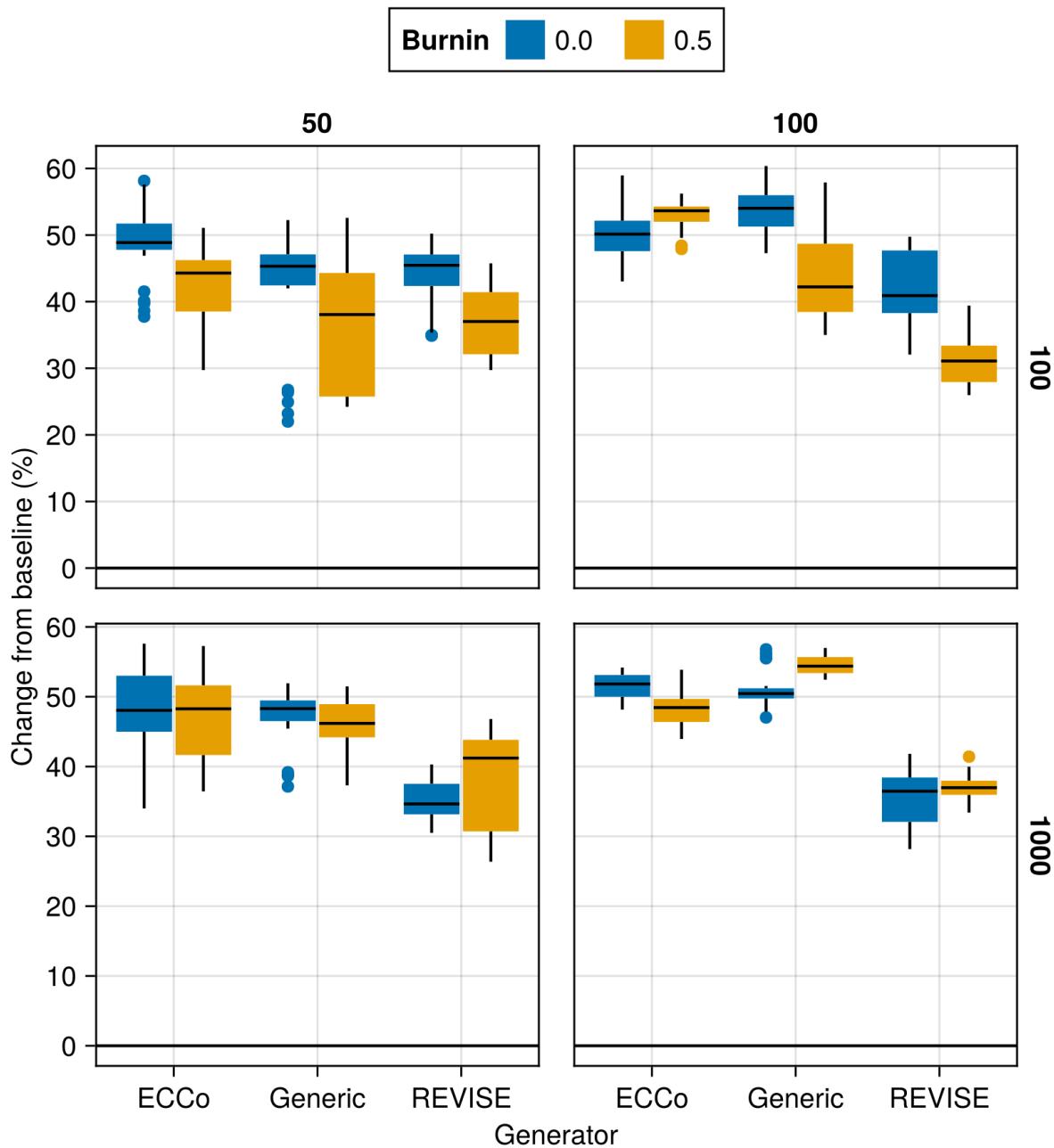


Figure A20: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

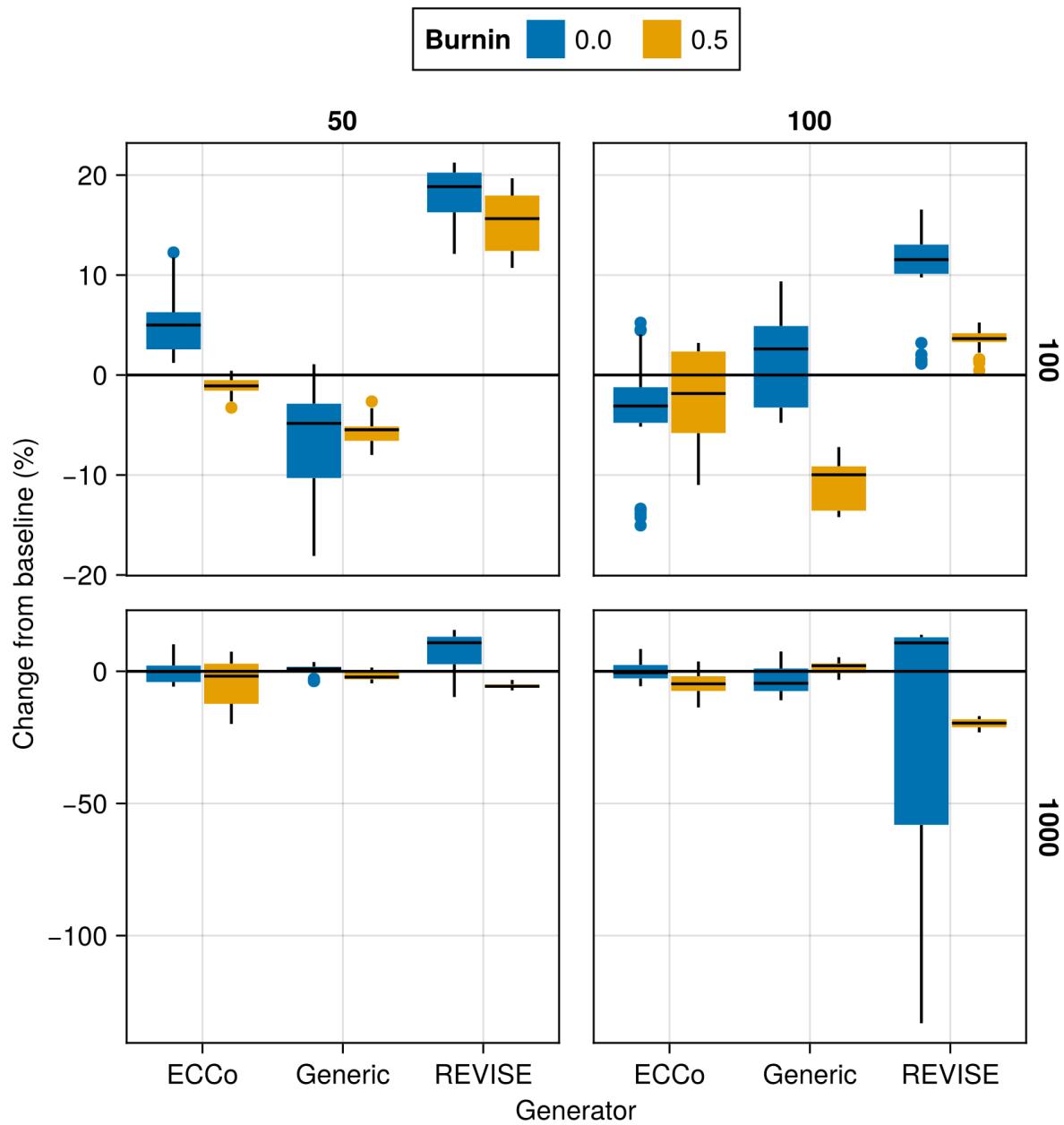


Figure A21: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

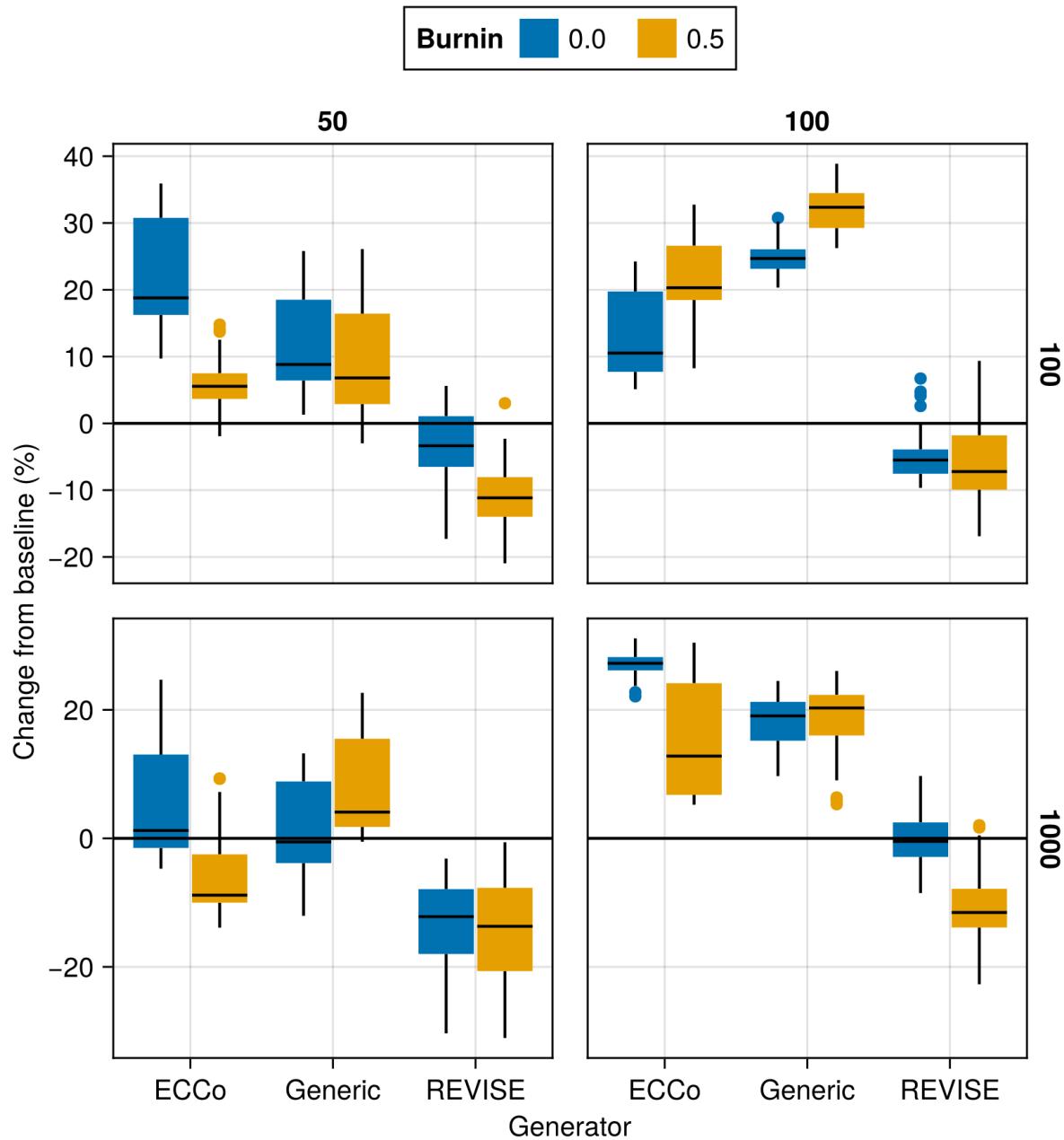


Figure A22: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

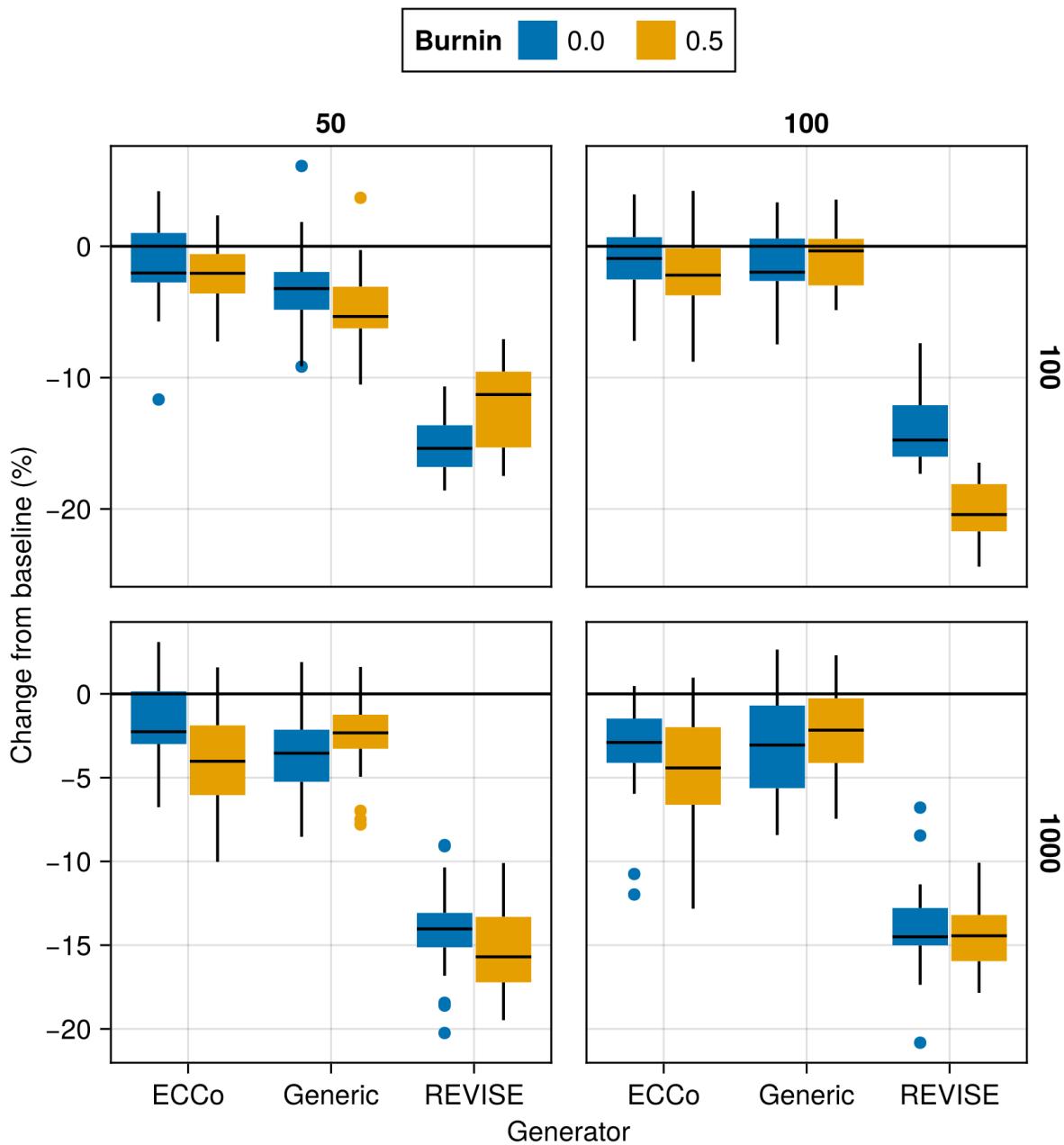


Figure A23: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

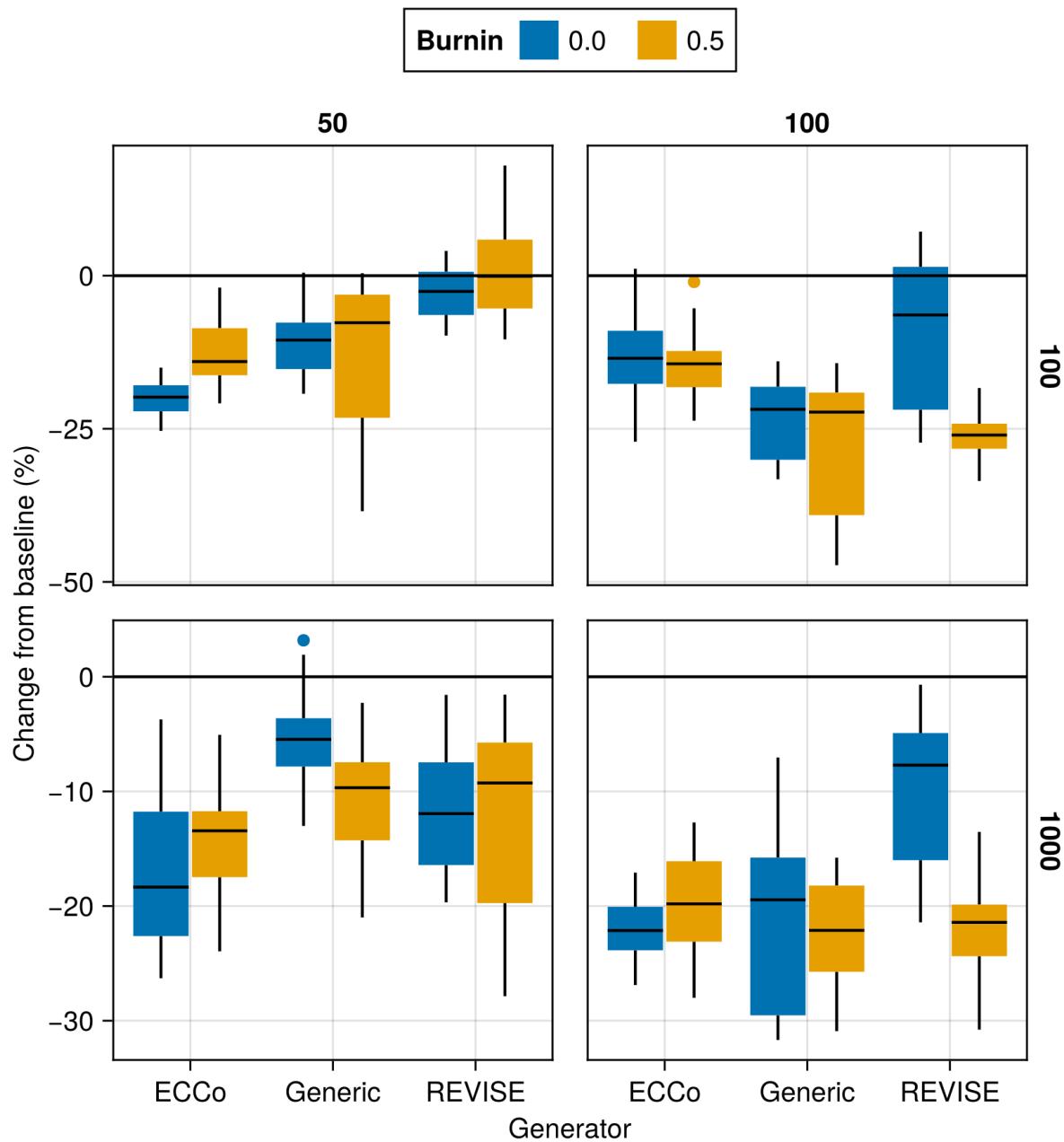


Figure A24: Average outcomes for the cost measure across hyperparameters. Data: Circles.

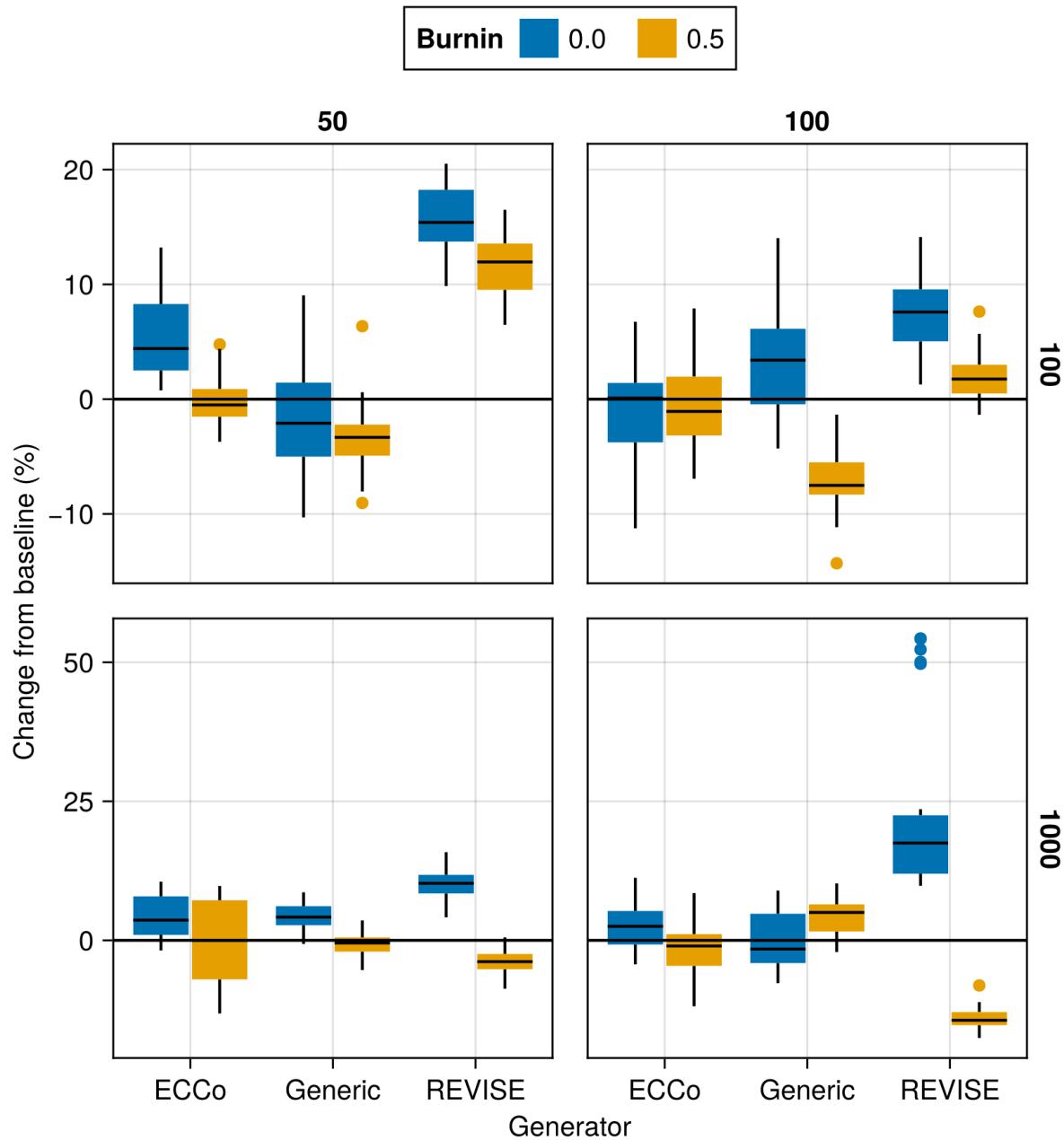


Figure A25: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

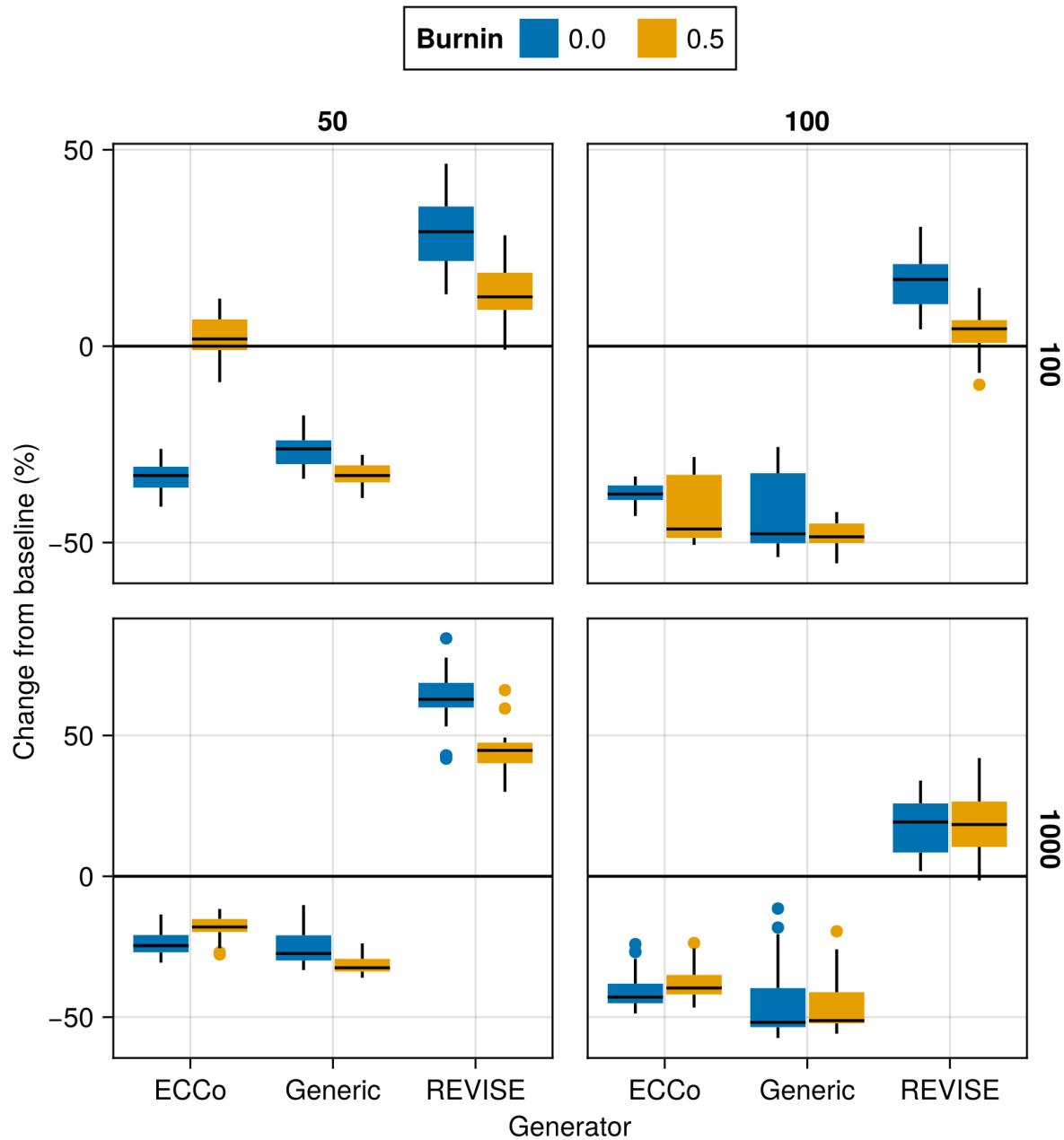


Figure A26: Average outcomes for the cost measure across hyperparameters. Data: Moons.

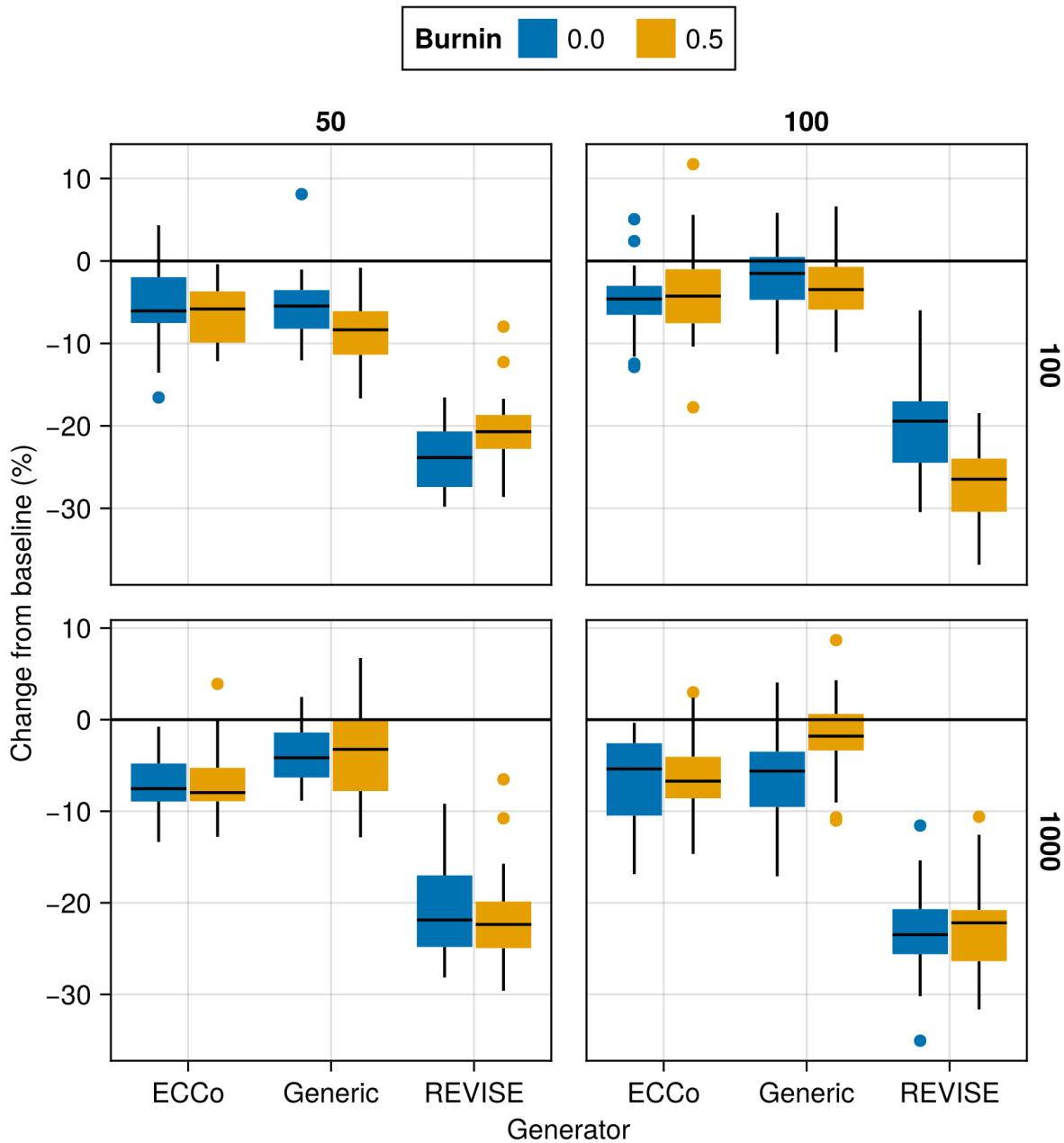


Figure A27: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

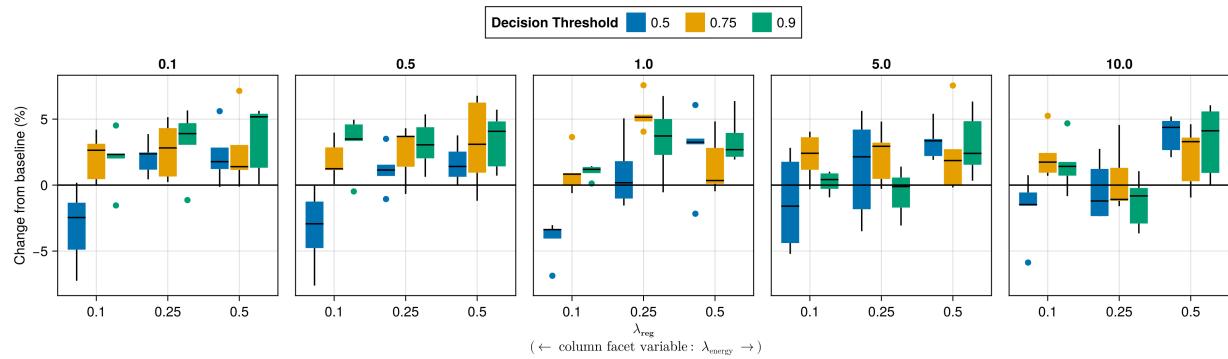


Figure A28: Average outcomes for the plausibility measure across key hyperparameters. Data: Adult.

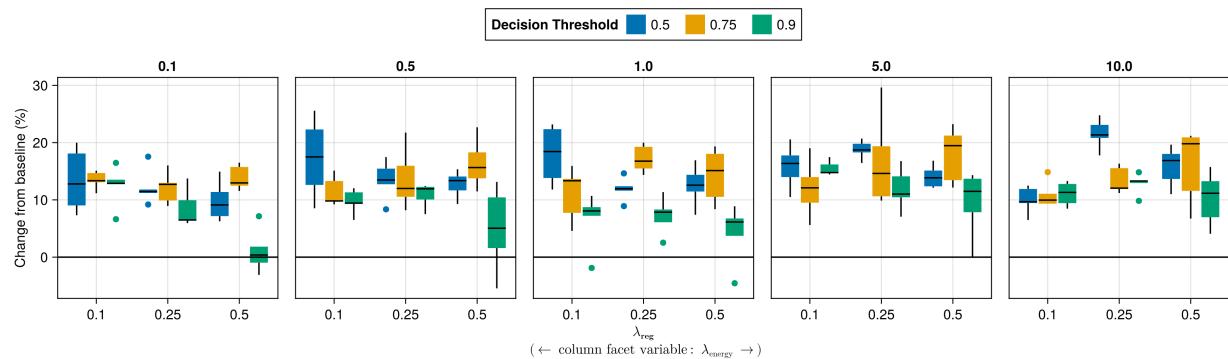


Figure A29: Average outcomes for the plausibility measure across key hyperparameters. Data: California Housing.

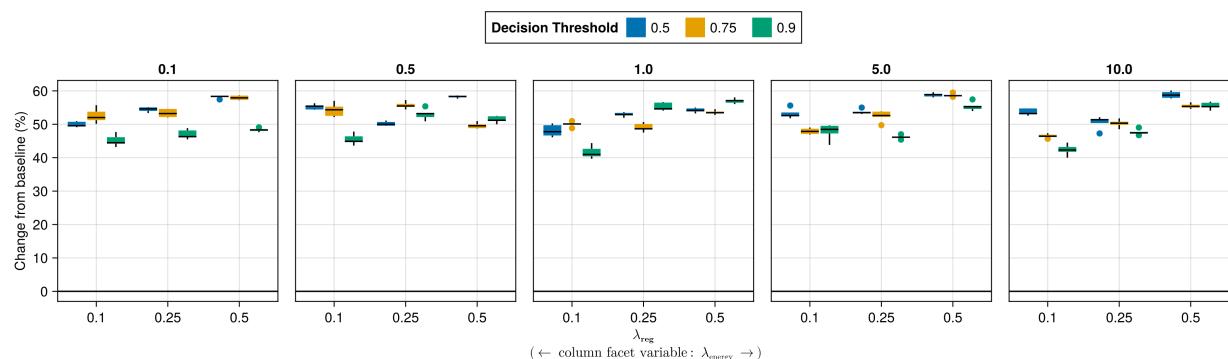


Figure A30: Average outcomes for the plausibility measure across key hyperparameters. Data: Circles.

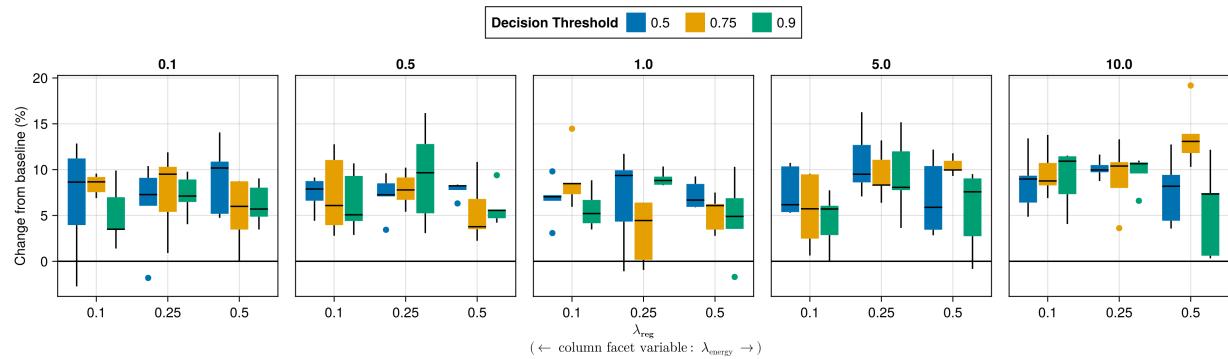


Figure A31: Average outcomes for the plausibility measure across key hyperparameters. Data: Credit.

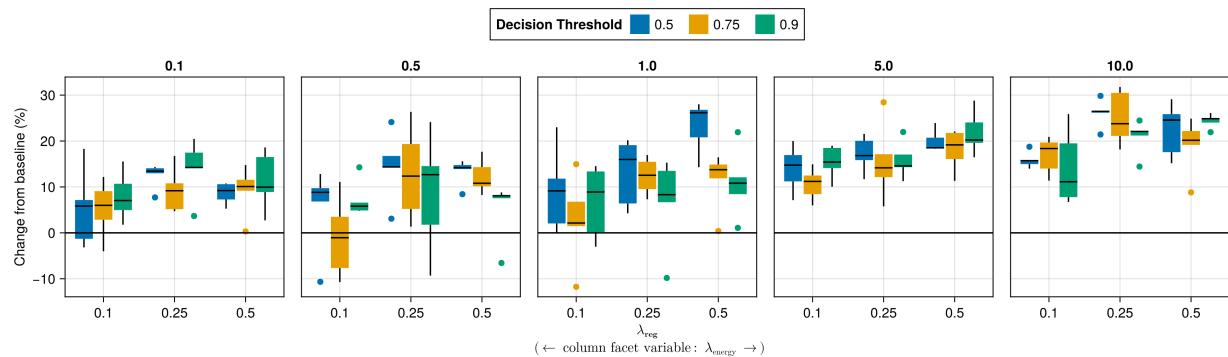


Figure A32: Average outcomes for the plausibility measure across key hyperparameters. Data: GMSC.

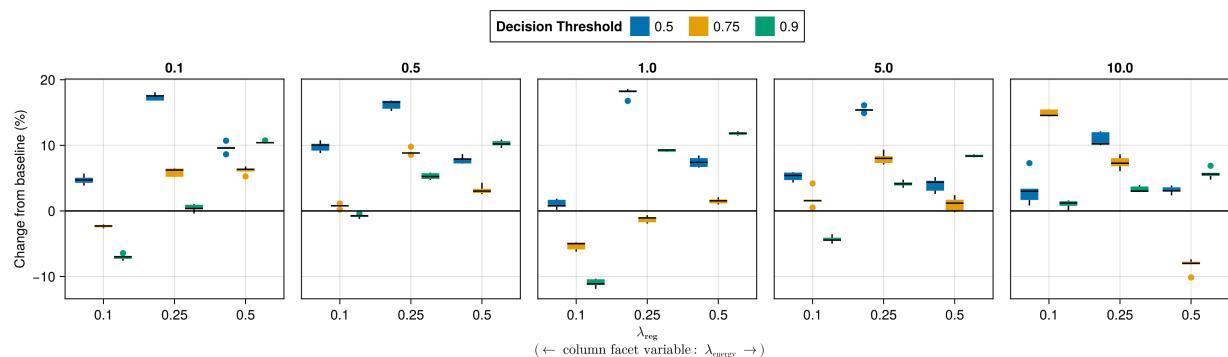


Figure A33: Average outcomes for the plausibility measure across key hyperparameters. Data: Linearly Separable.

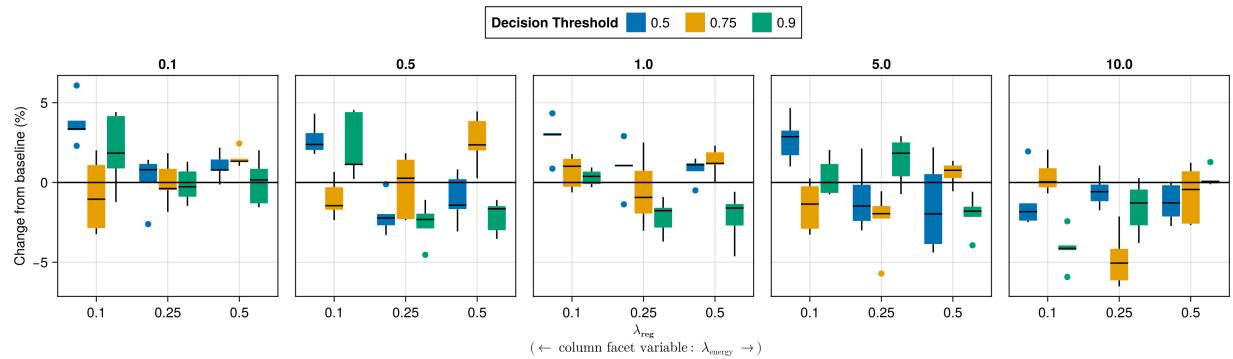


Figure A34: Average outcomes for the plausibility measure across key hyperparameters. Data: MNIST.

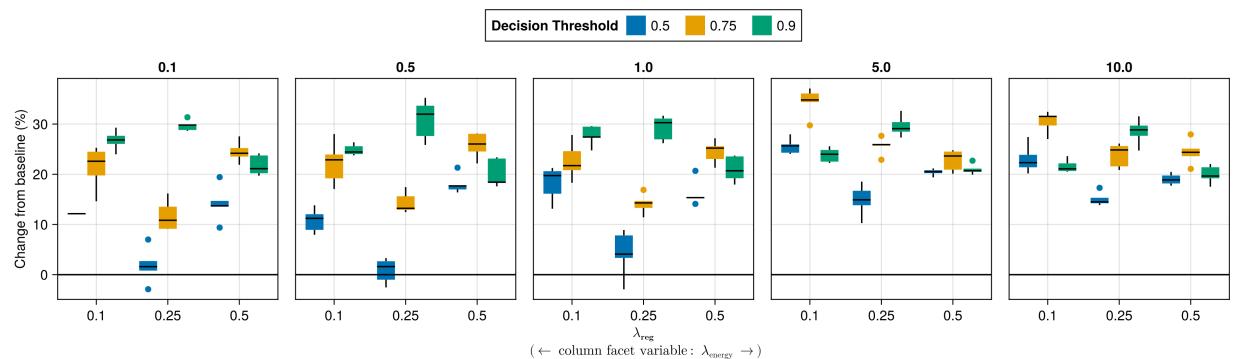


Figure A35: Average outcomes for the plausibility measure across key hyperparameters. Data: Moons.

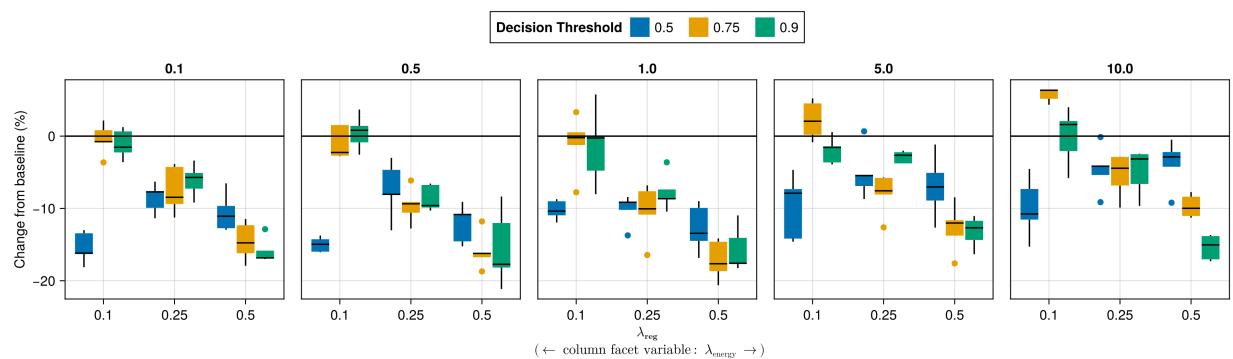


Figure A36: Average outcomes for the plausibility measure across key hyperparameters. Data: Overlapping.

582 **I.3.1.2 Proportion of Mature CE** The results with respect to the proportion of mature counterfactuals in each  
 583 epoch are shown in Figure A37 to Figure A45.

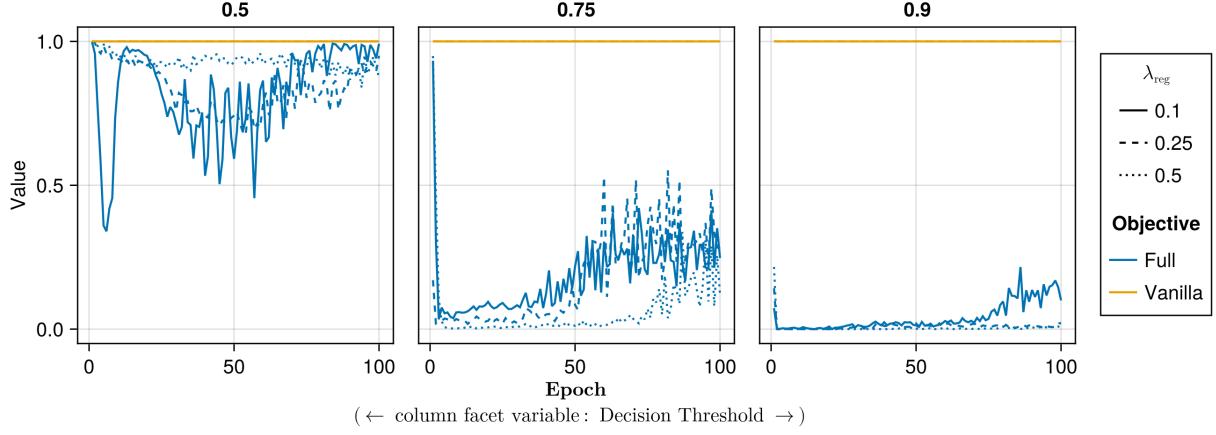


Figure A37: Proportion of mature counterfactuals in each epoch. Data: Adult.

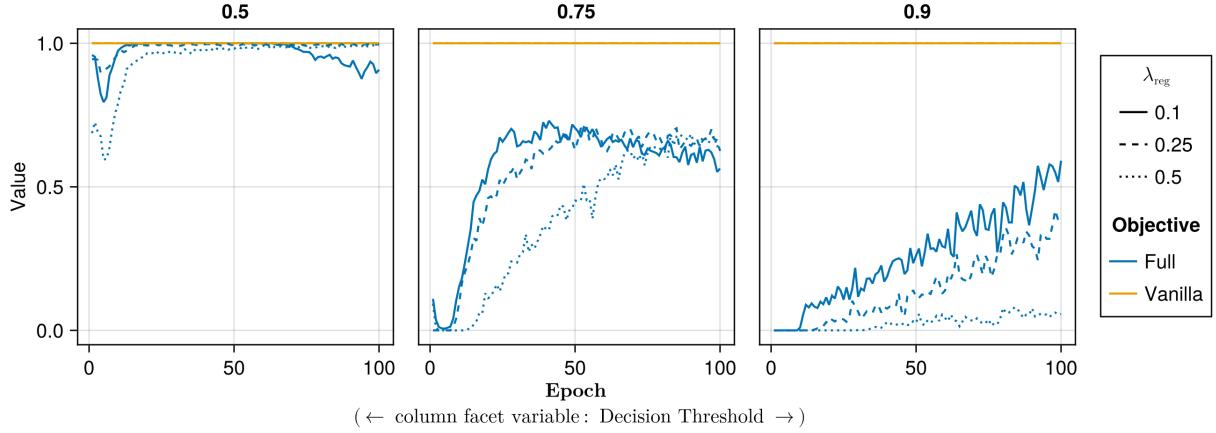


Figure A38: Proportion of mature counterfactuals in each epoch. Data: California Housing.

## 584 J Computation Details

### 585 J.1 Hardware

586 We performed our experiments on a high-performance cluster. Details about the cluster will be disclosed upon publi-  
 587 cation to avoid revealing information that might interfere with the double-blind review process. Since our experiments  
 588 involve highly parallel tasks and rather small models by today's standard, we have relied on distributed computing  
 589 across multiple central processing units (CPU). Graphical processing units (GPU) were not required.

### 590 J.1.1 Grid Searches

591 Model training for the largest grid searches with 270 unique parameter combinations was parallelized across 34 CPUs  
 592 with 2GB memory each. The time to completion varied by dataset for reasons discussed in Section 5: 0h49m (*Moons*),  
 593 1h4m (*Linearly Separable*), 1h49m (*Circles*), 3h52m (*Overlapping*). Model evaluations for large grid searches were  
 594 parallelized across 20 CPUs with 3GB memory each. Evaluations for all data sets took less than one hour (<1h) to  
 595 complete.

### 596 J.1.2 Tuning

597 For tuning of selected hyperparameters, we distributed the task of generating counterfactuals during training across 40  
 598 CPUs with 2GB memory each for all tabular datasets. Except for the *Adult* dataset, all training runs were completed

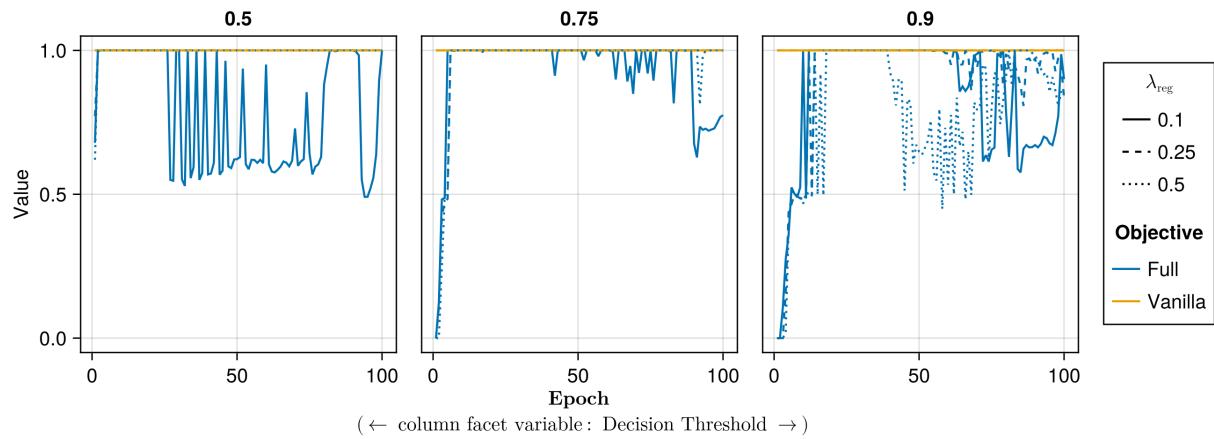


Figure A39: Proportion of mature counterfactuals in each epoch. Data: Circles.

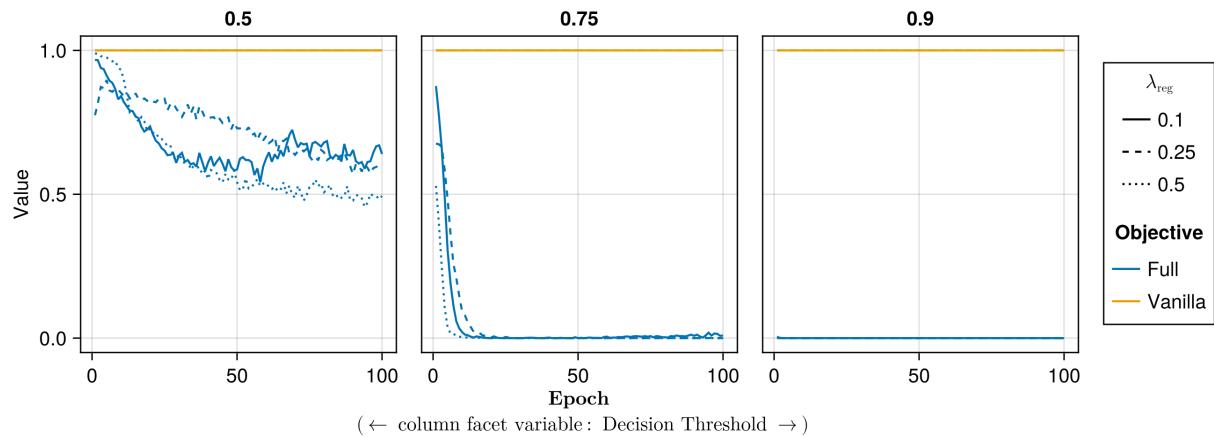


Figure A40: Proportion of mature counterfactuals in each epoch. Data: Credit.

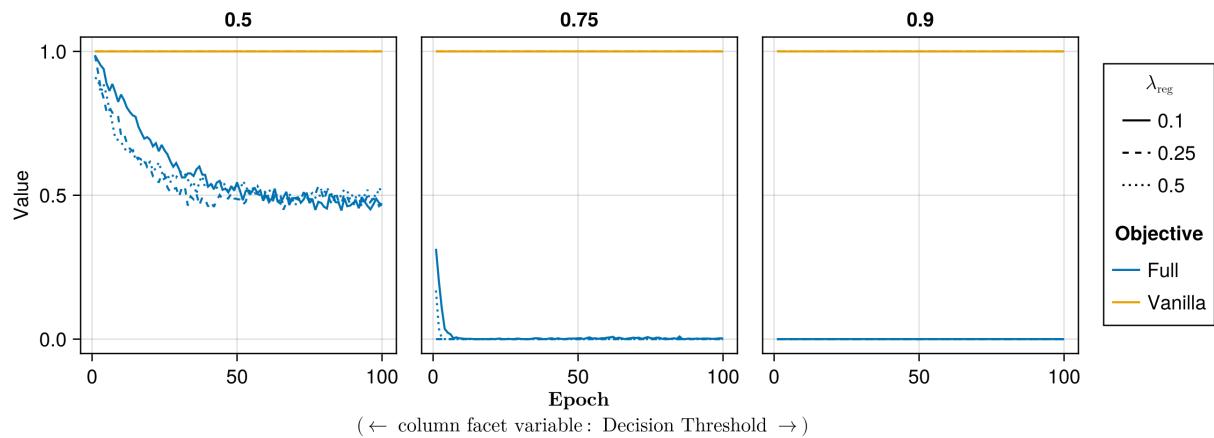


Figure A41: Proportion of mature counterfactuals in each epoch. Data: GMSC.

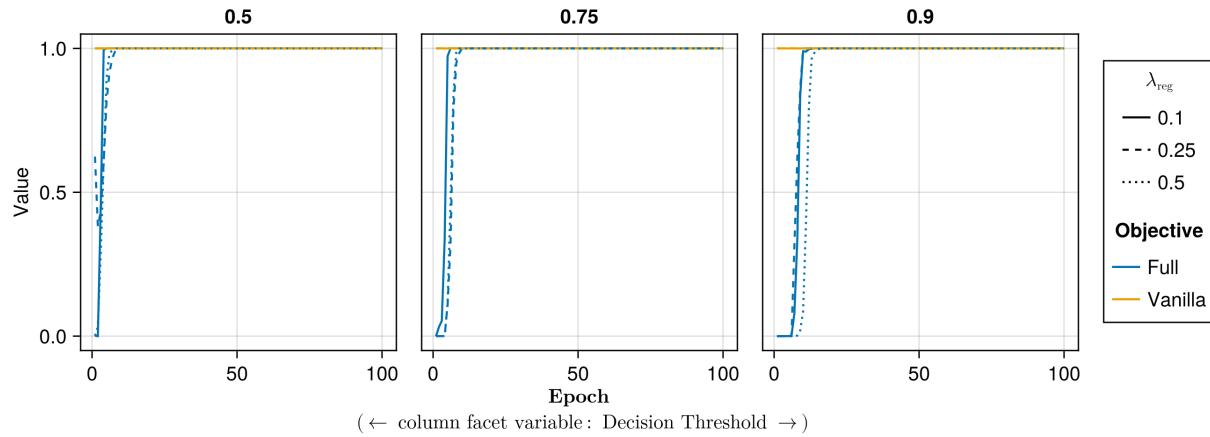


Figure A42: Proportion of mature counterfactuals in each epoch. Data: Linearly Separable.

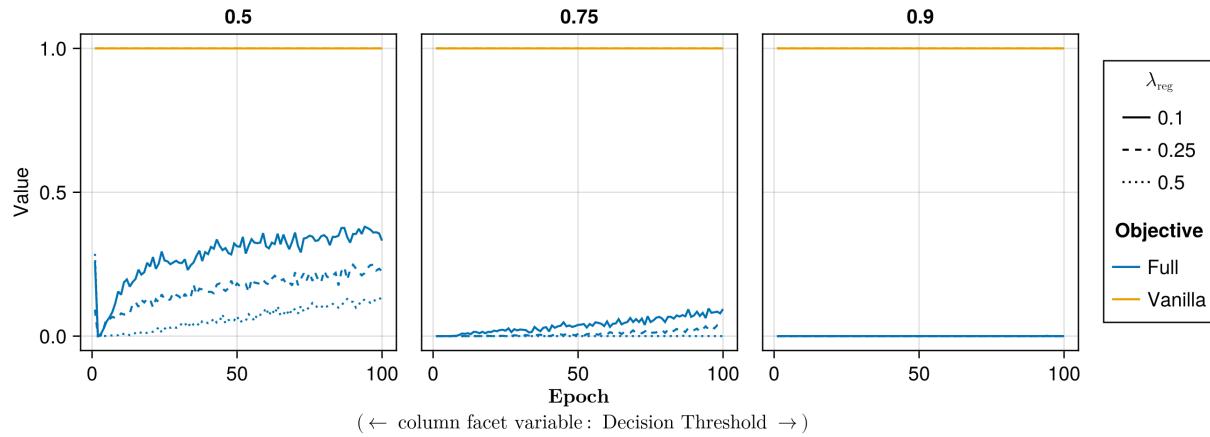


Figure A43: Proportion of mature counterfactuals in each epoch. Data: MNIST.

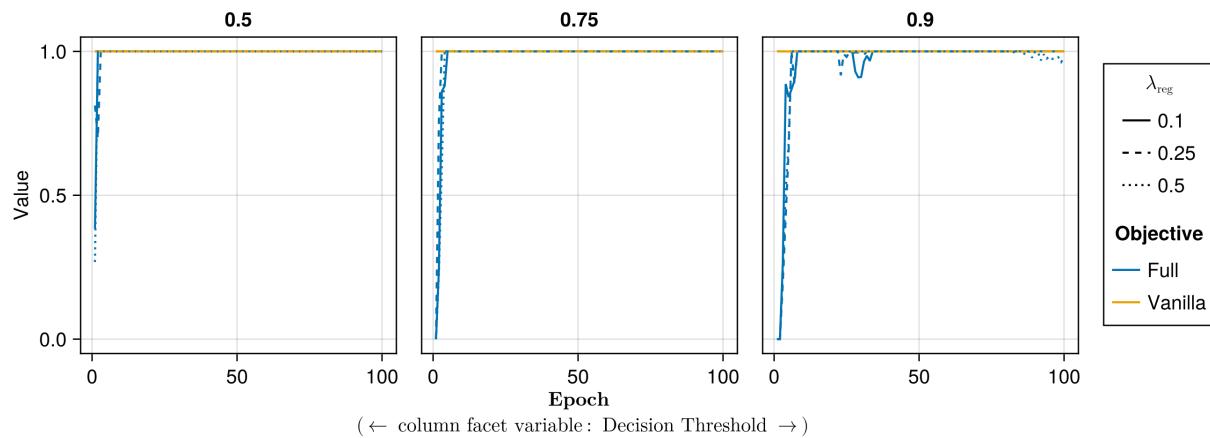


Figure A44: Proportion of mature counterfactuals in each epoch. Data: Moons.

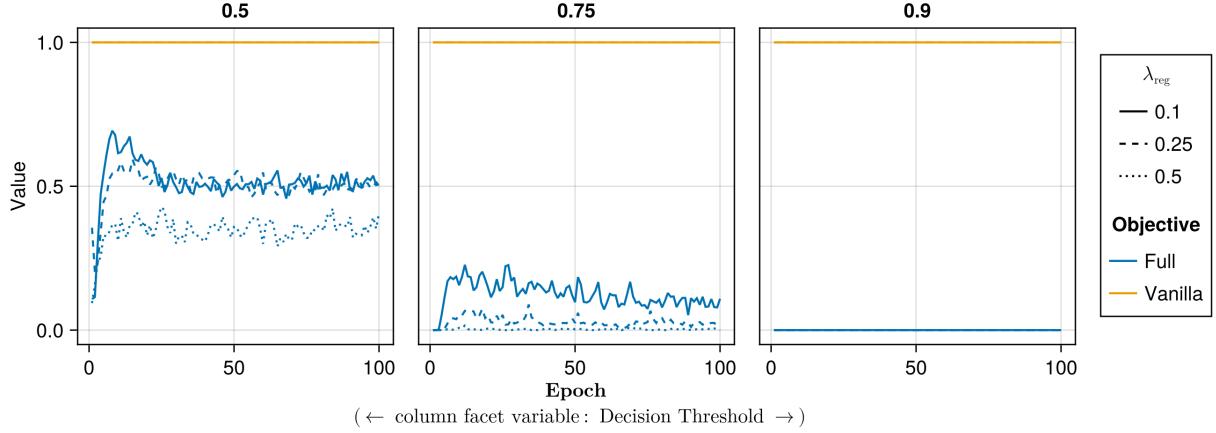


Figure A45: Proportion of mature counterfactuals in each epoch. Data: Overlapping.

599 in less than half an hour (<0h30m). The *Adult* dataset took around 0h35m to complete. Evaluations across 20 CPUs  
 600 with 3GB memory each generally took less than 0h30m to complete. For *MNIST*, we relied on 100 CPUs with 2GB  
 601 memory each. For the *MLP*, training of all models could be completed in 1h30m, while the evaluation across 20 CPUs  
 602 (6GB memory) took 4h12m. For the *CNN*, training of all models took ~8h, with conventionally trained models taking  
 603 ~0h15m each and model with CT taking ~0h30m-0h45m each.

## 604 J.2 Software

605 All computations were performed in the Julia Programming Language ([Bezanson et al. 2017](#)). We have developed  
 606 a package for counterfactual training that leverages and extends the functionality provided by several existing pack-  
 607 ages, most notably [CounterfactualExplanations.jl](#) ([Altmeyer, Deursen, et al. 2023](#)) and the [Flux.jl](#) library for deep  
 608 learning ([Michael Innes et al. 2018; Mike Innes 2018](#)). For data-wrangling and presentation-ready tables we relied on  
 609 [DataFrames.jl](#) ([Bouchet-Valat and Kamiski 2023](#)) and [PrettyTables.jl](#) ([Chagas et al. 2024](#)), respectively. For plots and  
 610 visualizations we used both [Plots.jl](#) ([Christ et al. 2023](#)) and [Makie.jl](#) ([Danisch and Krumbiegel 2021](#)), in particular  
 611 [AlgebraOfGraphics.jl](#). To distribute computational tasks across multiple processors, we have relied on [MPI.jl](#) ([Byrne,  
 612 Wilcox, and Churavy 2021](#)).