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)

models are tasked with learning representations directly from data, 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-growing degrees of freedom to achieve that task, which has often led them to outperform traditionally more parsimonious models. Unfortunately, in doing so, models learn increasingly complex and highly sensitive representations that we can no longer easily interpret.

The 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 to adversarial examples: counterfactuals of model inputs that yield vastly different model predictions despite being "imperceptible" in that they are semantically indifferent from their factual counterparts. Although some partially effective mitigation strategies have been proposed, for example **adversarial training** (I. J. Goodfellow, Shlens, and Szegedy 2014), truly robust deep learning (DL) remains unattainable even for models that are considered shallow by today's standards (Kolter 2023).

Part of the problem is that the high degrees of freedom provide room for many solutions that are locally optimal with respect to narrow objectives (Wilson 2020).[1] Indeed, recent work on the so called "lottery ticket hypothesis" suggests that modern neural networks can be pruned by up to 90% while preserving their predictive performance (Frankle and Carbin 2019) and generalizability (Morcos et al. 2019). Similarly, Zhang et al. (2021) showed that state-of-the-art neural networks are so expressive that they can fit randomly labeled data. Thus, looking at the predictive performance, the solutions may seem to provide compelling explanations for the data, when in fact they are based on purely associative, semantically meaningless patterns. This poses two related challenges. Firstly, there is no dependable way to verify if such complex representations correspond to meaningful and plausible explanations. Secondly, even if we could resolve the first challenge, it remains undecided how to ensure that models can *only* learn valuable explanations.

The first challenge has attracted an abundance of research on **explainable AI** (XAI) which aims to develop tools to derive explanations from complex model representations. This can mitigate a scenario in which we deploy opaque models and blindly rely on their predictions. On countless occasions, this scenario has occurred in practice and caused real harm to people who were affected adversely and often unfairly by automated decision-making (ADM) systems involving opaque models (O'Neil 2016; McGregor 2021). Effective XAI tools can aid us in monitoring models and providing recourse to individuals to turn adverse outcomes (e.g., "loan application rejected") into positive ones (e.g., "application accepted"). Wachter, Mittelstadt, and Russell (2017) propose **counterfactual explanations** (CE) as an effective approach to achieve this goal: CEs explain how factual inputs need to change in order for some fitted model to produce some desired output, typically involving minimal perturbations.

To our surprise, the second challenge has not yet attracted any major consolidated research effort. Specifically, there has been no concerted effort towards improving improving models' explanatory capacity, which we will henceforth simply call "explainability", defined as the degree to which learned representations correspond to explanations that are interpretable and deemed **plausible** by humans (see Definition 3.1). Instead, the choice has typically been to improve the ability of XAI tools to identify the subset explanations that are both plausible and valid for any given model, independent of whether the learned representations are also compatible with implausible explanations (Altmeyer et al. 2024). Fortunately, recent findings indicate that explainability can arise as byproduct of regularization techniques aimed at other objectives such as robustness, generalization, and generative capacity (Schut et al. 2021; Augustin, Meinke, and Hein 2020; Altmeyer et al. 2024).

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

- We discuss existing related work on improving models and consolidate it through the lens of counterfactual explanations (Section 2).
- We present our proposed methodological framework that leverages faithful counterfactual explanations during the training phase of models to achieve the explainability objective (Section 3).
- 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).

Despite some limitations of our approach discussed in Section 5, we conclude in Section 6 that counterfactual training provides a practical framework for researchers and practitioners interested in making opaque models more trustworthy. We also believe that this work serves as an opportunity for XAI researchers to re-evaluate the trend of improving XAI tools without improving the underlying models.

[1] We follow the standard ML convention, where "degrees of freedom" refer to the number of parameters estimated from data.

2 Related Literature

To the best of our knowledge, our proposed framework of counterfactual training represents the first attempt to use counterfactual explanations during training to improve model explainability. In high-level terms, we define model explainability as the extent to which valid explanations derived for an opaque model are also deemed plausible with respect to the underlying data and stakeholder requirements. To make this more concrete, we follow Augustin, Meinke, and Hein (2020) in tying the concept of explainability to the quality of counterfactual explanations that we can generate for a given model. The authors show that counterfactual explanations—understood here as minimal input perturbations that yield some desired model prediction—are generally more meaningful if the underlying model is more robust to adversarial examples. We can make intuitive sense of this finding when looking at adversarial training (AT) through the lens of representation learning with high degrees of freedom: by inducing models to "unlearn" representations that are susceptible to worst-case counterfactuals (i.e., adversarial examples), AT effectively removes some implausible explanations from the solution space.

2.1 Adversarial Examples are Counterfactual Explanations

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

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

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

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

2.2 Beyond Robustness

Improving the adversarial robustness of models is not the only path towards aligning representations with plausible explanations. In a work closely related to this one, Altmeyer et al. (2024) show that explainability can be improved through model averaging and refined model objectives. The authors propose a way to generate counterfactuals that are maximally **faithful** to the model in that they are consistent with what the model has learned about the underlying

data. Formally, they rely on tools from energy-based modelling to minimize the divergence between the distribution of counterfactuals and the conditional posterior over inputs learned by the model. Their proposed counterfactual explainer, *ECCCo*, yields plausible explanations if and only if the underlying model has learned representations that 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.

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

3 Counterfactual Training

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

Definition 3.1 (Model Explainability)**.** Let $\mathbf{M}_\theta : \mathcal{X} \mapsto \mathcal{Y}$ denote a supervised classification model that maps from the D-dimensional input space $\mathcal{X}$ to representations $\phi(\mathbf{x};\theta)$ and finally to the K-dimensional output space $\mathcal{Y}$. Assume that 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 $\arg\max_y \mathbf{y}^+ = y^+$ and y^+ denotes the index of the target class.

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

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

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

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

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

3.1 Our Proposed Objective

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

[2]For detailed background information on gradient-based counterfactual search and convergence see supplementary appendix.

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

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

where $\text{yloss}(\cdot)$ is any conventional classification loss that induces discriminative performance (e.g., cross-entropy). The second and third terms in Equation 1 are explained in more detail below. For now, they can be sufficiently described as inducing explainability directly and indirectly by penalizing: (1) the contrastive divergence, $\text{div}(\cdot)$, between mature counterfactuals $\mathbf{x}'_T$ and observed samples x and, (2) the adversarial loss, $\text{advloss}(.)$, with respect to nascent counterfactuals $\mathbf{x}'_{t\leq T}$. Finally, $\text{ridge}(\cdot)$ denotes a Ridge penalty (ℓ_2-norm) that regularises the magnitude of the energy terms involved in $\text{div}(\cdot)$ (Du and Mordatch 2020). The tradeoff between the different components can be governed by adjusting the strengths of the penalties λ_{div}, λ_{adv} and λ_{reg}.

3.1.1 Directly Inducing Explainability through Contrastive Divergence

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

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

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

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

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

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

3.1.2 Indirectly Inducing Explainability through Adversarial Robustness

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

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

Under this choice, we consider nascent counterfactuals $\mathbf{x}'_{t\leq T}$ as adversarial examples as long as the magnitude of the perturbation to any individual feature is at most ε. This is closely aligned with Szegedy et al. (2013), who define an

adversarial attack as an "imperceptible non-random perturbation". Thus, we choose to work with a different distinction between CE and AE than Freiesleben (2022), who considers misclassification as the key distinguishing feature of AE. One of the key observations in this work is that we can leverage counterfactual explanations during training and get adversarial examples, essentially for free.

3.2 Encoding Actionability Constraints

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

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

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

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 respect to feature d. Intuitively, we think of this simply in terms ignoring implausibility costs with respect to immutable features, which effectively forces the model to instead seek plausibility with respect to the remaining features. This in turn results in lower overall sensitivity to immutable features, which we demonstrate empirically for different classifiers in Section 4. Under certain conditions, this results holds theoretically:[3]

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 softmax activation $\mathcal{S}$ (i.e.,* multinomial logistic regression*) where $y \in \{1, ..., K\} = \mathcal{K}$ and $\mathbf{x} \in \mathbb{R}^D$. If we assume multivariate Gaussian class densities with common diagonal covariance matrix $\Sigma_k = \Sigma$ for all $k \in \mathcal{K}$, then protecting an immutable feature from the contrastive divergence penalty (Equation 2) will result in lower classifier sensitivity to that feature relative to the remaining features, provided that at least one of those is discriminative and mutable.*

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

3.3 Illustration

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

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

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 architecture each time (a linear classifier). In each case, we show the linear decision boundary (green) and the training data colored according to their ground-truth label: orange points belong to the target class, $y^+ = 2$, blue points belong to the non-target class, $y^- = 1$. Stars indicate counterfactuals in the target class generated at test time using generic gradient descent until convergence.

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

[3] For the proof, see the supplementary appendix.

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

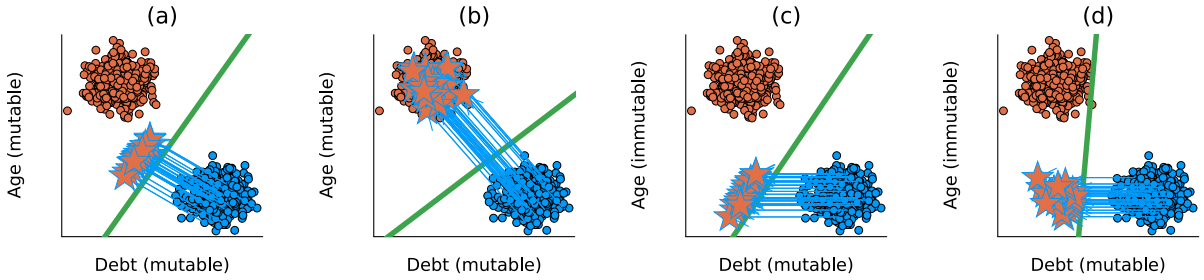

Figure 1: Visual illustration of how counterfactual training improves explainability. See Example 3.1 for details.

4 Experiments

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

Research Question 4.1 (Plausibility)**.** *Does our proposed counterfactual training objective (Equation 1) induce models to learn plausible explanations?*

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

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

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

4.1 Experimental Setup

4.1.1 Evaluation

Our key outcome of interest is how well models perform with respect to explainability (Definition 3.1): to this end, we focus primarily on the plausibility and cost of faithfully generated counterfactuals at test time. To measure the cost of counterfactuals, we follow the standard convention of using distances (ℓ_1-norm) between factuals and counterfactuals as a proxy. For plausibility, we assess how similar counterfactuals are to observed samples in the target domain. We rely on the distance-based metric used by Altmeyer et al. (2024),

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

and introduce a novel divergence metric,

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

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

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

We run the experiments with three CE generators: *Generic* of Wachter, Mittelstadt, and Russell (2017) as a simple baseline approach, *REVISE* (Joshi et al. 2019) that aims to generate plausible counterfactuals using a surrogate Variational Autoencoder (VAE), and *ECCo*—the generator of Altmeyer et al. (2023) but without the conformal prediction component—as a method that directly targets both faithfulness and plausibility of the CEs.

4.2 Experimental Results

4.2.1 Plausibility

4.2.2 Actionability

4.2.3 Impact of hyperparameter settings

We extensively test the impact of three types of hyperparameters on the proposed training regime. Our complete results are available in the technical appendix; this section focuses on the main findings.

Hyperparameters of the CE generators. First, we observe that CT is highly sensitive to hyperparameter settings but (a) there are manageable patterns and (b) we can typically identify settings that improve either plausibility or cost, and commonly both of them at the same time. Second, we note that the choice of a CE generator has a major impact on the results. For example, *REVISE* tends to perform the worst, most likely because it uses a surrogate VAE to generate counterfactuals which impedes faithfulness (Altmeyer et al. 2024). Third, increasing T, the maximum number of steps, generally yields better outcomes because more CEs can mature in each training epoch. Fourth, the impact of τ, the required decision threshold is more difficult to predict. On "harder" datasets it may be difficult to satisfy high τ for any given sample (i.e., also factuals) and so increasing this threshold does not seem to correlate with better outcomes. In fact, we have generally found that a choice of $\tau = 0.5$ leads to optimal results because it is associated with high proportions of mature counterfactuals.

Hyperparameters for penalties. We find that the strength of the energy regularization, λ_{reg} is highly impactful; energy must be sufficiently regularized to avoid poor performance in terms of decreased plausibility and increased costs. The sensitivity with respect to λ_{div} and λ_{adv} is much less evident. While high values of λ_{reg} may increase the variability in outcomes when combined with high values for any of the other penalties in Equation 1, this effect is not very pronounced.

Other hyperparameters. We observe that the effectiveness and stability of CT is positively associated with the number of counterfactuals generated during each training epoch. We also confirm that a higher number of training epochs is beneficial. Interestingly, we find that it is not necessary to employ CT during the entire training phase to achieve the desired improvements in explainability. We have tested training models conventionally during the first half of training before switching to CT after this initial "burn-in" period and observed positive results. Put differently, CT may be a way to improve the explainability of trained models in a fine-tuning manner.

5 Discussion

We begin the discussion by addressing the direct extensions of the counterfactual training approach in Section 5.1. Then, we look at its broader limitations and challenges in Section 5.2.

5.1 Future research

CT is defined only for classification settings. Our formulation relies on the distinction between non-target class(es) y^- and target class(es) y^+ to generate counterfactuals through Equation 1. While y^- and y^+ can be arbitrarily defined by the user, CT requires the output space $\mathcal{Y}$ to be discrete. Thus, it applies to binary and multi-class classification but it is not well-defined for other ML tasks where the change in outcome with respect to a decision threshold τ cannot be readily quantified. In fact, this is a common restriction in research on CEs and AR that predominantly focuses on classification models. Although other settings have attracted some interest (e.g., regression in Spooner et al. 2021; Zhao, Broelemann, and Kasneci 2023), there is still no consensus on what constitutes a counterfactual in such settings.

CT is subject to training instabilities. Joint energy-based models are susceptible to instabilities during training (Grathwohl et al. 2020) and even though we depart from the SGLD-based sampling, we still encounter major variability in the outcomes. CT is exposed to two potential sources of instabilities: (1) the energy-based contrastive divergence term in Equation 2, and (2) the underlying counterfactual explainers. For example, Altmeyer et al. (2023) recognize this to be a challenge for *ECCCo* and so it may have downstream impacts on our proposed method. Still, we find that training instabilities can be successfully mitigated by regularizing energy (λ_{reg}), generating a sufficiently large number of counterfactuals during each training epoch and including only mature counterfactuals for contrastive divergence.

CT is sensitive to hyperparameter selection. As discussed in Section 4.2.3, our method benefits from tuning certain key hyperparameters. In this work, we have relied exclusively on grid search for this task. Future work on CT could benefit from investigating more sophisticated approaches towards hyperparameter tuning. Notably, counterfactual training is iterative which makes a variety of methods applicable, including Bayesian (e.g., Snoek, Larochelle, and Adams 2012) or gradient-based (e.g., Franceschi et al. 2017) optimization.

5.2 Limitations and challenges

CT increases the training time of models. Counterfactual training promotes explainability through CEs and robustness through AEs at the cost of longer training times compared to conventional training regimes. While higher numbers of iterations and counterfactuals per iteration positively impact the quality of found solutions, they also increase the required amount of computations. We find that relatively small grids with 270 settings can take almost four hours for more demanding datasets on a high-performance computing cluster with 34 2GB CPUs[4]. However, there are three factors that attenuate the impact of this limitation. First, CT provides counterfactual explanations for the training samples essentially for free, which may be beneficial in many ADM systems. Second, we find that CT can retain its value when used as a "fine-tuning" training regime for conventionally-trained models. Third, in principle, CT yields itself to parallel execution, which we have leveraged for our own experiments.

Immutable features may have proxies. In Proposition 3.1 we define an approach to protect immutable features and thus increase the actionability of the generated counterfactuals. However, this approach requires that model owners define the mutability constraints for (all) features considered by the model. Even with sufficient domain knowledge to protect all immutable features—ones that cannot be changed at all and ones that cannot be reasonably expected to change—there may exist proxies that are theoretically mutable (and hence should not be protected) but preserve enough information about the principals to counteract the protections. As one example, consider the Adult dataset used in our experiments where the mutable education status is a proxy for the immutable age, in that the attainment of degrees is correlated with age. Delineating actionability is a major undecided challenge in the AR literature (see, e.g., Venkatasubramanian and Alfano 2020) impacting the capacity of CT to increase the explainability of the model.

Interventions on features may have downstream impacts on fairness.
- Equality of opportunity?
- Social segregation?
- Supporting AR within one context/system may still unfairly target recourse-affected individuals within other contexts/systems? In Example 3.1 younger individuals gain access to a loan but their age could still lead to, e.g., enforcing stronger supervisory mechanisms?

6 Conclusion

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G Notation

- y^+: The target class and also the index of the target class.
- y^-: The non-target class and also the index of non-the target class.
- $\mathbf{y}^+$: The one-hot encoded output vector for the target class.
- θ: Model parameters (unspecified).
- Θ: Matrix of parameters.

G.1 Other Technical Details

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

H Technical Details of Our Approach

H.1 Generating Counterfactuals through Gradient Descent

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

H.1.1 Background

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

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

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

For all generators used in this work we use standard logit crossentropy loss for $\text{yloss}(\cdot)$. All generators also penalize the distance (ℓ_1-norm) of counterfactuals from their original factual state. For *Generic* and *ECCo*, we have $\mathcal{Z} := \mathcal{X}$ and $g(\mathbf{z}) = g(\mathbf{z})^{-1} = \mathbf{z}$, that is counterfactual are searched directly in the feature space. Conversely, *REVISE* traverses the latent space of a variational autoencoder (VAE) fitted to the training data, where $g(\cdot)$ corresponds to the decoder (Joshi et al. 2019). In addition to the distance penalty, *ECCo* uses an additional penalty component that regularizes the energy associated with the counterfactual, $\mathbf{x}'$ (Altmeyer et al. 2024).

H.1.2 Convergence

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

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

H.2 Protecting Mutability Constraints with Linear Classifiers

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

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

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

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

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

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

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

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

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

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 made above. Hence, we have that $(\theta_{y^-,d_{\text{immtbl}}} - \theta_{y^+,d_{\text{immtbl}}}) < 0$ and $(\theta_{y^-,d_{\text{mtbl}}} - \theta_{y^+,d_{\text{mtbl}}}) > 0$

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

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

and equal to zero everywhere else.

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. Similarly, we are more likely to have $(x'_{d_{\text{mtbl}}} - x_{d_{\text{mtbl}}}) > 0$ since $(\mu_{y^-,d_{\text{mtbl}}} > \mu_{y^+,d_{\text{mtbl}}})$.

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

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

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

H.3 Domain Constraints

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

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

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

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

H.4 Training Details

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

I Detailed Results

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.

I.2 Grid Searches

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

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

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

I.2.1 Evaluation Details

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

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

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

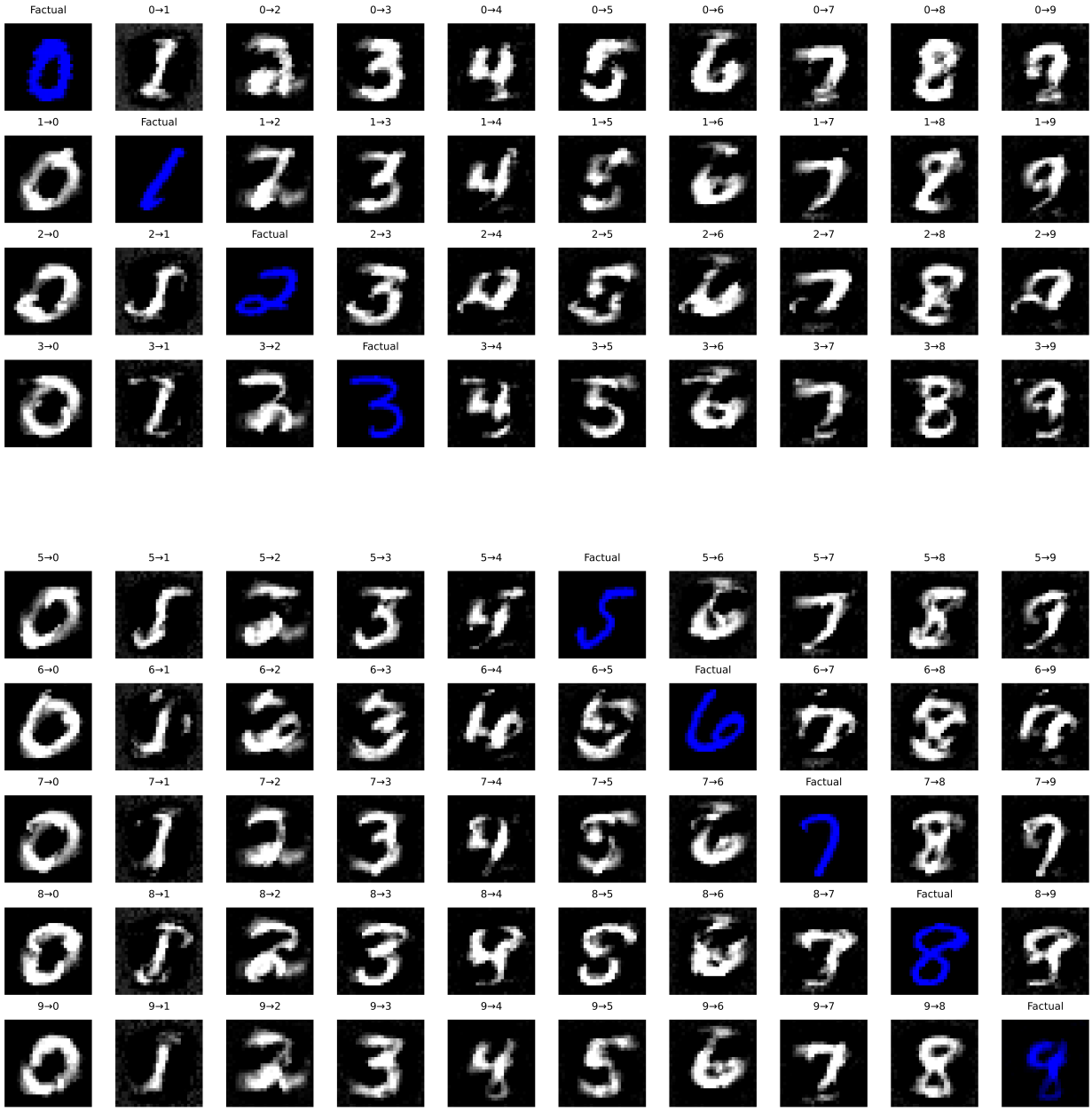

Figure A2: Counterfactual images for *MLP* with counterfactual training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

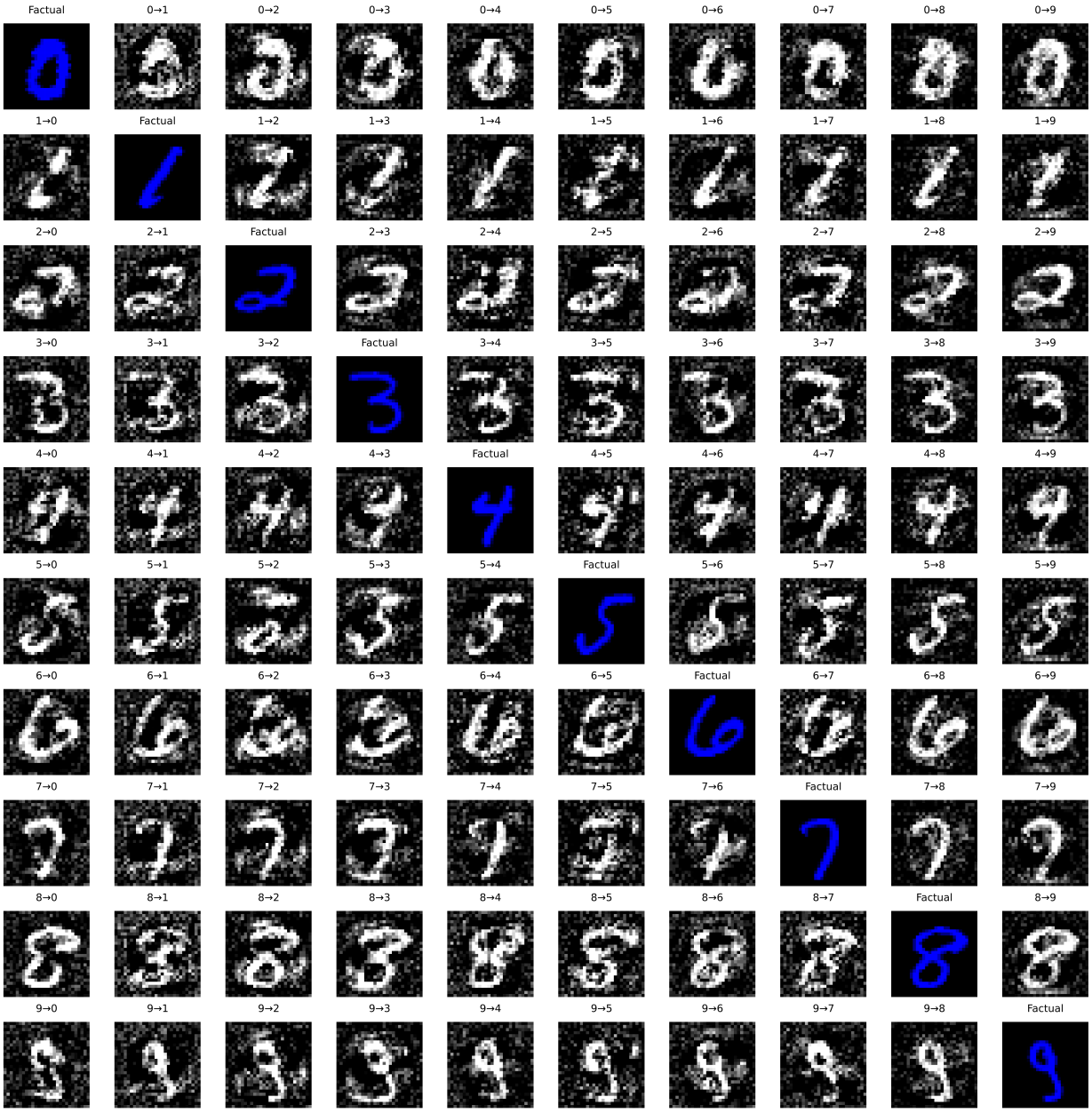

Figure A3: Counterfactual images for *MLP* with conventional training. The underlying generator, *ECCo*, aims to generate counterfactuals that are faithful to the model (Altmeyer et al. 2024).

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

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

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

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

I.2.2 Generator Parameters

The hyperparameter grid with varying generator parameters during training is shown in Note 1. The corresponding 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`
  - λ_{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`

Note 2: Evaluation Phase

- Generator Parameters:
  - λ_{energy}: `0.1, 0.5, 1.0, 5.0, 10.0`

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

I.2.2.2 Plausibility

The results with respect to the plausibility measure are shown in Figure A4 to Figure A7.

I.2.2.3 Cost

The results with respect to the cost measure are shown in Figure A8 to Figure A11.

I.2.3 Penalty Strengths

The hyperparameter grid with varying penalty strengths during training is shown in Note 3. The corresponding evaluation grid used for these experiments is shown in Note 4.

Note 3: Training Phase

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

Note 4: Evaluation Phase

- Generator Parameters:
  - λ_{energy}: `0.1, 0.5, 1.0, 5.0, 10.0`

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.

Dataset	Variable	Objective	Mean	Std
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

I.2.3.2 Plausibility

The results with respect to the plausibility measure are shown in Figure A12 to Figure A15.

I.2.3.3 Cost

The results with respect to the cost measure are shown in Figure A16 to Figure A19.

I.2.4 Other Parameters

The hyperparameter grid with other varying training parameters is shown in Note 5. The corresponding evaluation 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`

Note 6: Evaluation Phase

- Generator Parameters:
  - λ_{energy}: `0.1, 0.5, 1.0, 5.0, 10.0`

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).

Dataset	Variable	Objective	Mean	Std
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

I.2.4.2 Plausibility

The results with respect to the plausibility measure are shown in Figure A20 to Figure A23.

I.2.4.3 Cost

The results with respect to the cost measure are shown in Figure A24 to Figure A27.

I.3 Hyperparameter Tuning

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

Finally, to increase the proportion of mature counterfactuals for some datasets, we have also investigated the effect on the learning rate η for the counterfactual search and even smaller regularization strengths for a fixed decision threshold of 0.5 (Figure A46 to Figure A50). For the given low decision threshold, we find that the learning rate has no discernable impact on the proportion of mature counterfactuals (Figure A51 to Figure A55). We do notice, however, that the results for MNIST are much improved when using a low value λ_{reg}, the strength for the engery regularization: plausibility is increased by up to ~10ppt (Figure A49) and the proportion of mature counterfactuals reaches 100%.

One consideration worth exploring is to combine high decision thresholds with high learning rates, which we have not investigated here.

> 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`.

I.3.1 Key Parameters

The hyperparameter grid for tuning key parameters is shown in Note 7. The corresponding evaluation grid used for 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:
> - λ_{reg}: `0.1, 0.25, 0.5`
> - Objective: `full, vanilla`

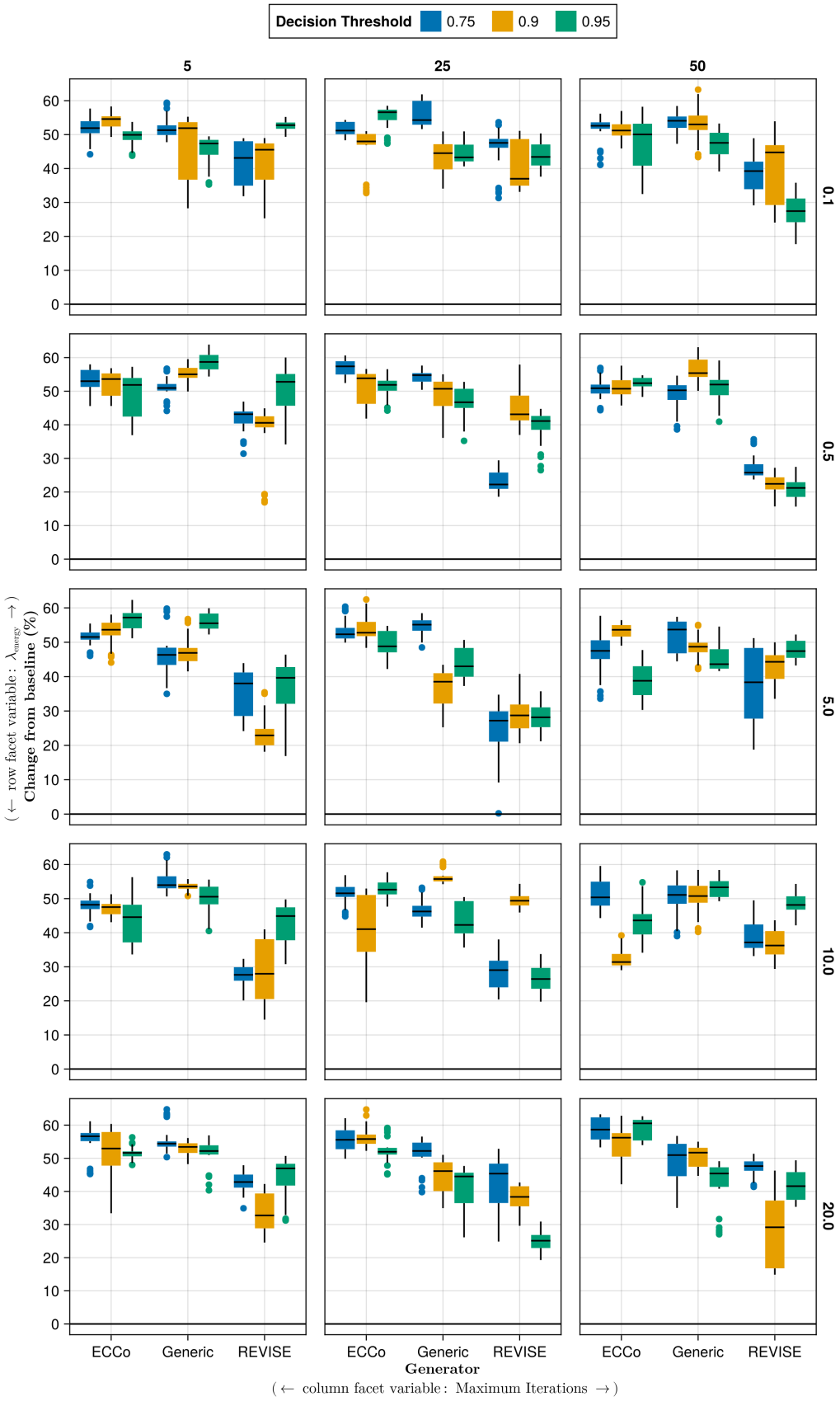

Figure A4: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

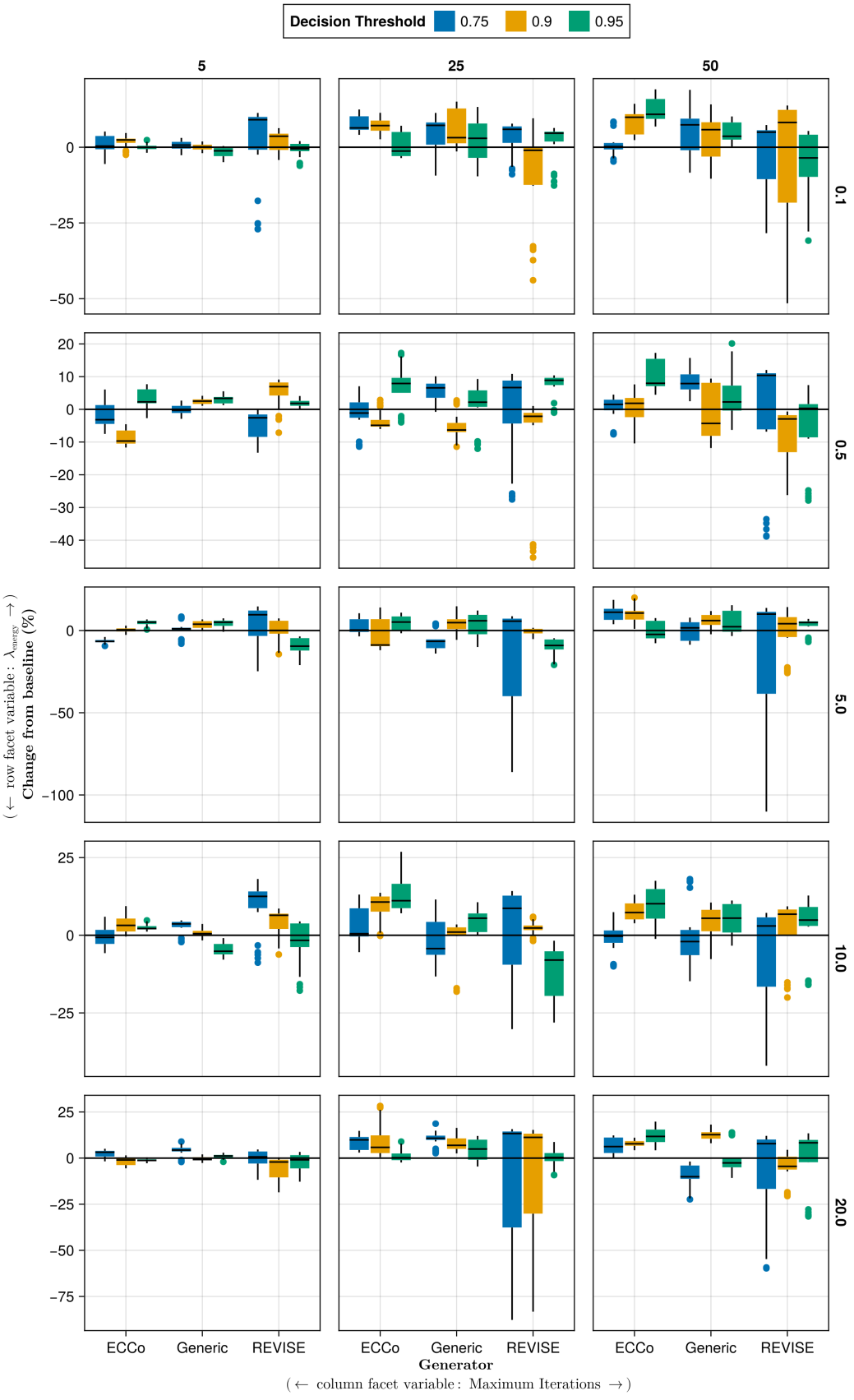

Figure A5: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

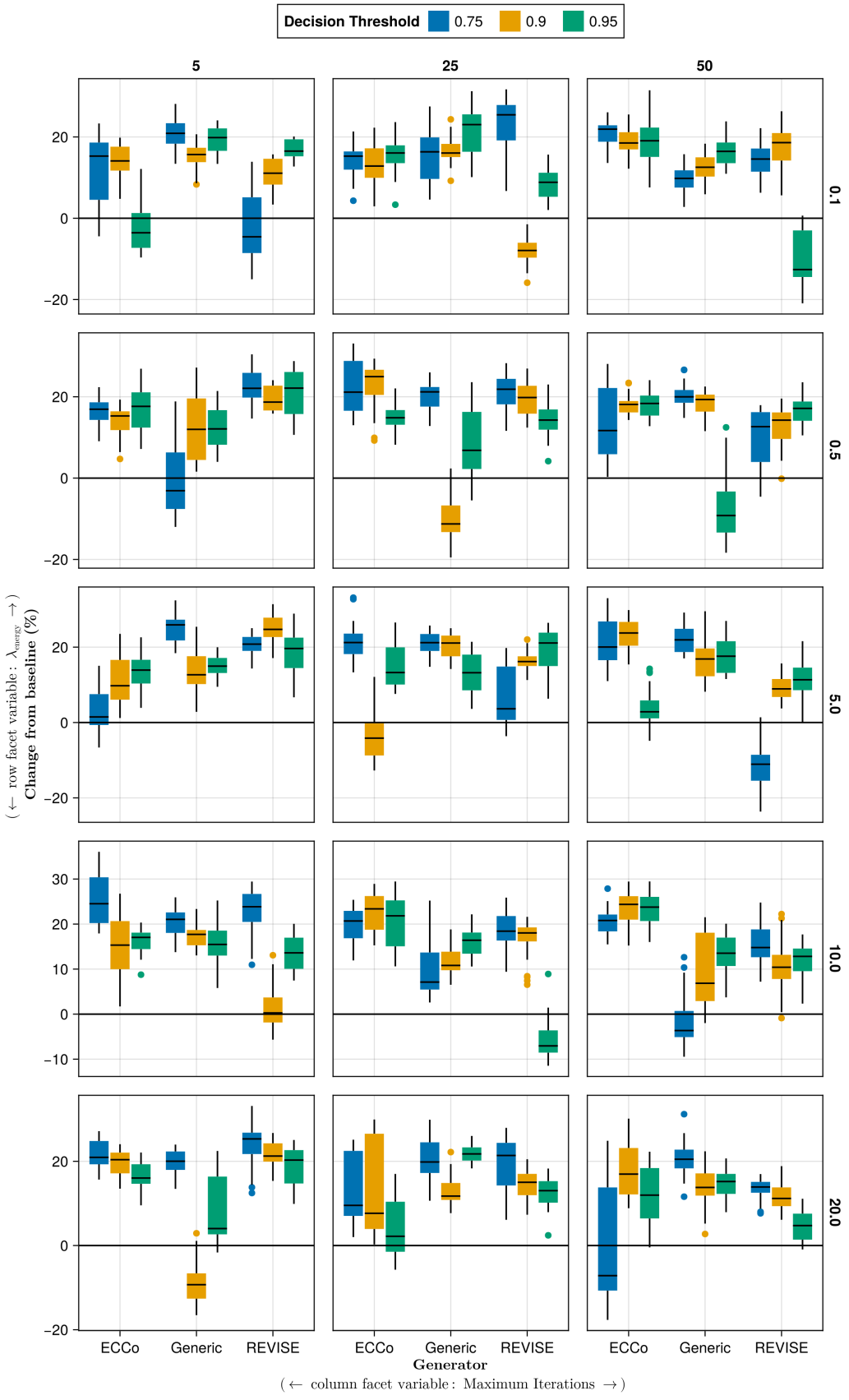

Figure A6: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

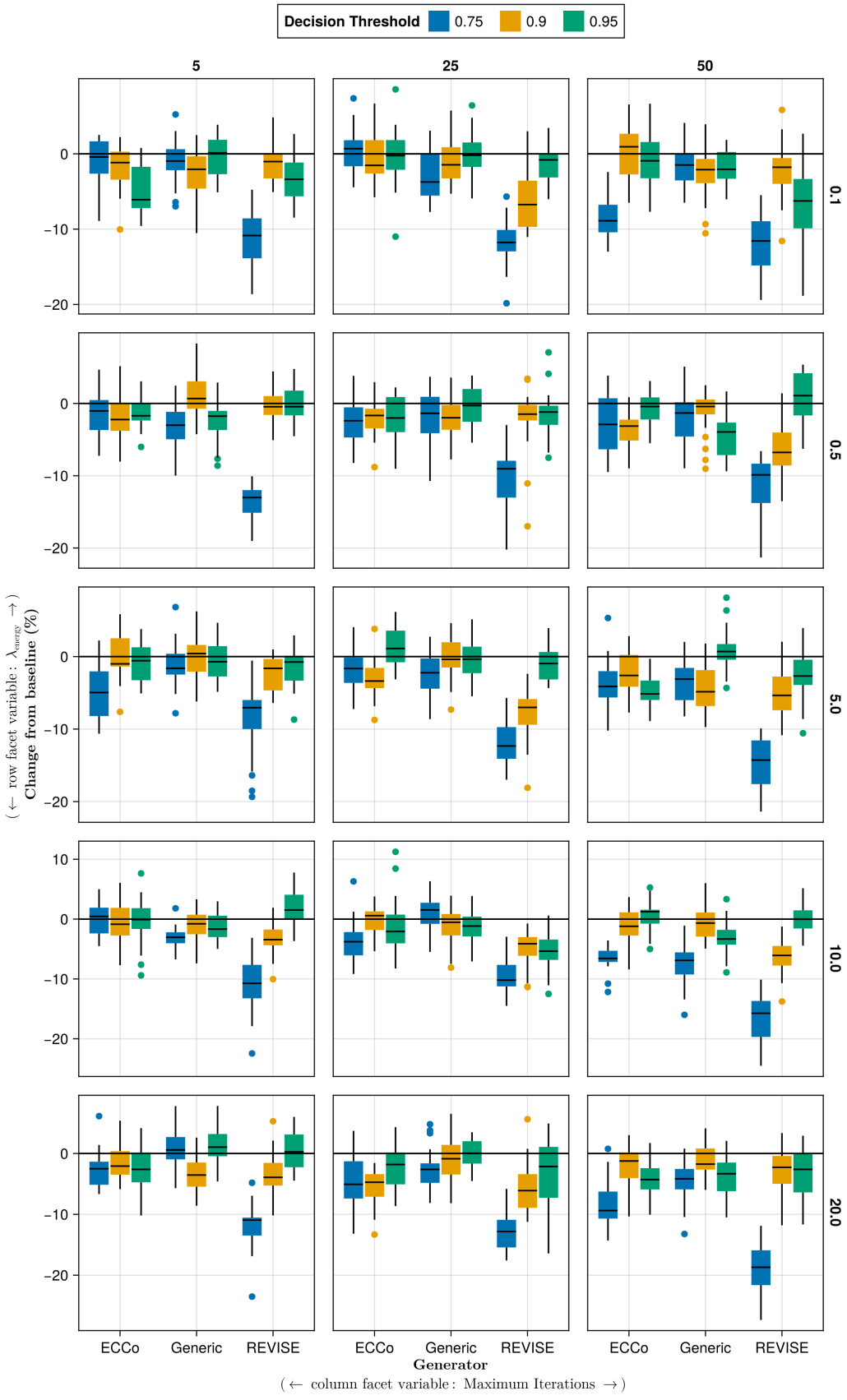

Figure A7: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

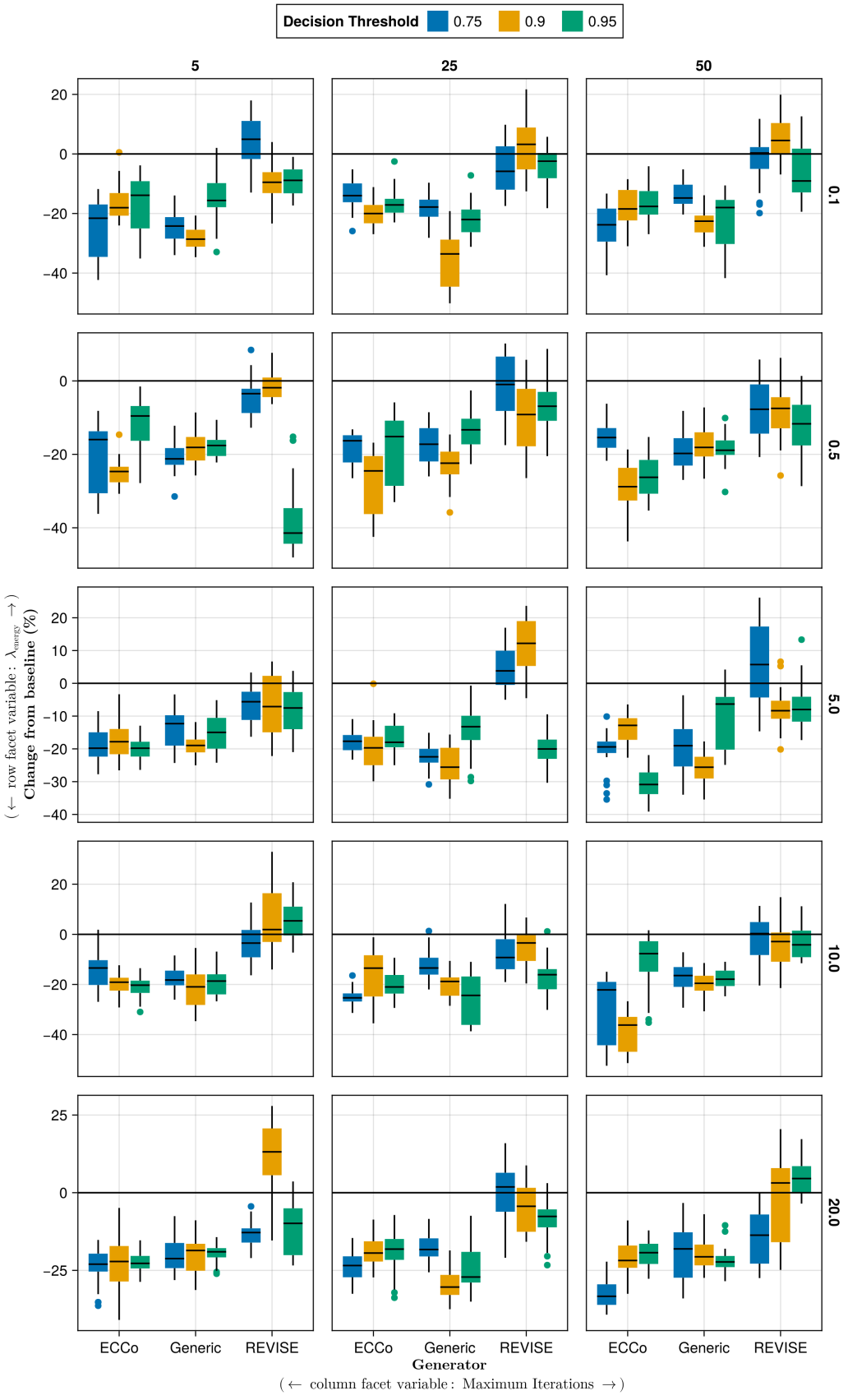

Figure A8: Average outcomes for the cost measure across hyperparameters. Data: Circles.

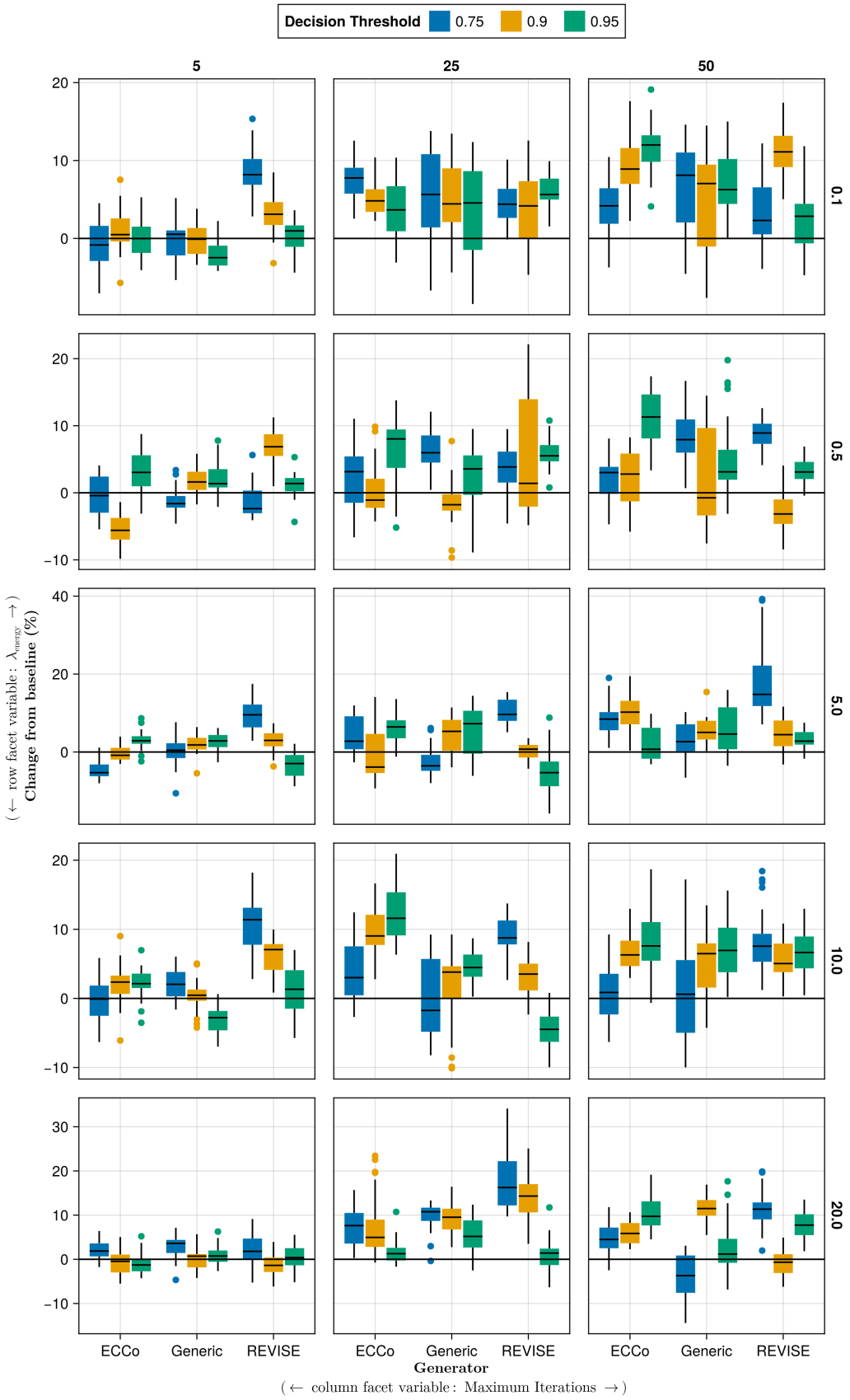

Figure A9: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

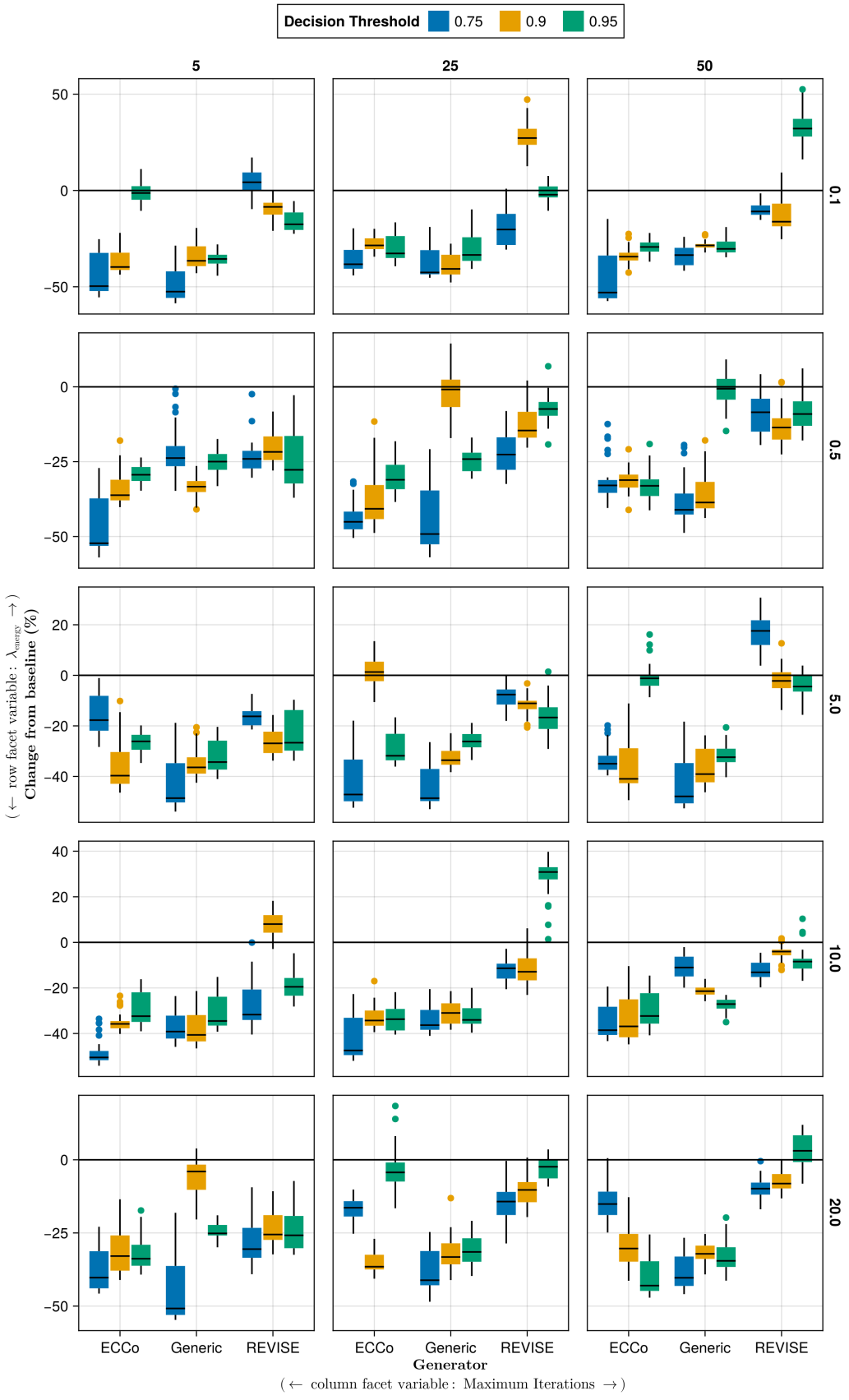

Figure A10: Average outcomes for the cost measure across hyperparameters. Data: Moons.

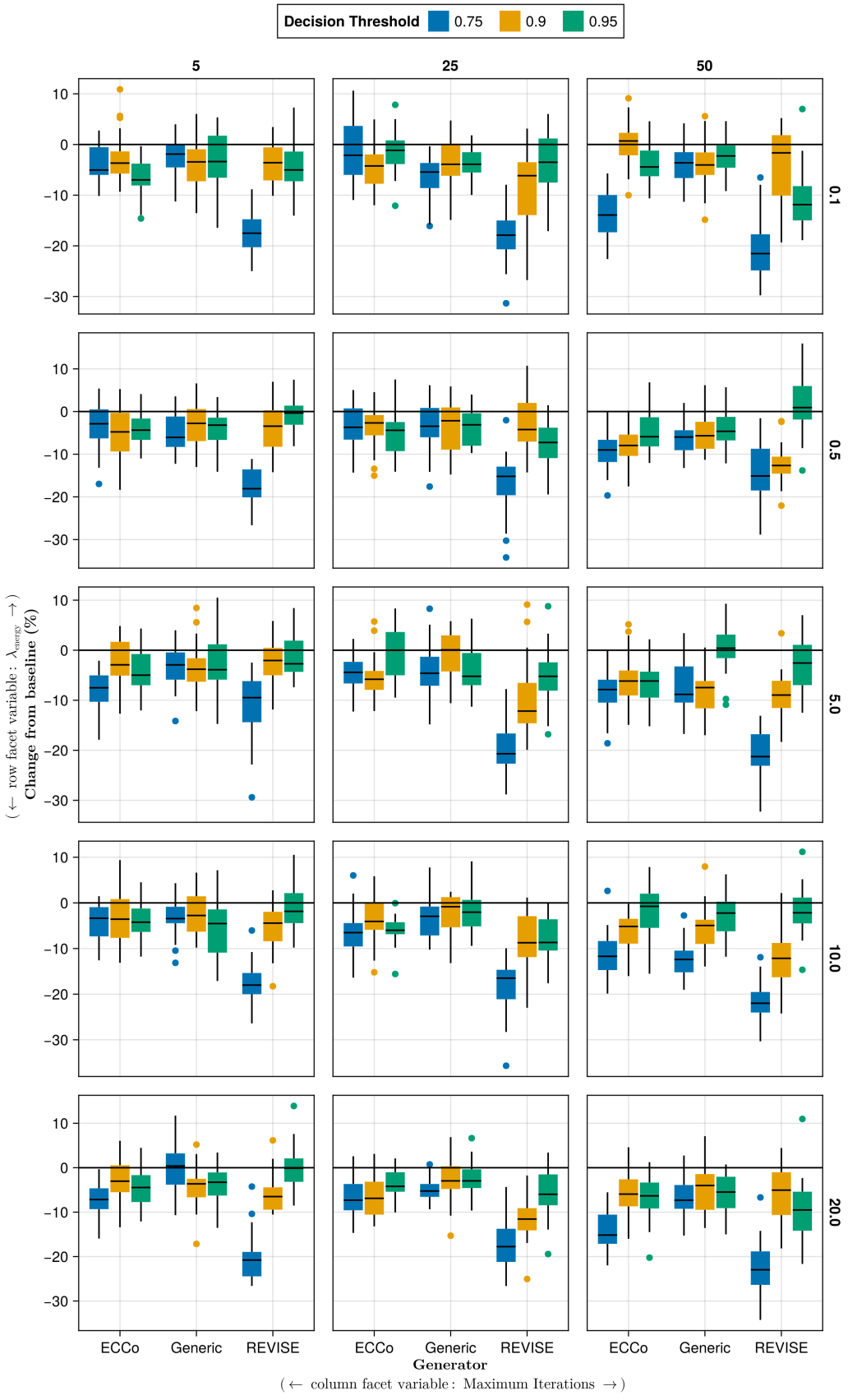

Figure A11: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

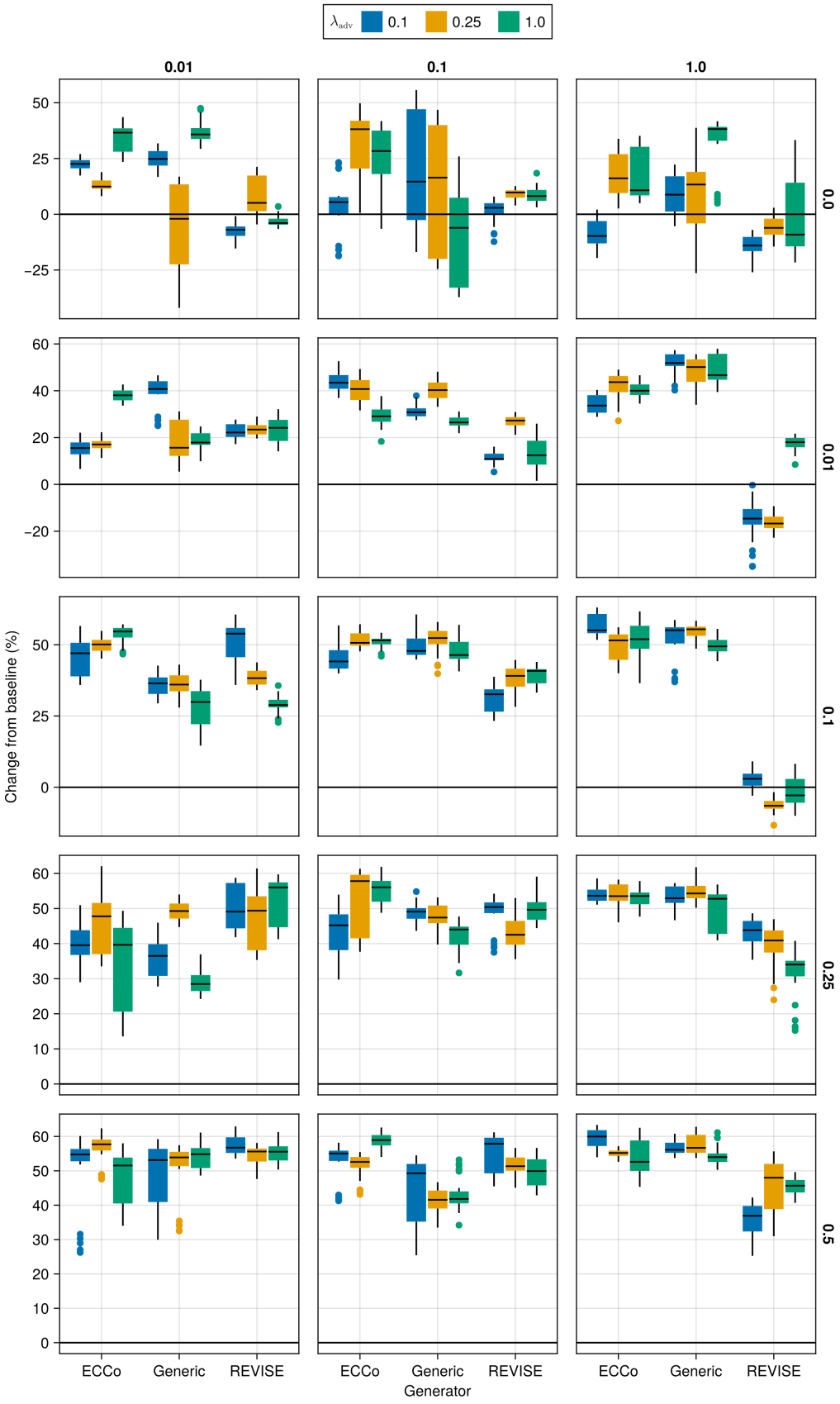

Figure A12: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

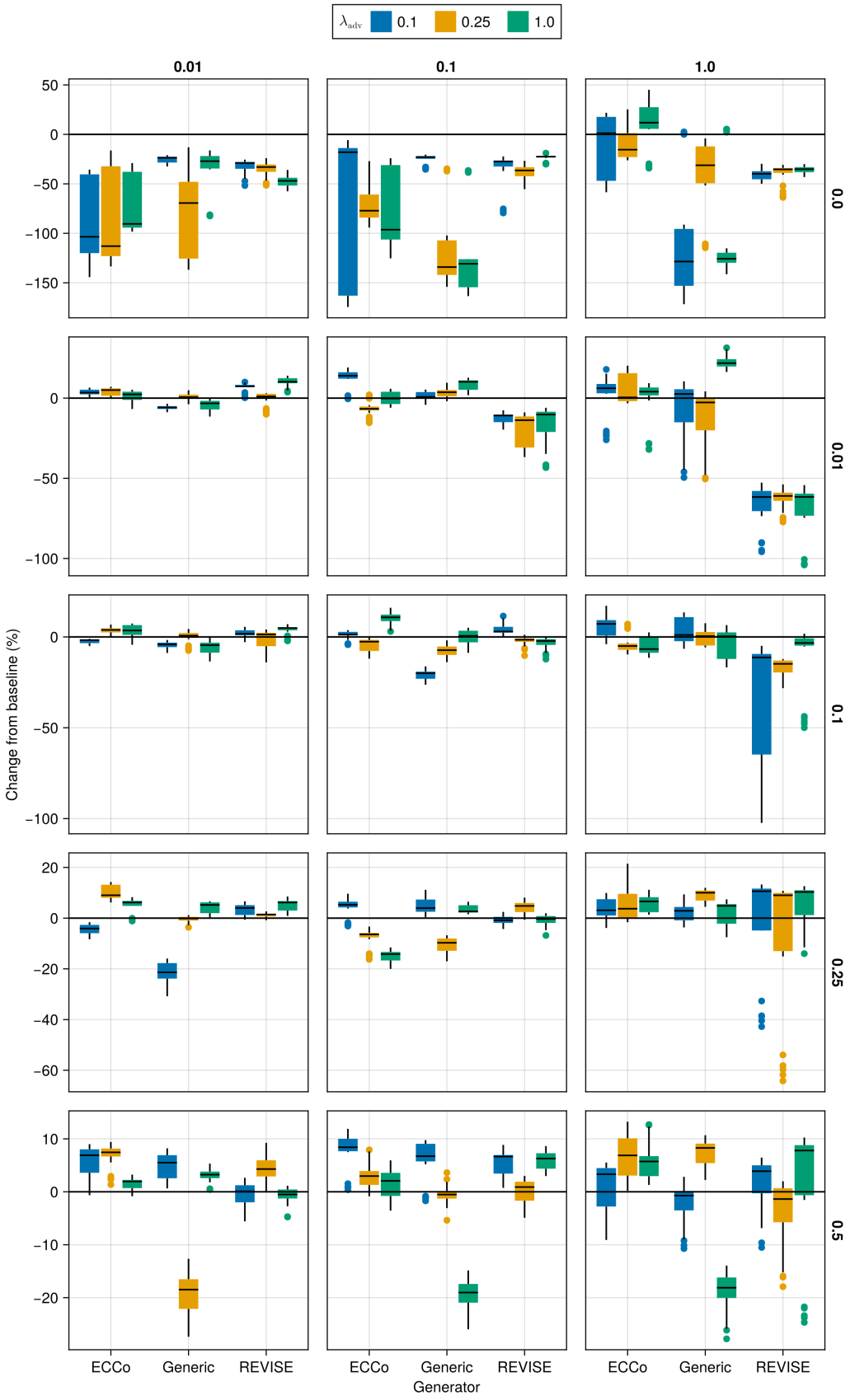

Figure A13: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

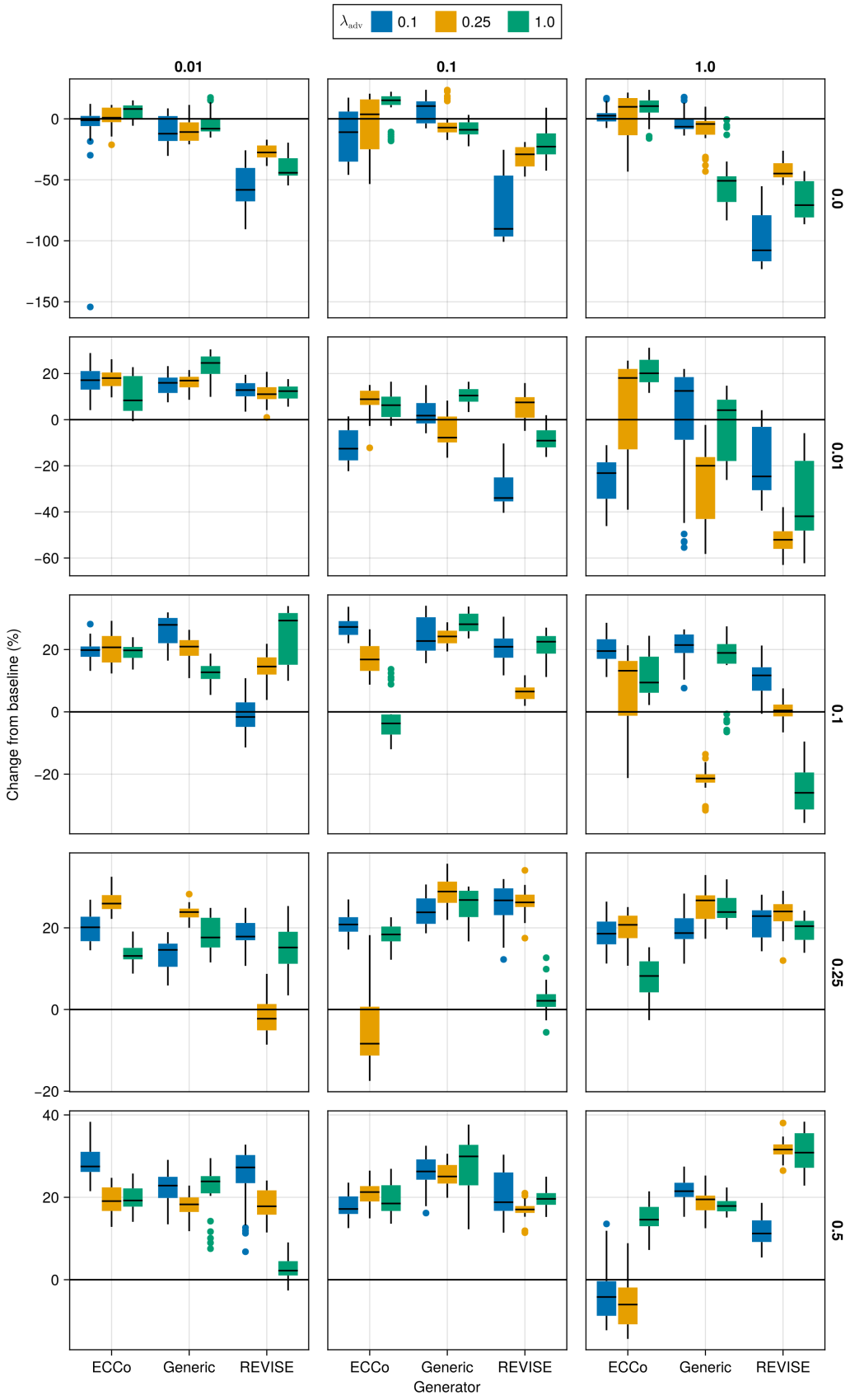

Figure A14: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

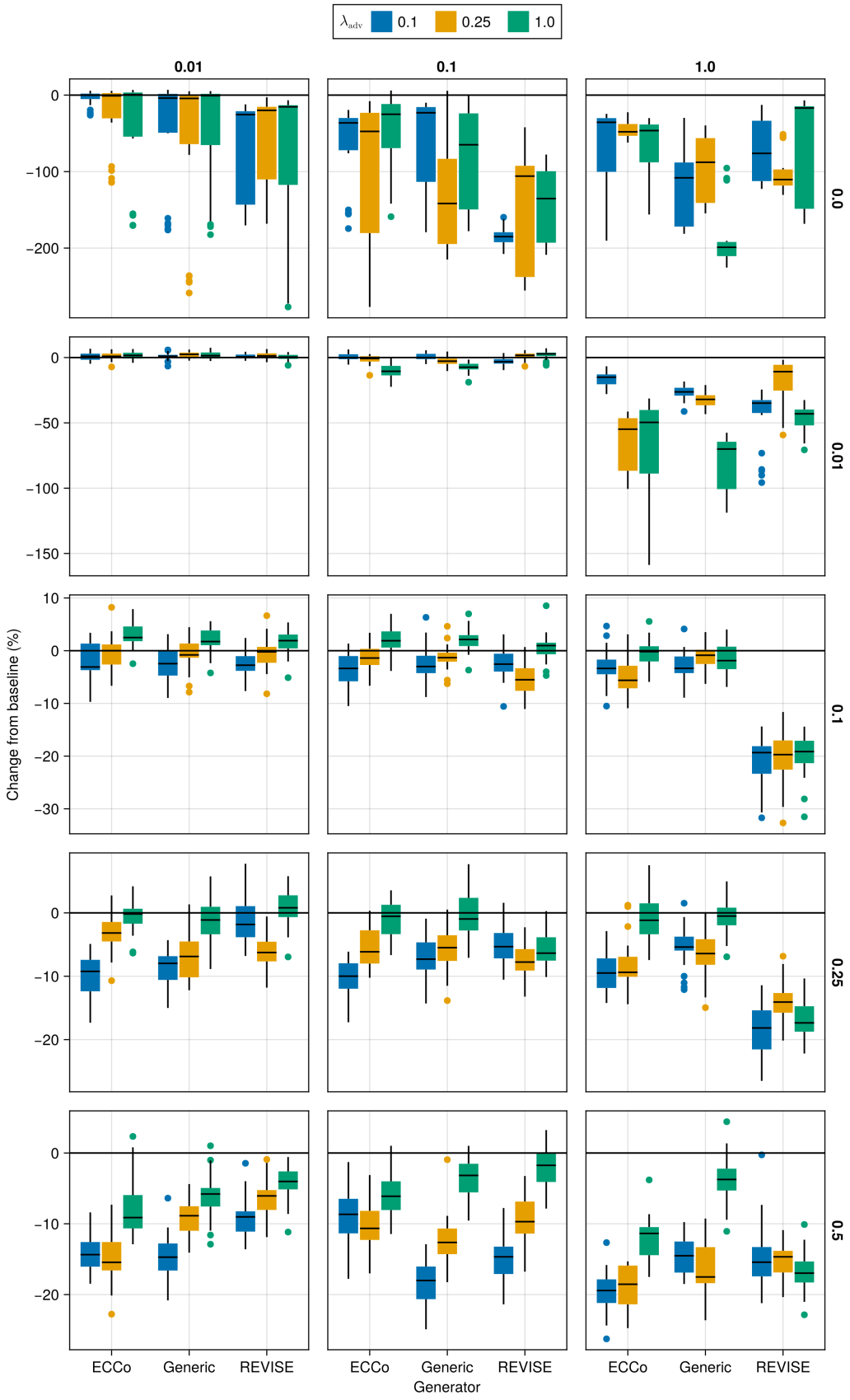

Figure A15: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

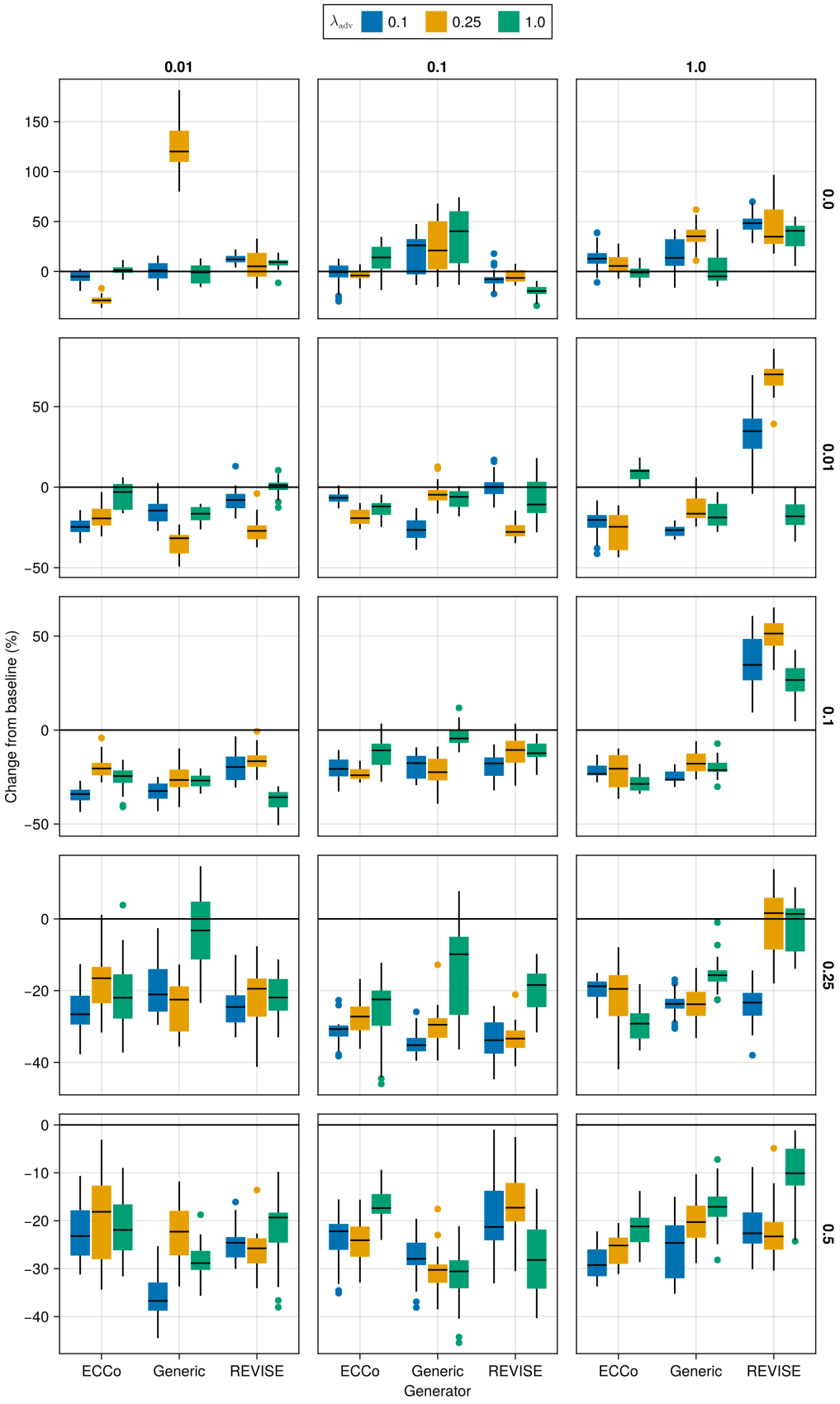

Figure A16: Average outcomes for the cost measure across hyperparameters. Data: Circles.

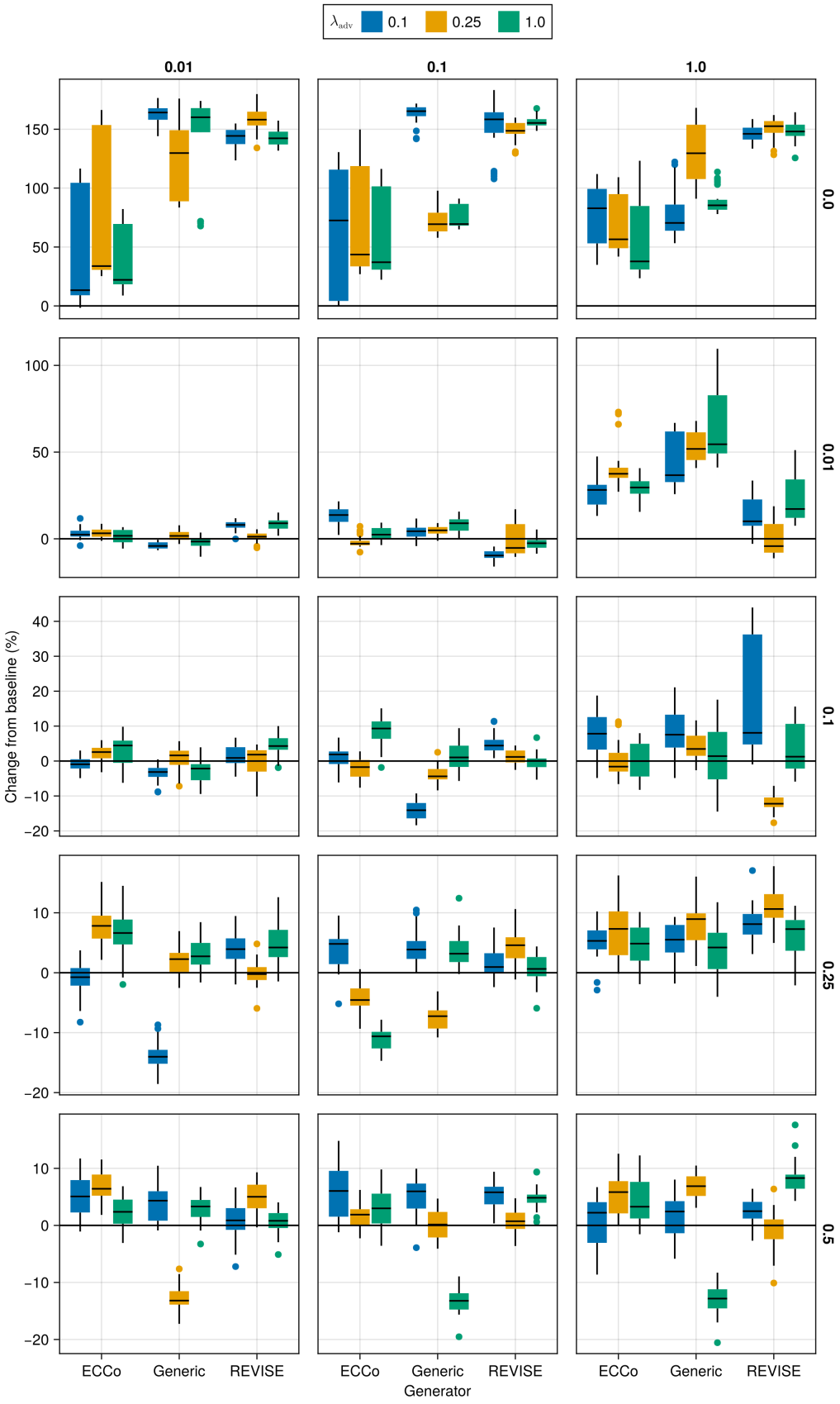

Figure A17: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

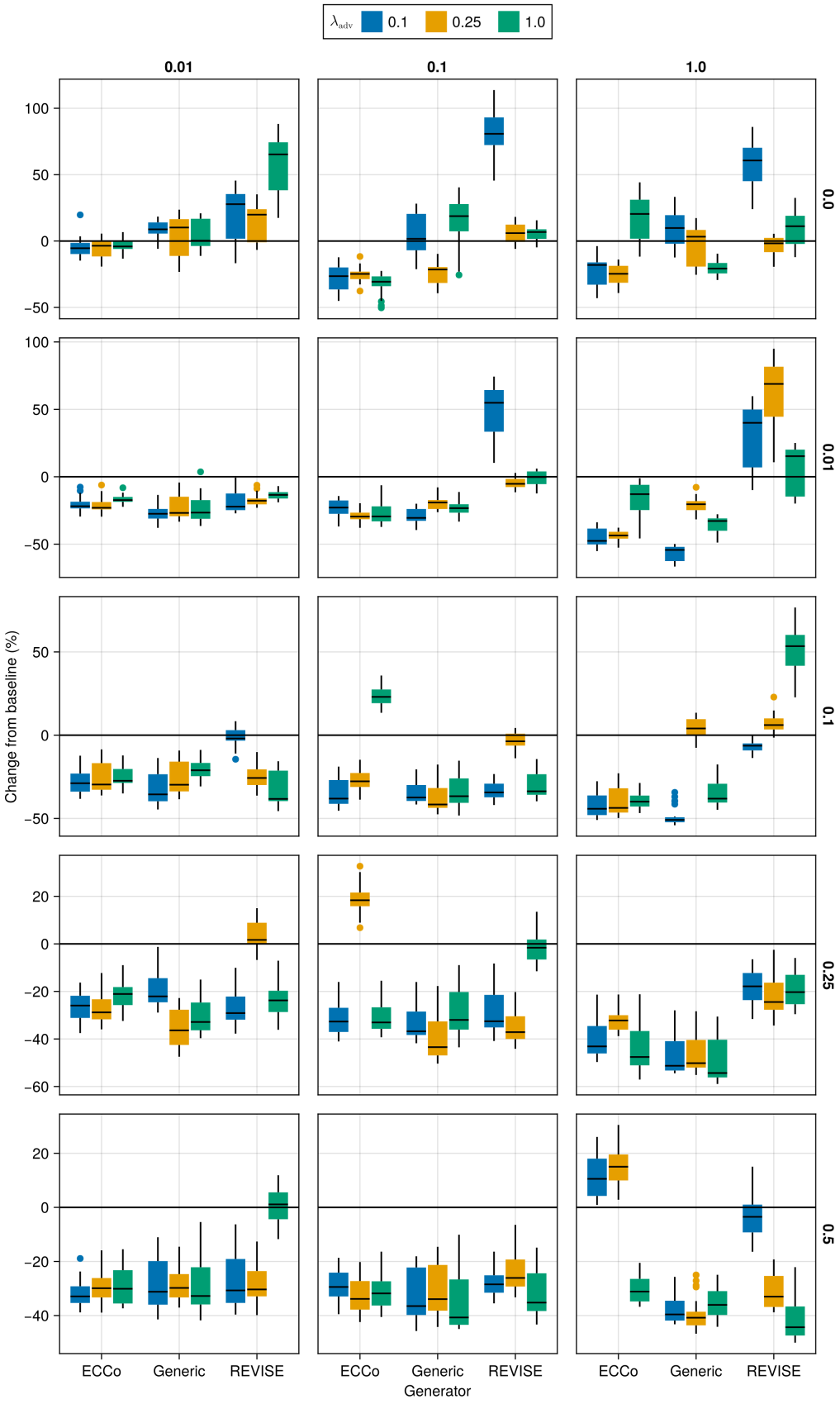

Figure A18: Average outcomes for the cost measure across hyperparameters. Data: Moons.

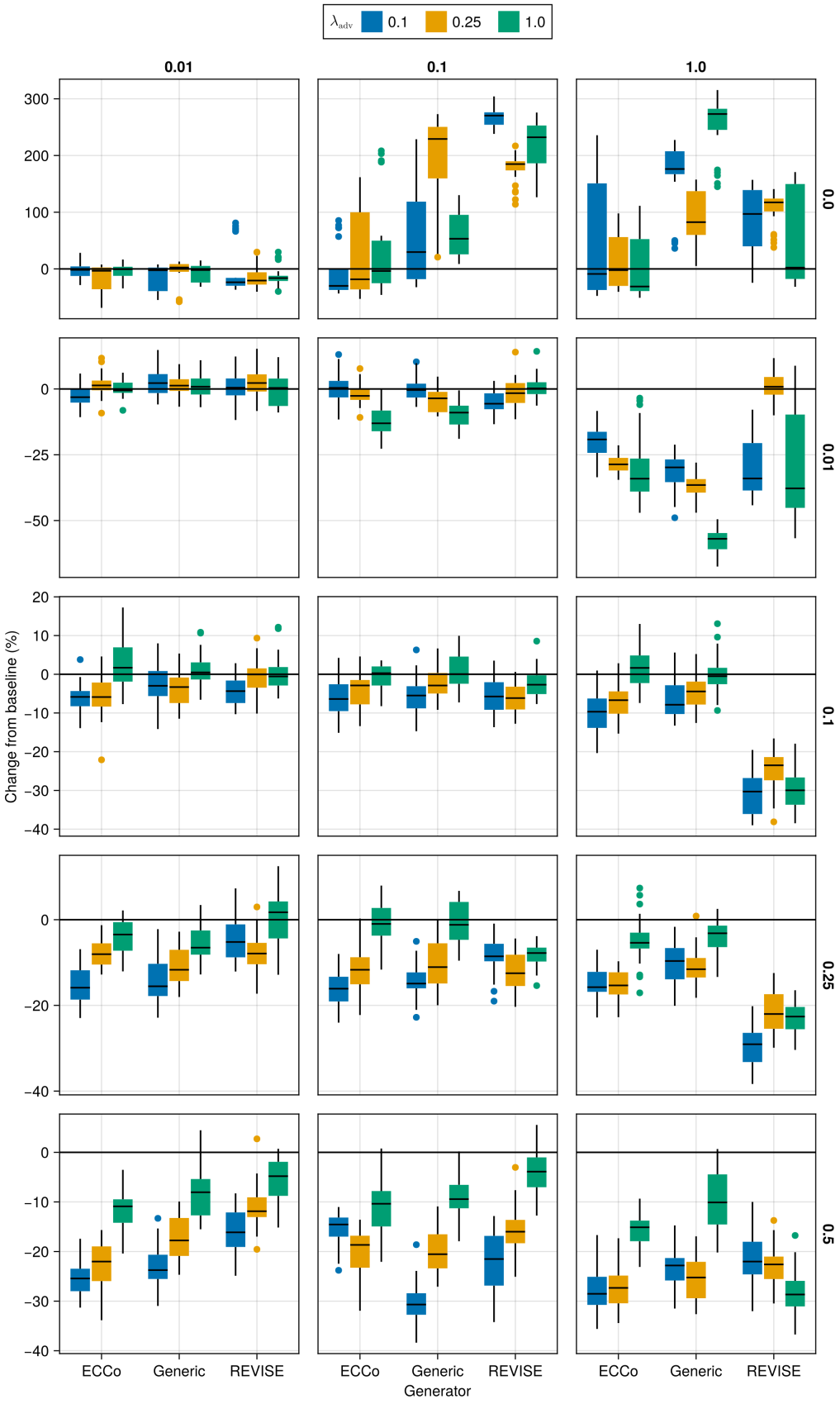

Figure A19: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

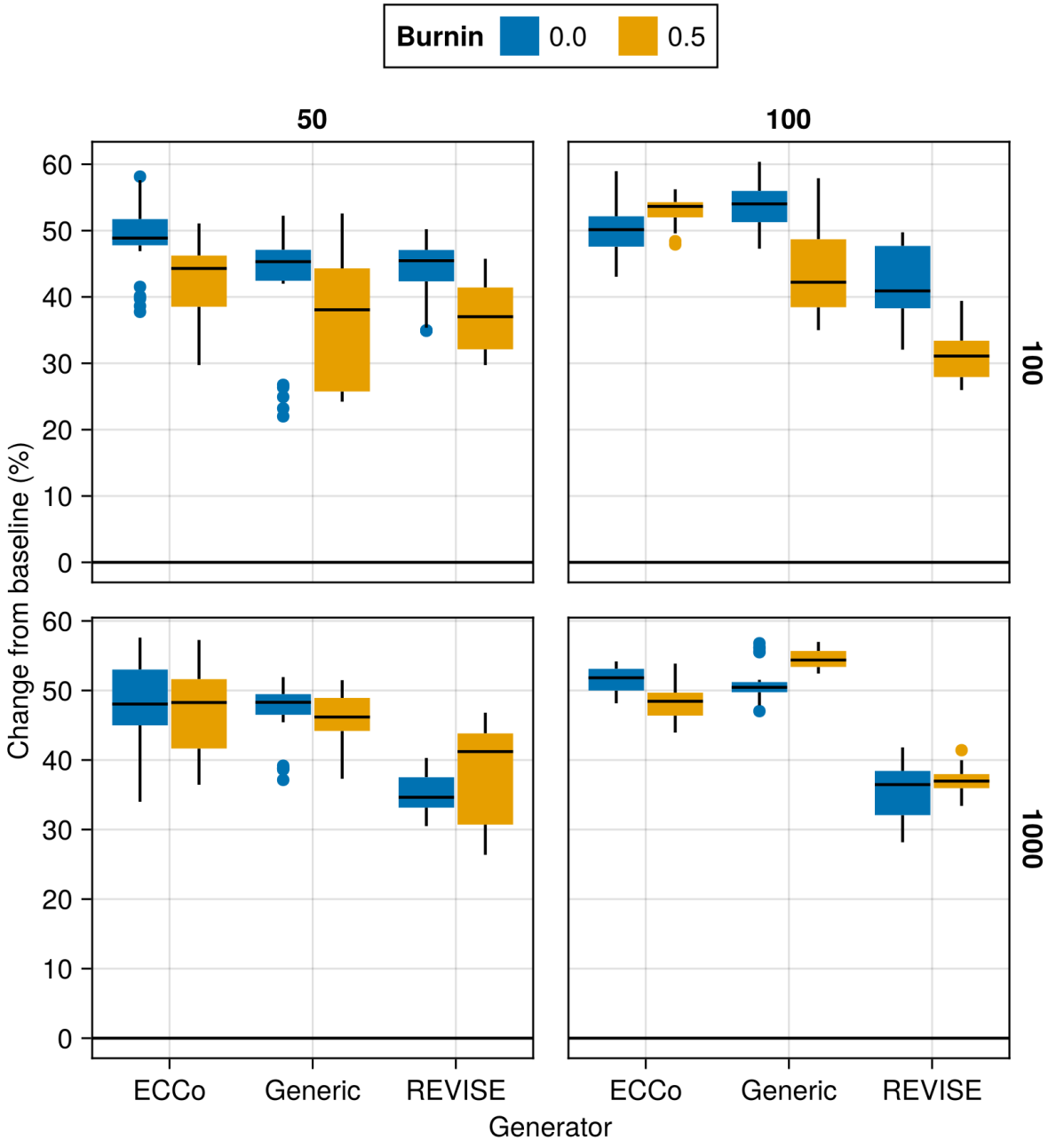

Figure A20: Average outcomes for the plausibility measure across hyperparameters. Data: Circles.

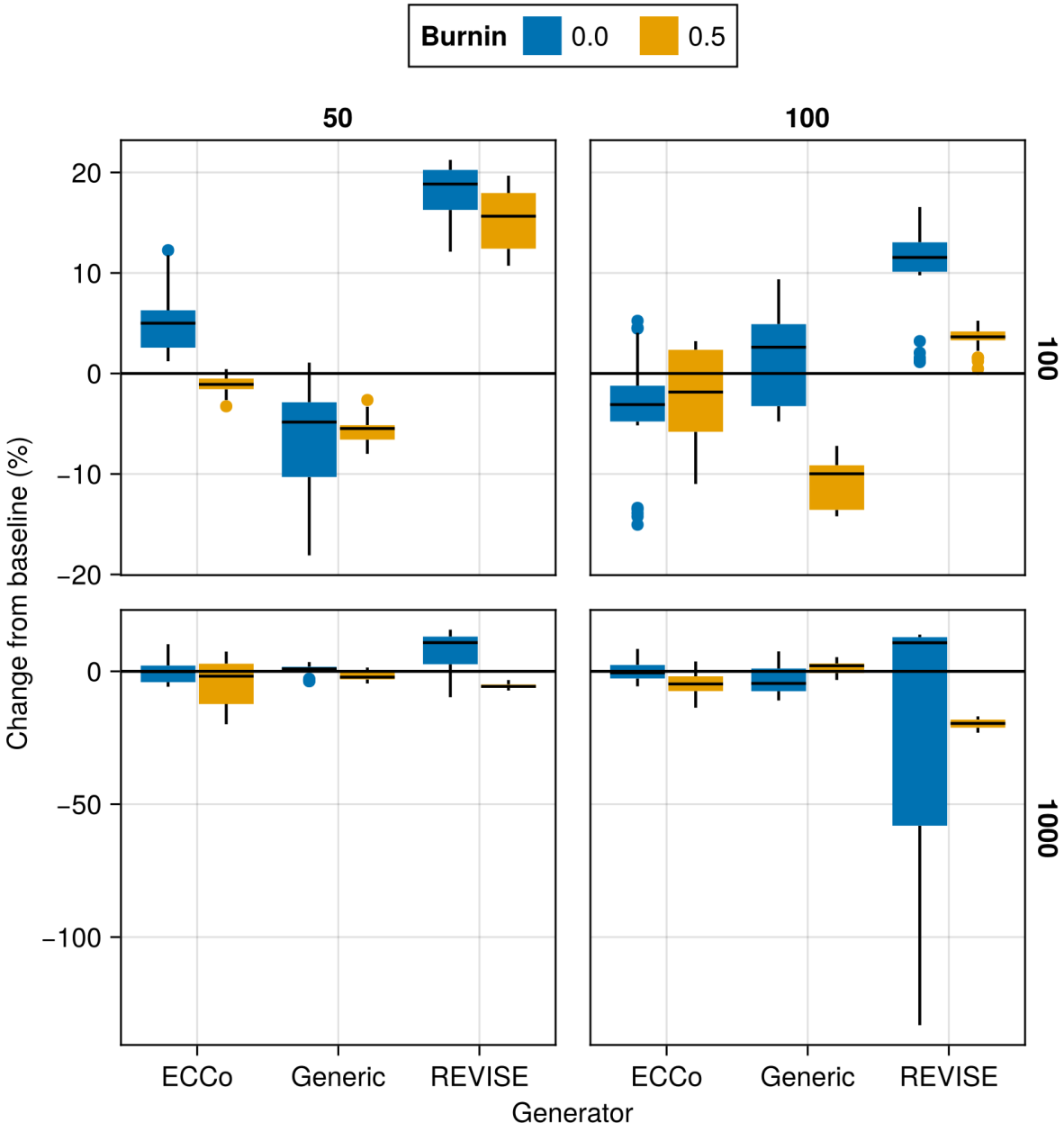

Figure A21: Average outcomes for the plausibility measure across hyperparameters. Data: Linearly Separable.

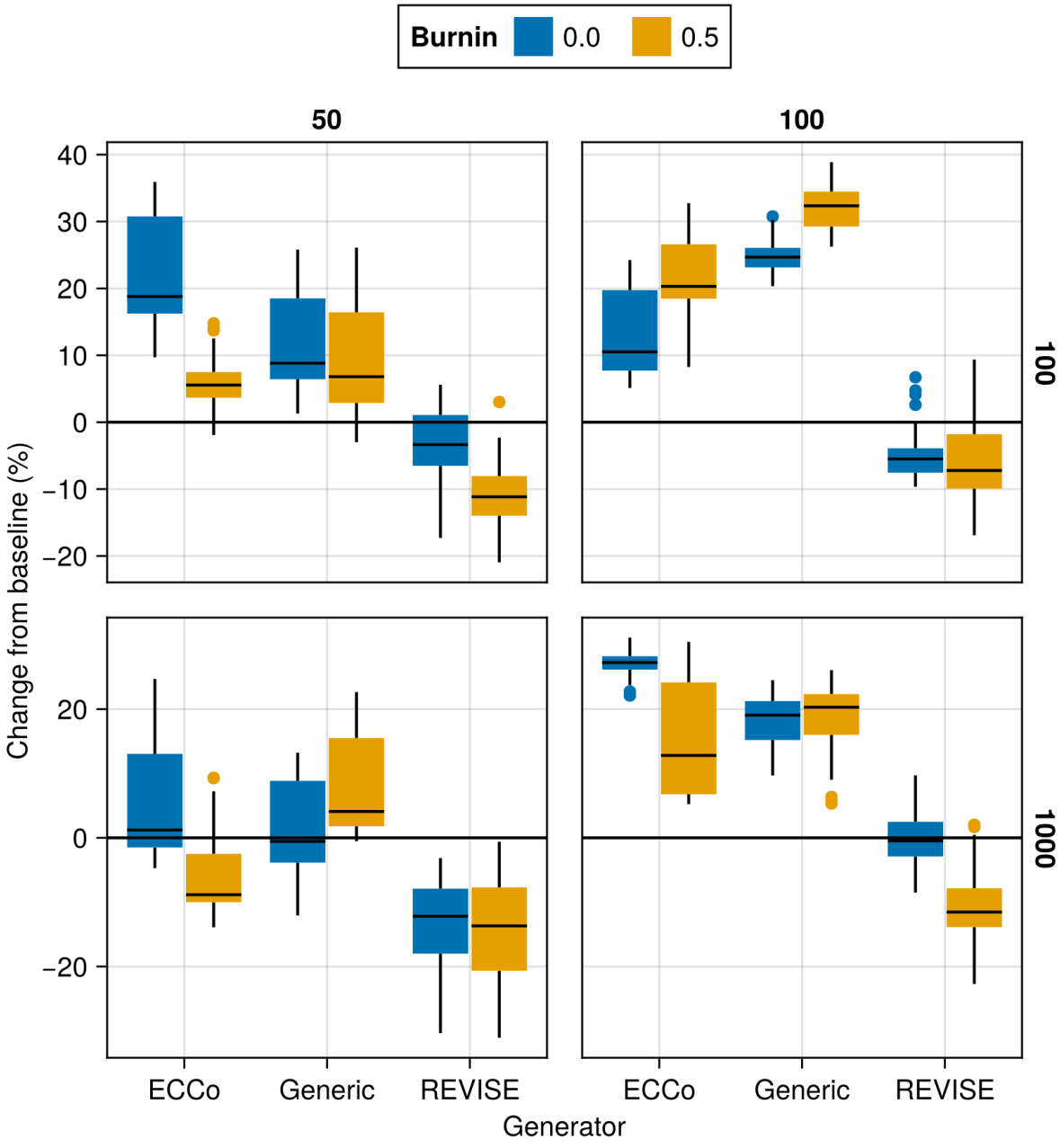

Figure A22: Average outcomes for the plausibility measure across hyperparameters. Data: Moons.

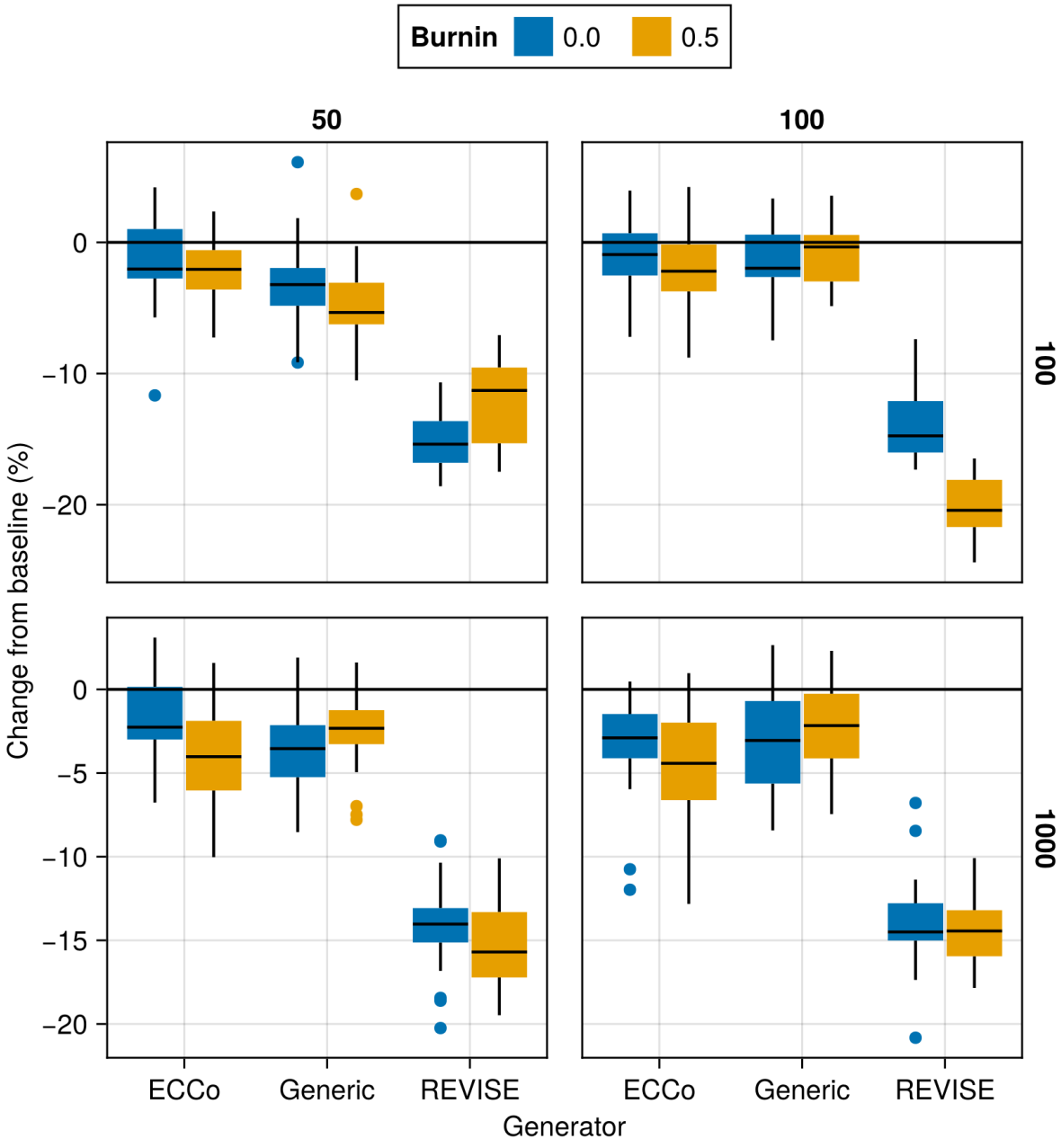

Figure A23: Average outcomes for the plausibility measure across hyperparameters. Data: Overlapping.

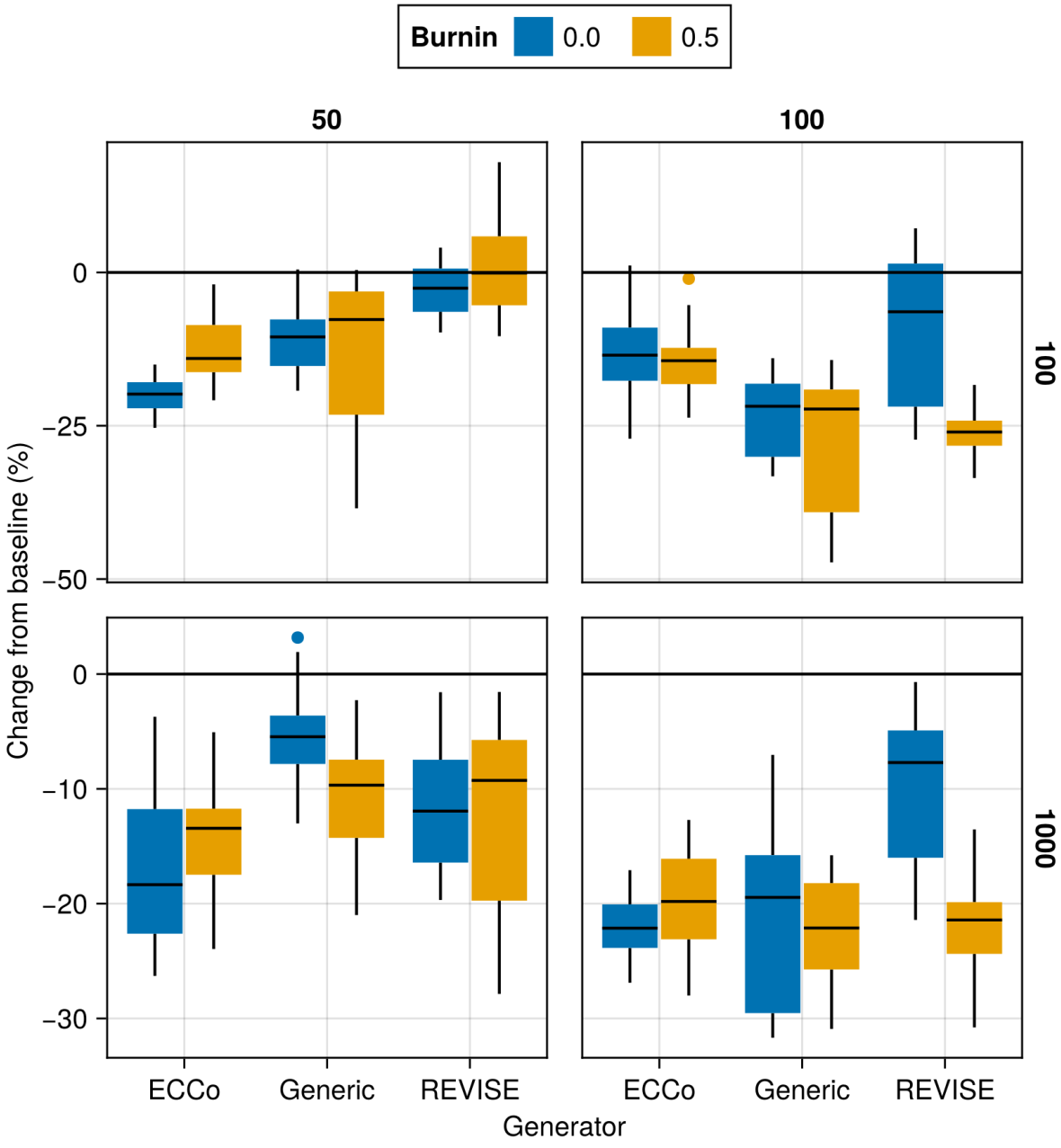

Figure A24: Average outcomes for the cost measure across hyperparameters. Data: Circles.

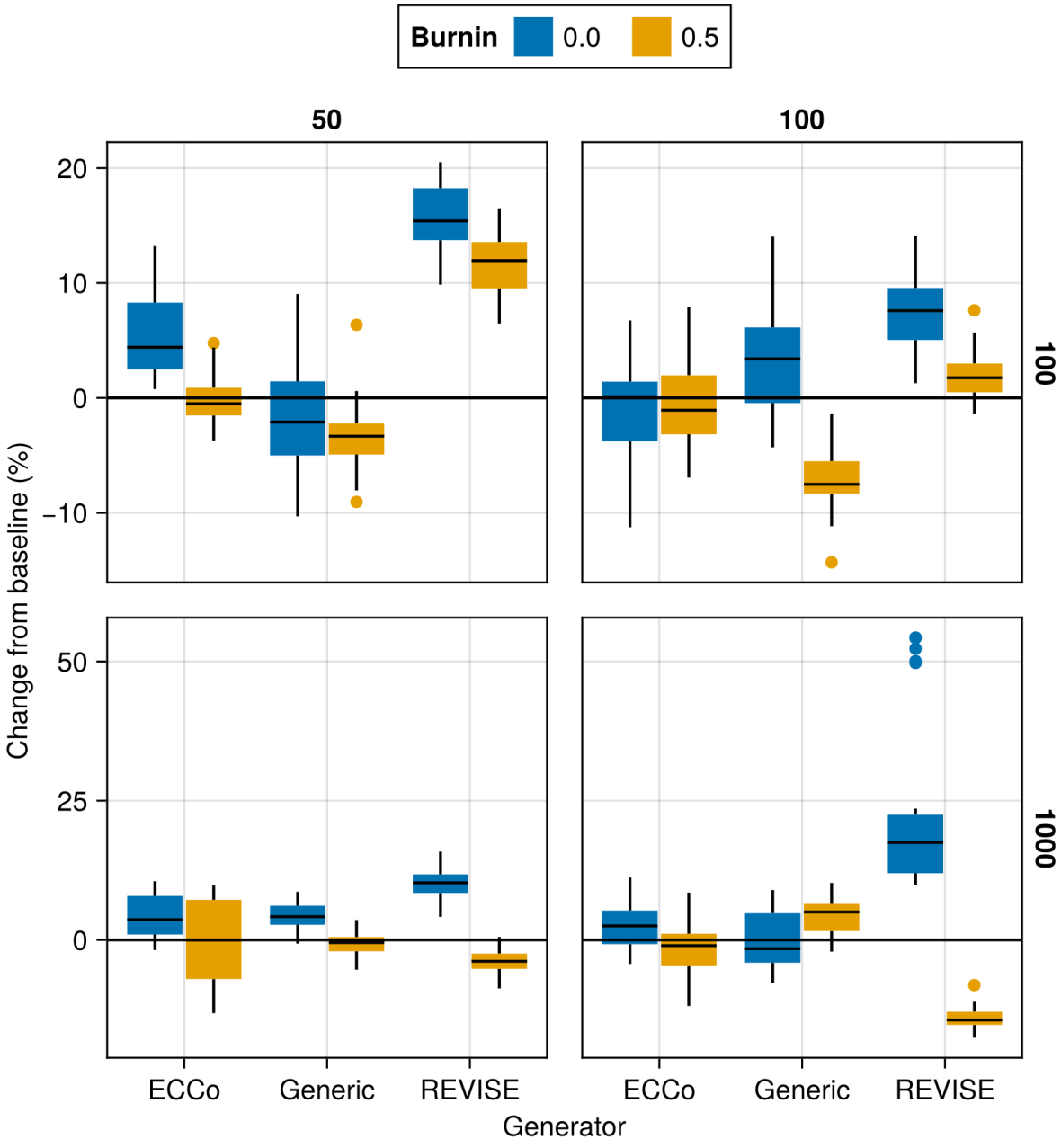

Figure A25: Average outcomes for the cost measure across hyperparameters. Data: Linearly Separable.

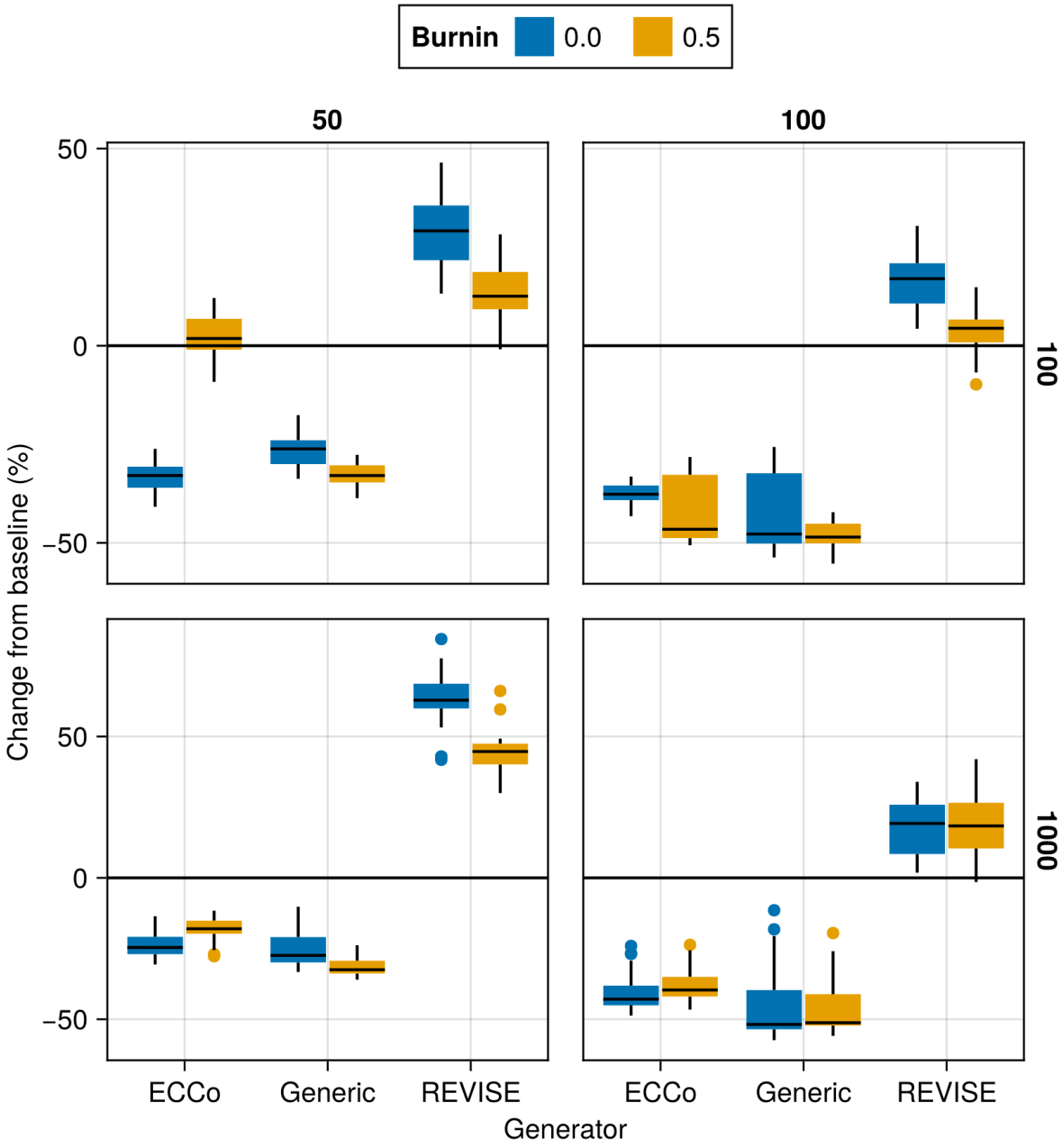

Figure A26: Average outcomes for the cost measure across hyperparameters. Data: Moons.

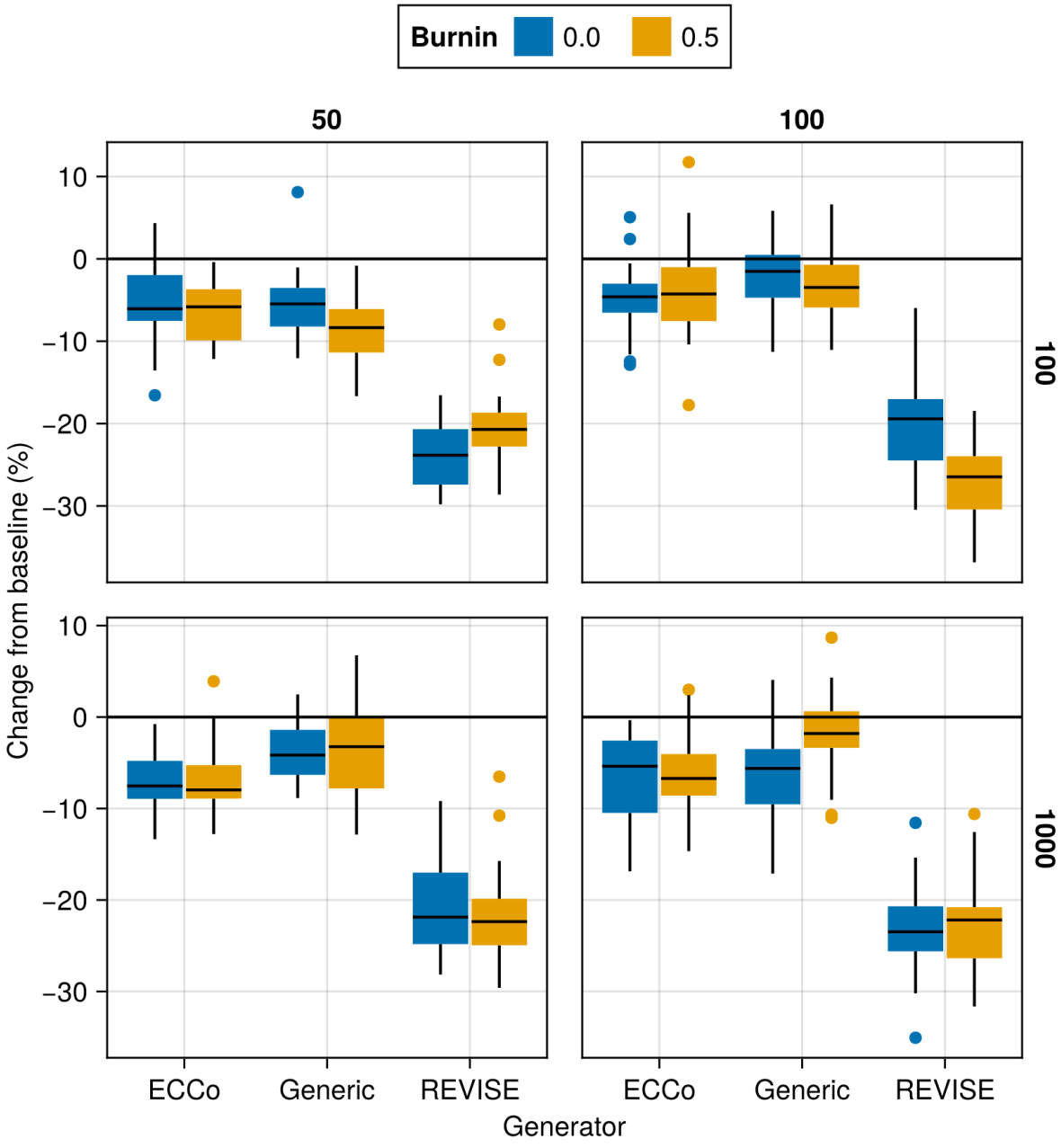

Figure A27: Average outcomes for the cost measure across hyperparameters. Data: Overlapping.

Note 8: Evaluation Phase

- Generator Parameters:
  - λ_{energy}: `0.1, 0.5, 1.0, 5.0, 10.0`

I.3.1.1 Plausibility

The results with respect to the plausibility measure are shown in Figure A28 to Figure A36.

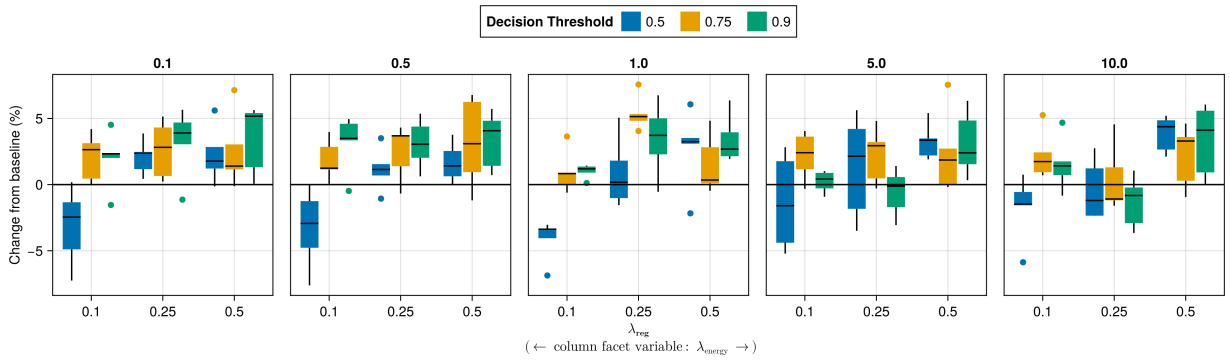

Figure A28: Average outcomes for the plausibility measure across key hyperparameters. Data: Adult.

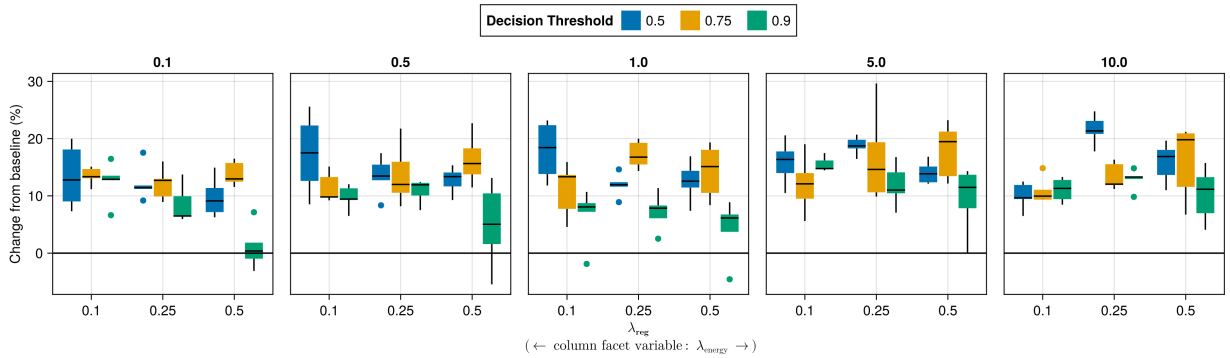

Figure A29: Average outcomes for the plausibility measure across key hyperparameters. Data: California Housing.

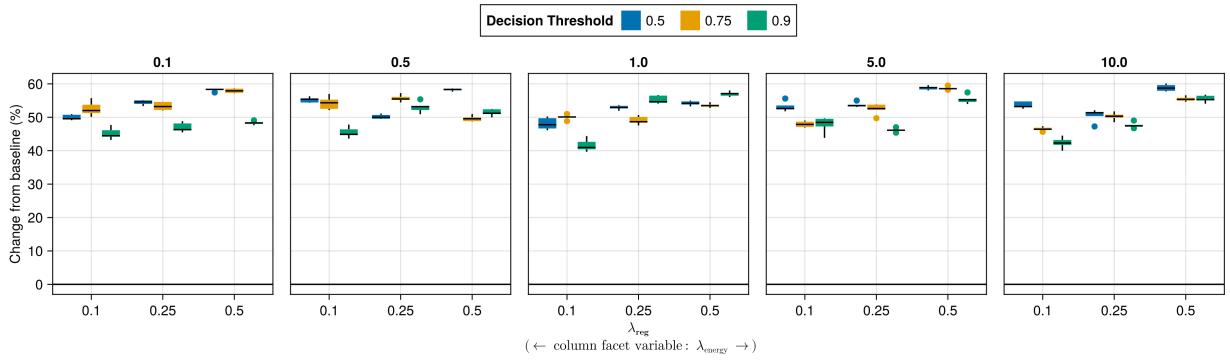

Figure A30: Average outcomes for the plausibility measure across key hyperparameters. Data: Circles.

I.3.1.2 Proportion of Mature CE

The results with respect to the proportion of mature counterfactuals in each epoch are shown in Figure A37 to Figure A45.

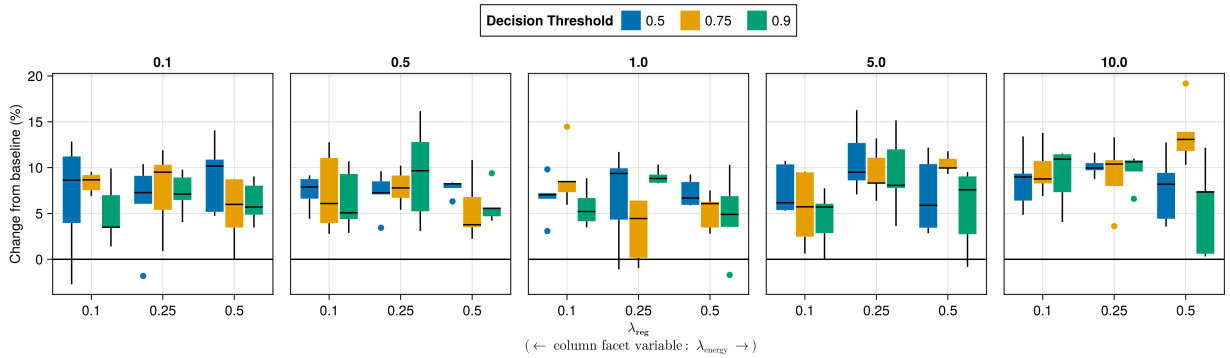

Figure A31: Average outcomes for the plausibility measure across key hyperparameters. Data: Credit.

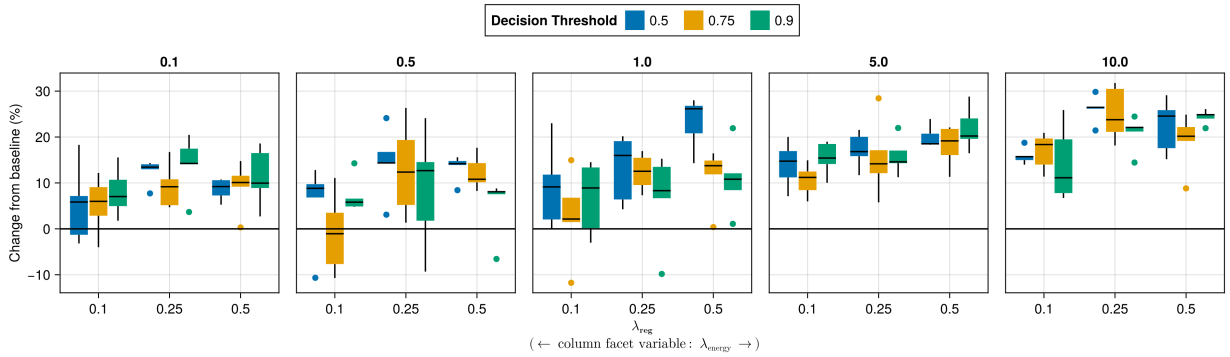

Figure A32: Average outcomes for the plausibility measure across key hyperparameters. Data: GMSC.

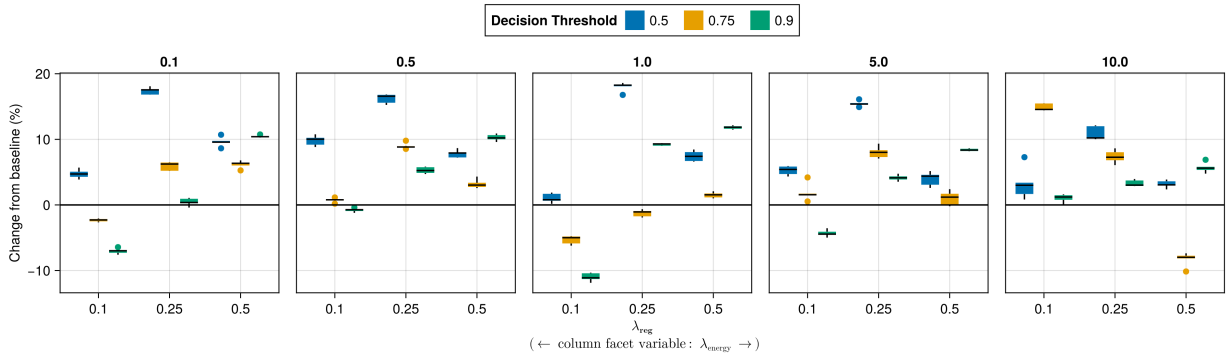

Figure A33: Average outcomes for the plausibility measure across key hyperparameters. Data: Linearly Separable.

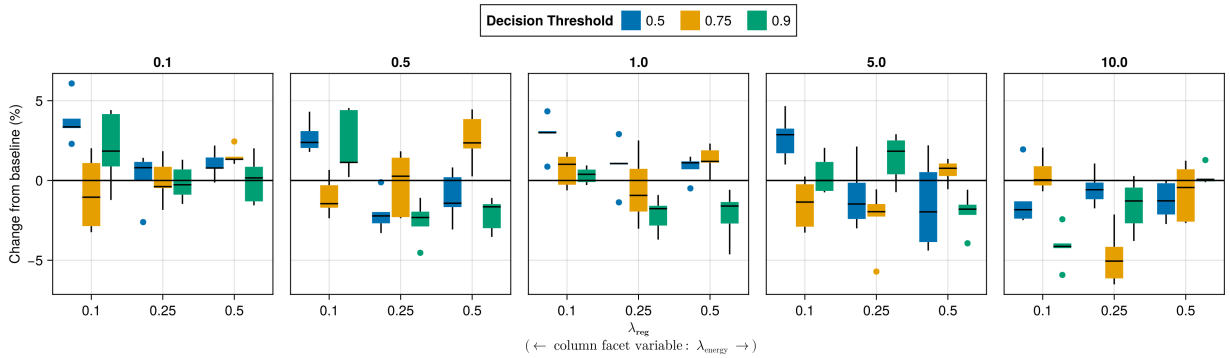

Figure A34: Average outcomes for the plausibility measure across key hyperparameters. Data: MNIST.

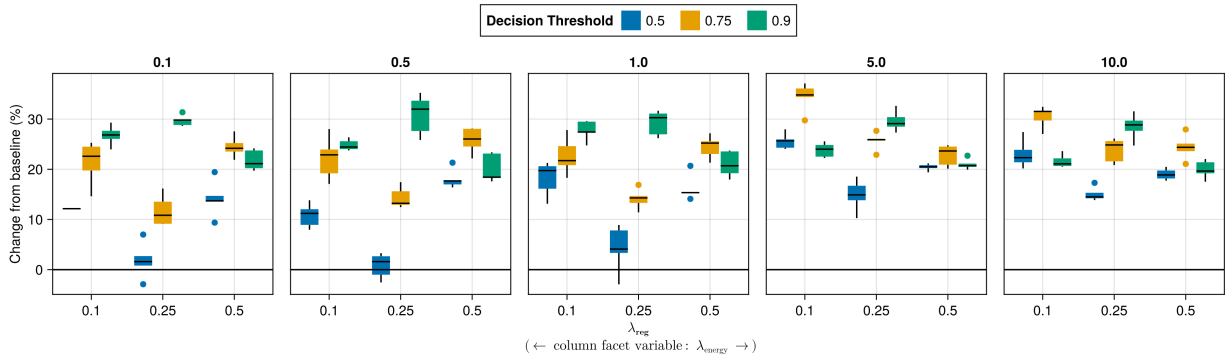

Figure A35: Average outcomes for the plausibility measure across key hyperparameters. Data: Moons.

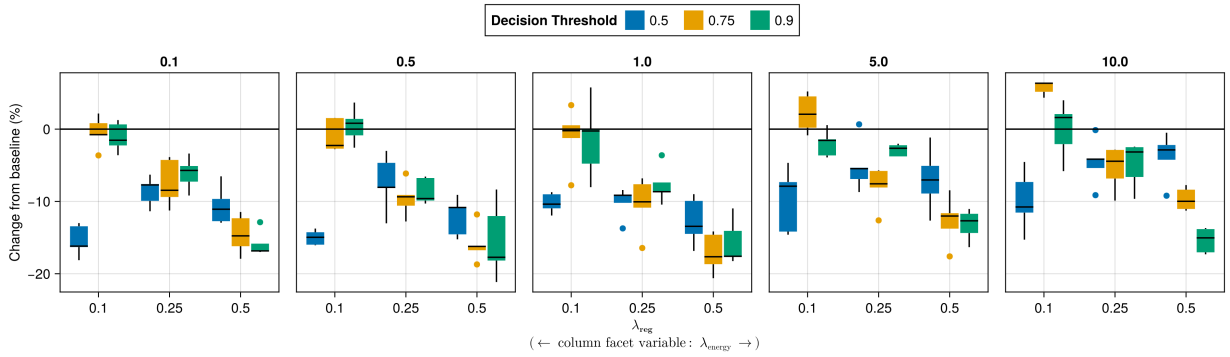

Figure A36: Average outcomes for the plausibility measure across key hyperparameters. Data: Overlapping.

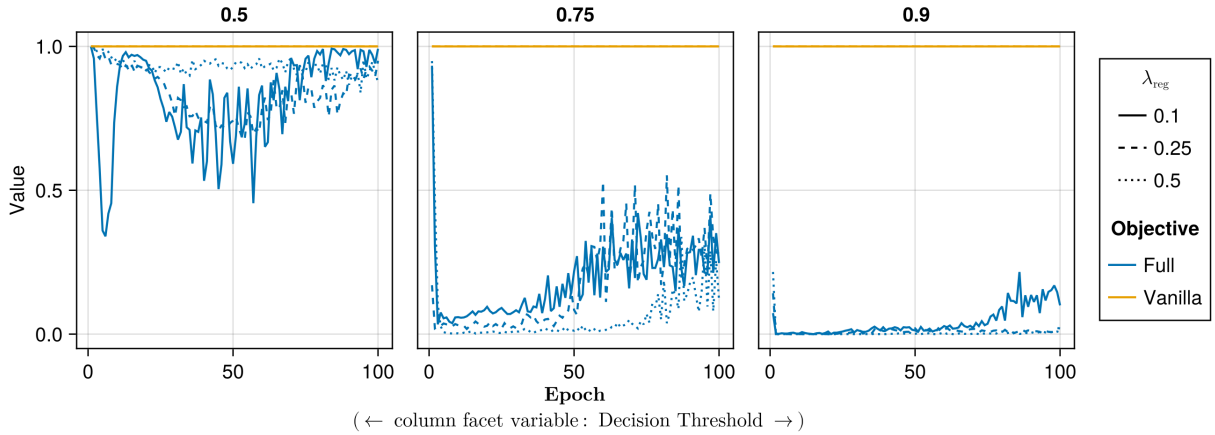

Figure A37: Proportion of mature counterfactuals in each epoch. Data: Adult.

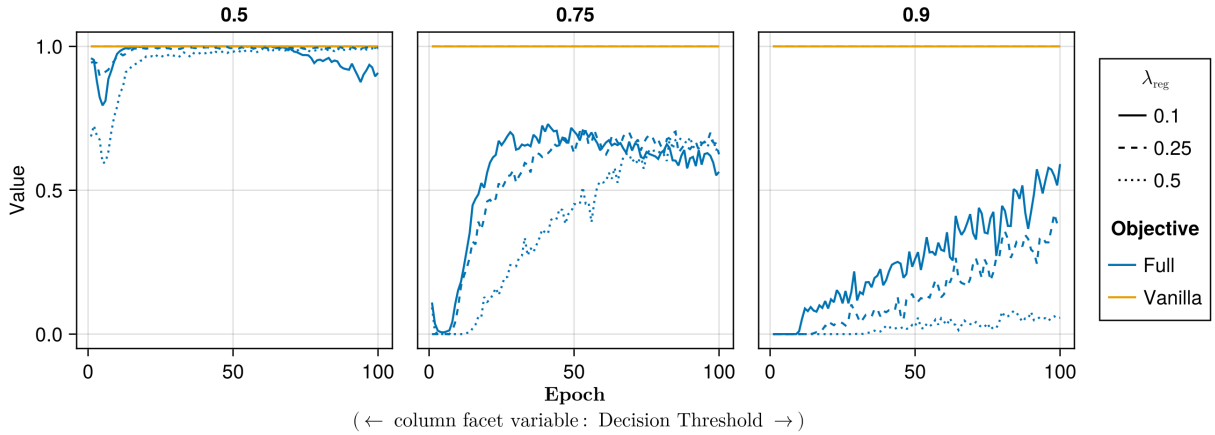

Figure A38: Proportion of mature counterfactuals in each epoch. Data: California Housing.

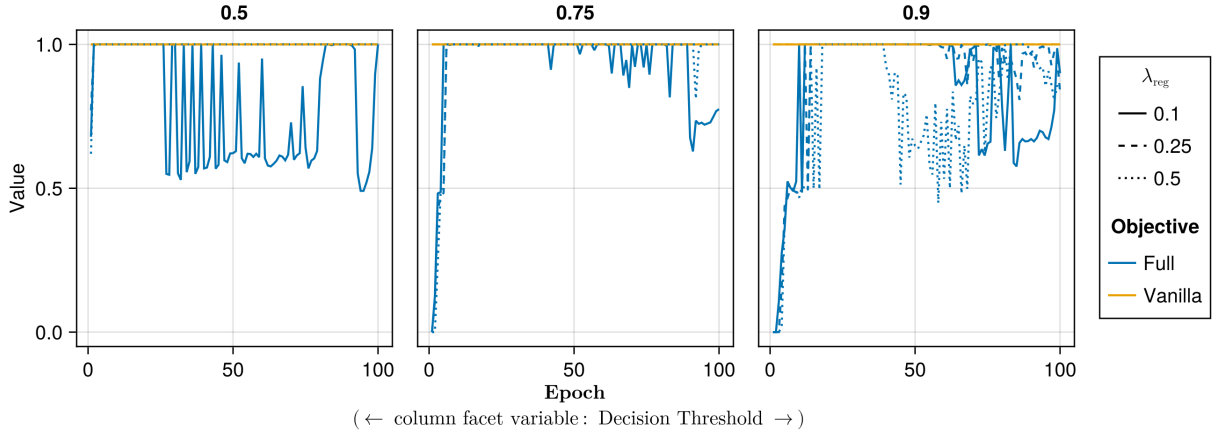

Figure A39: Proportion of mature counterfactuals in each epoch. Data: Circles.

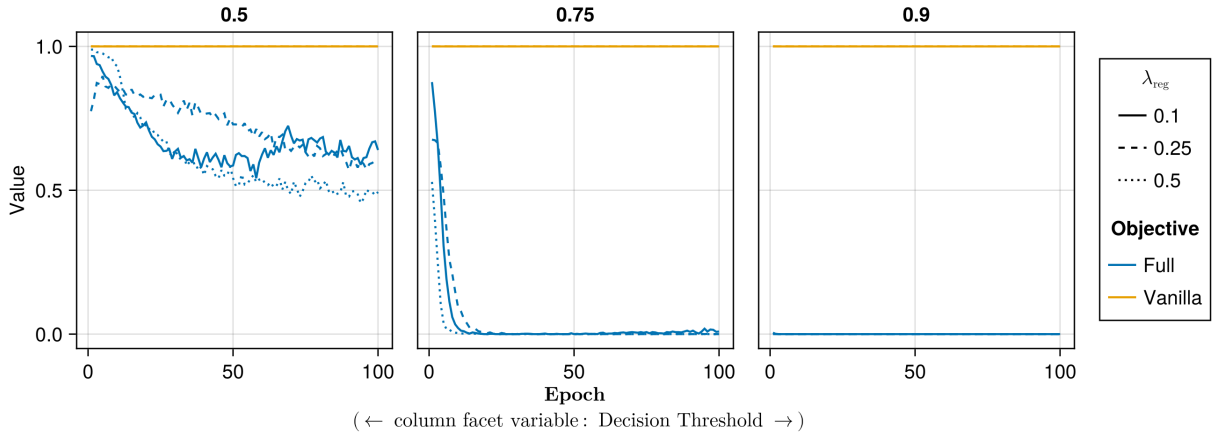

Figure A40: Proportion of mature counterfactuals in each epoch. Data: Credit.

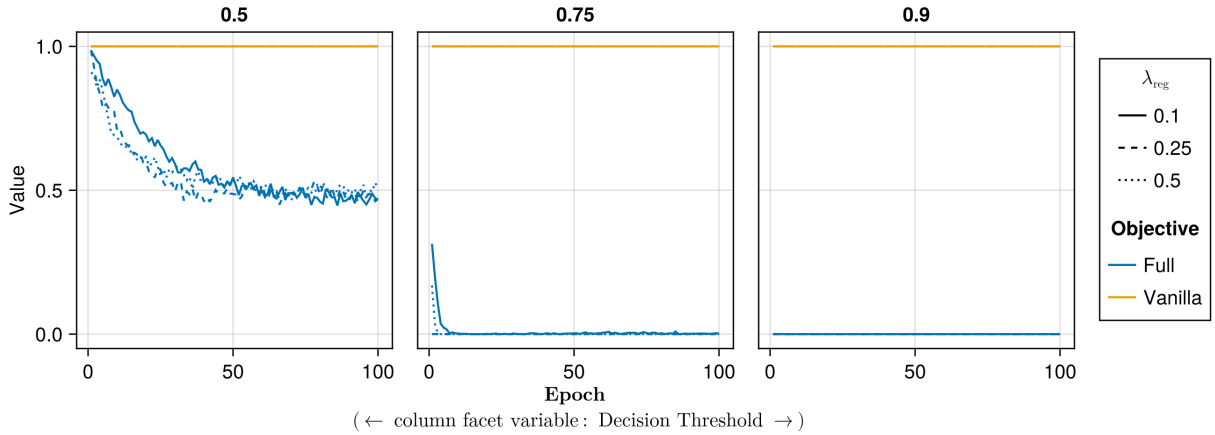

Figure A41: Proportion of mature counterfactuals in each epoch. Data: GMSC.

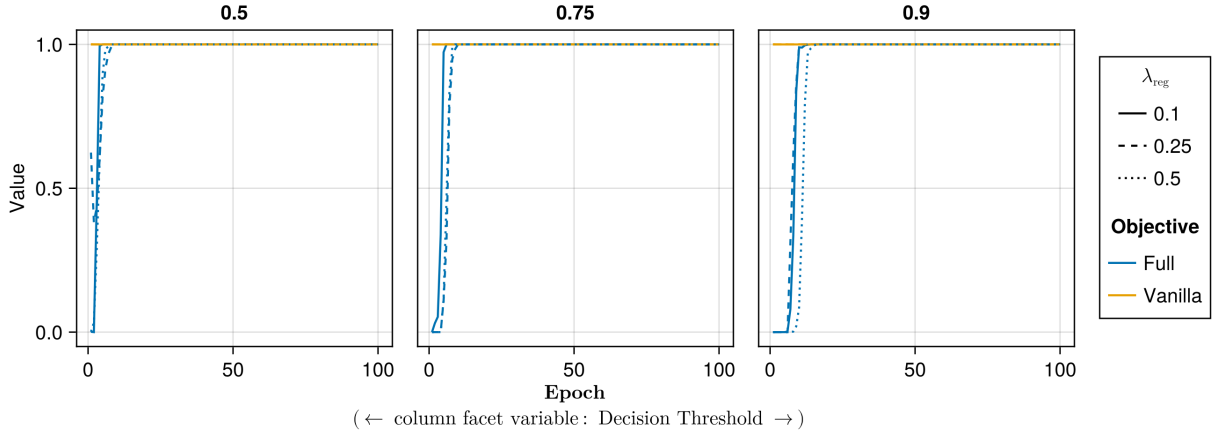

Figure A42: Proportion of mature counterfactuals in each epoch. Data: Linearly Separable.

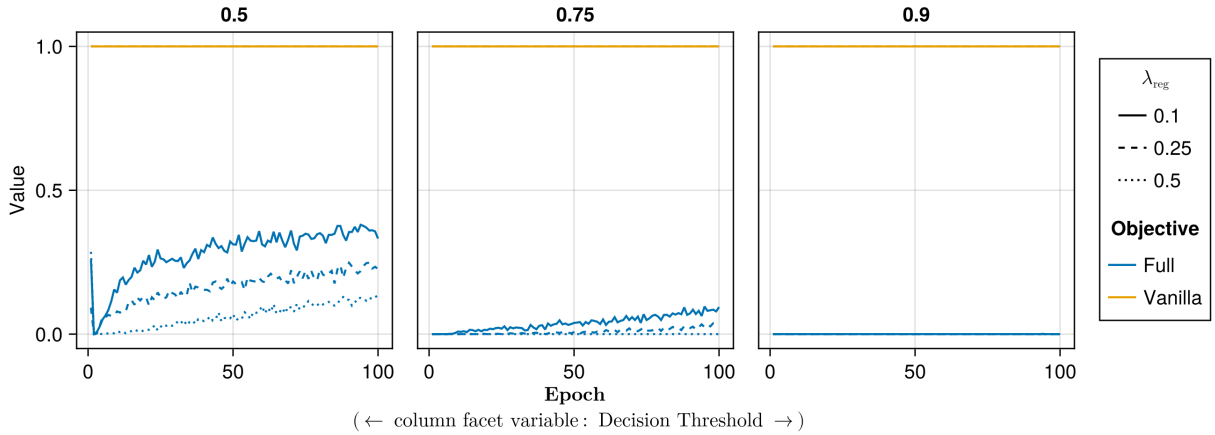

Figure A43: Proportion of mature counterfactuals in each epoch. Data: MNIST.

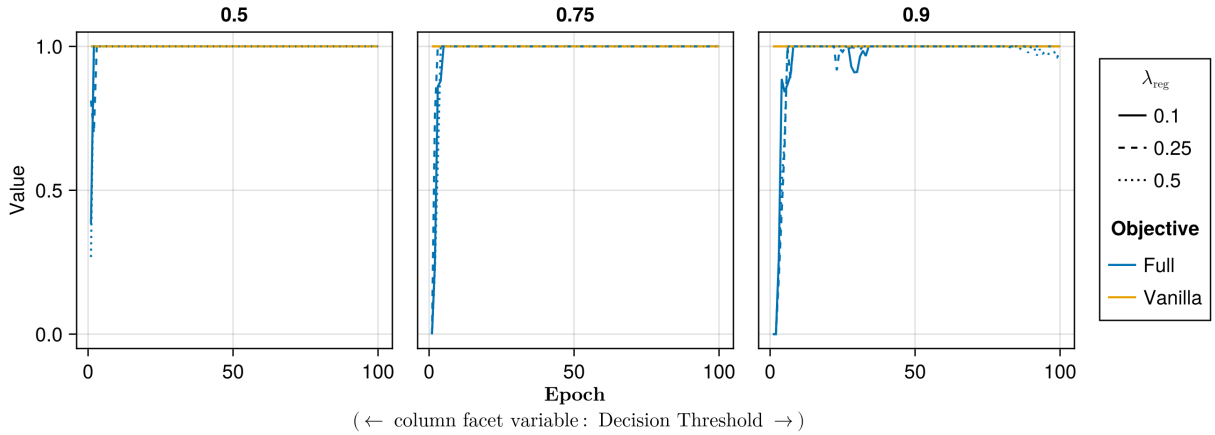

Figure A44: Proportion of mature counterfactuals in each epoch. Data: Moons.

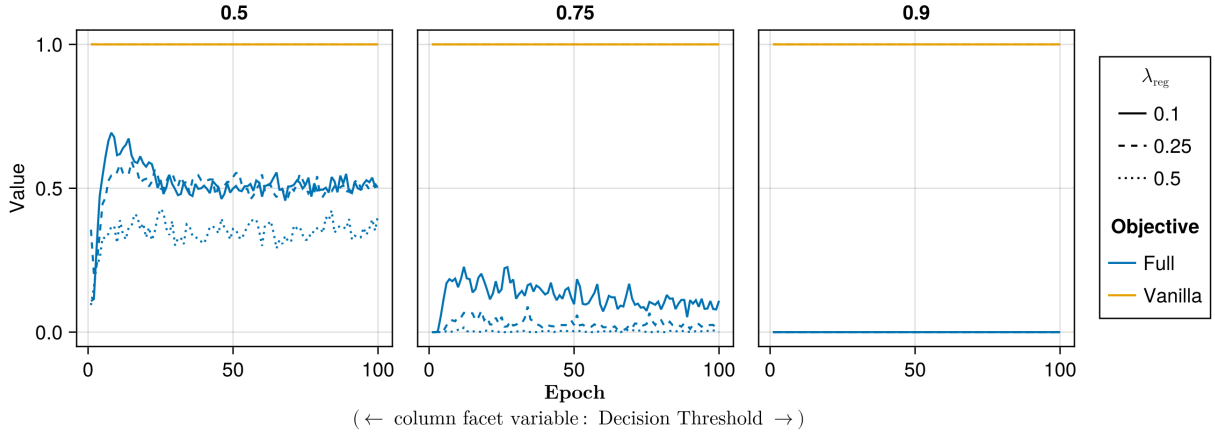

Figure A45: Proportion of mature counterfactuals in each epoch. Data: Overlapping.

I.3.2 Learning Rate

The hyperparameter grid for tuning the learning rate is shown in Note 9. The corresponding evaluation grid used for these experiments is shown in Note 10.

Note 9: Training Phase

- Generator Parameters:
  - Learning Rate: `0.1, 0.5, 1.0`
- Model: `mlp`
- Training Parameters:
  - λ_{reg}: `0.01, 0.1, 0.5`
  - Objective: `full, vanilla`

Note 10: Evaluation Phase

- Generator Parameters:
  - λ_{energy}: `0.1, 0.5, 1.0, 5.0, 10.0`

I.3.2.1 Plausibility The results with respect to the plausibility measure are shown in Figure A46 to Figure A50.

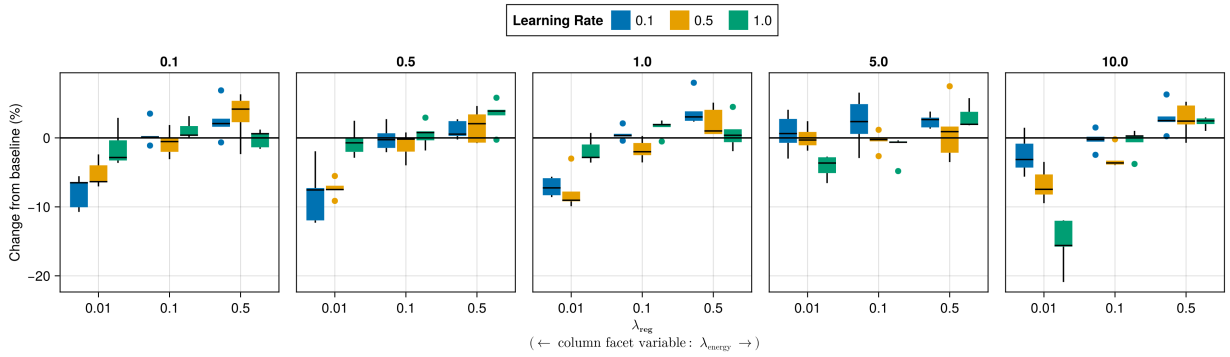

Figure A46: Average outcomes for the plausibility measure across key hyperparameters. Data: Adult.

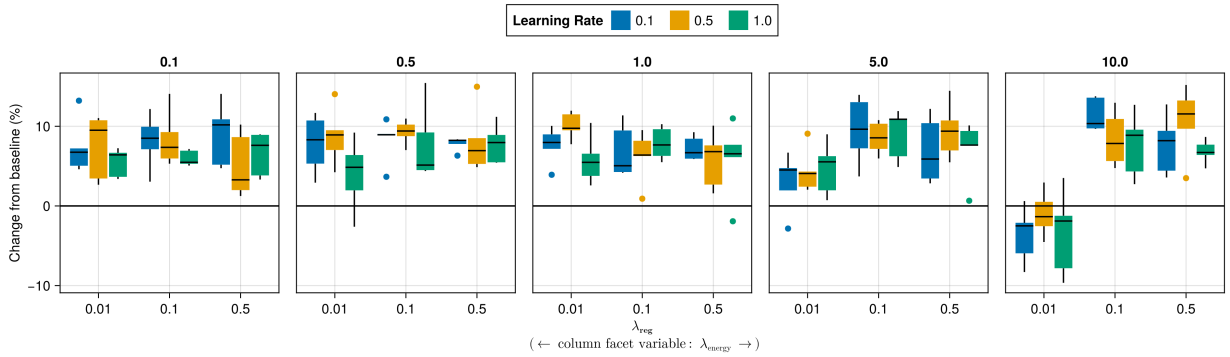

Figure A47: Average outcomes for the plausibility measure across key hyperparameters. Data: Credit.

I.3.2.2 Proportion of Mature CE The results with respect to the proportion of mature counterfactuals in each epoch are shown in Figure A51 to Figure A55.

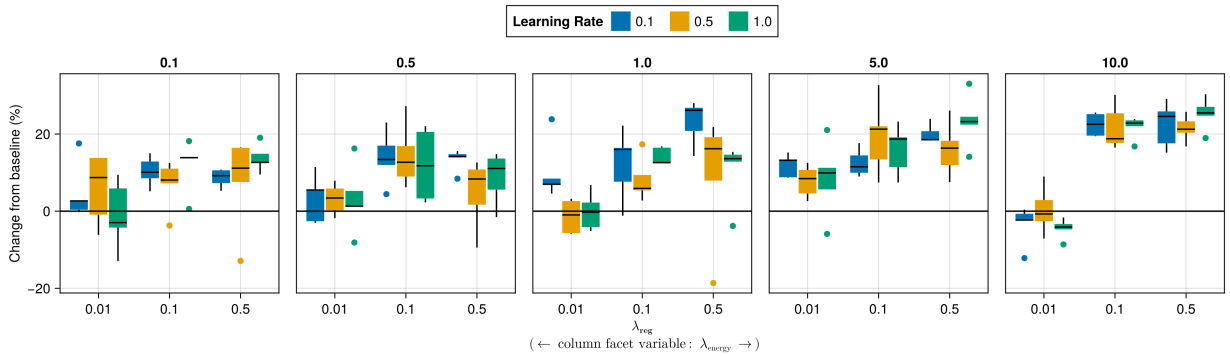

Figure A48: Average outcomes for the plausibility measure across key hyperparameters. Data: GMSC.

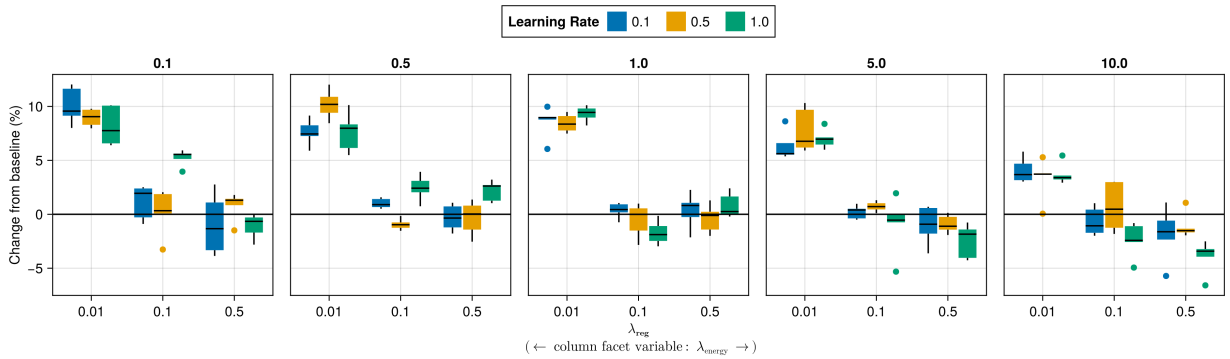

Figure A49: Average outcomes for the plausibility measure across key hyperparameters. Data: MNIST.

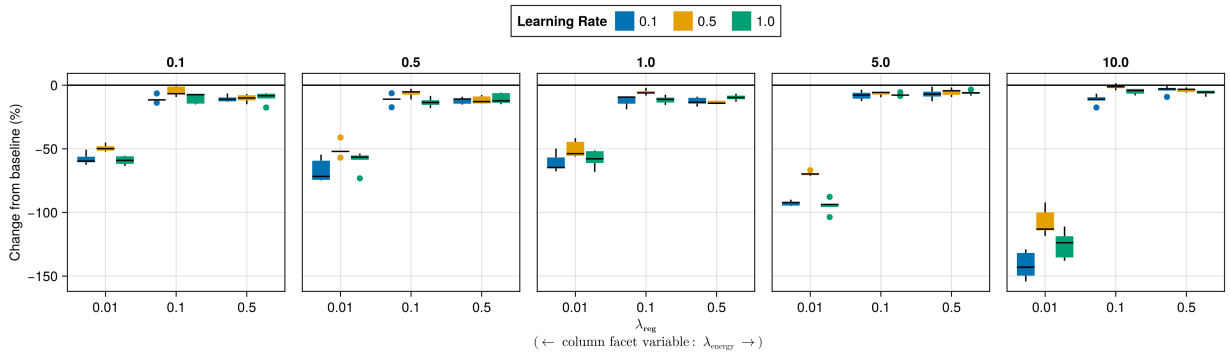

Figure A50: Average outcomes for the plausibility measure across key hyperparameters. Data: Overlapping.

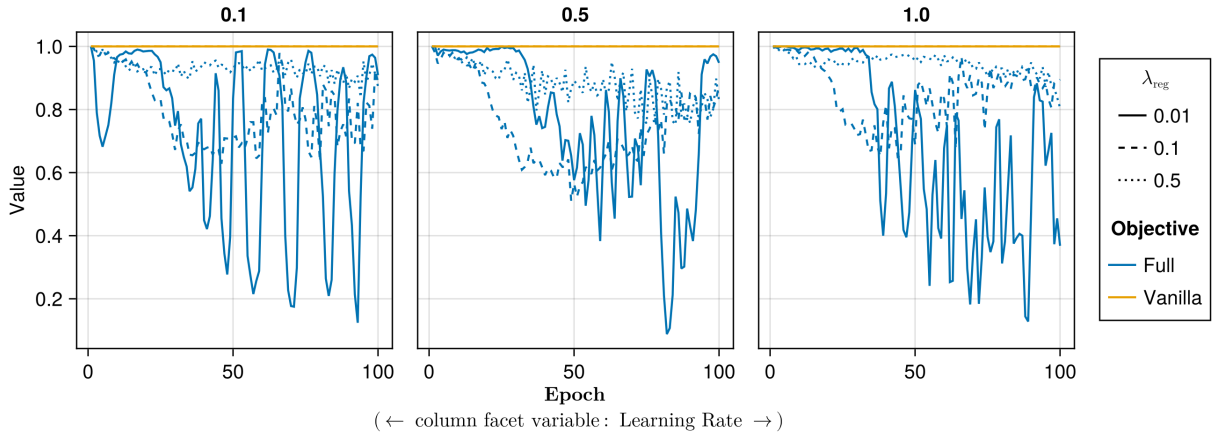

Figure A51: Proportion of mature counterfactuals in each epoch. Data: Adult.

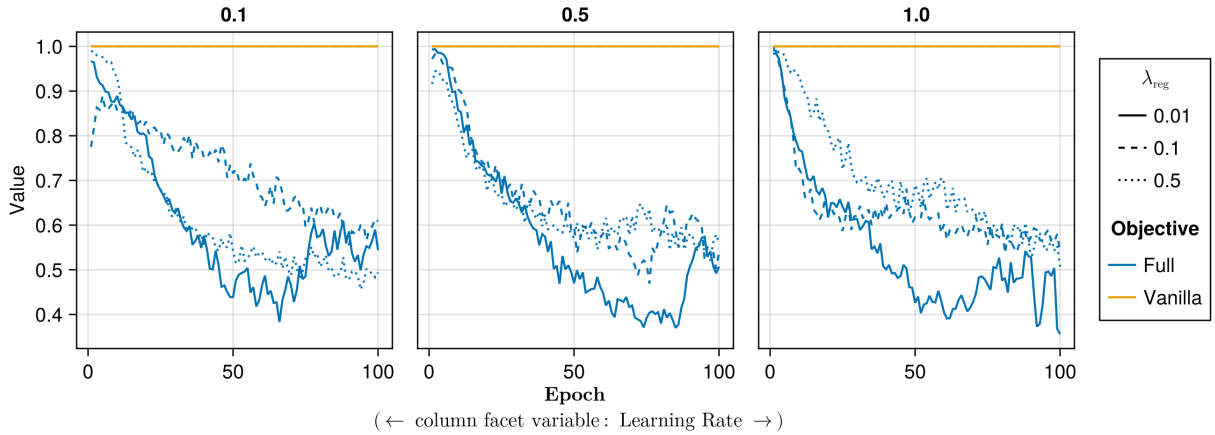

Figure A52: Proportion of mature counterfactuals in each epoch. Data: Credit.

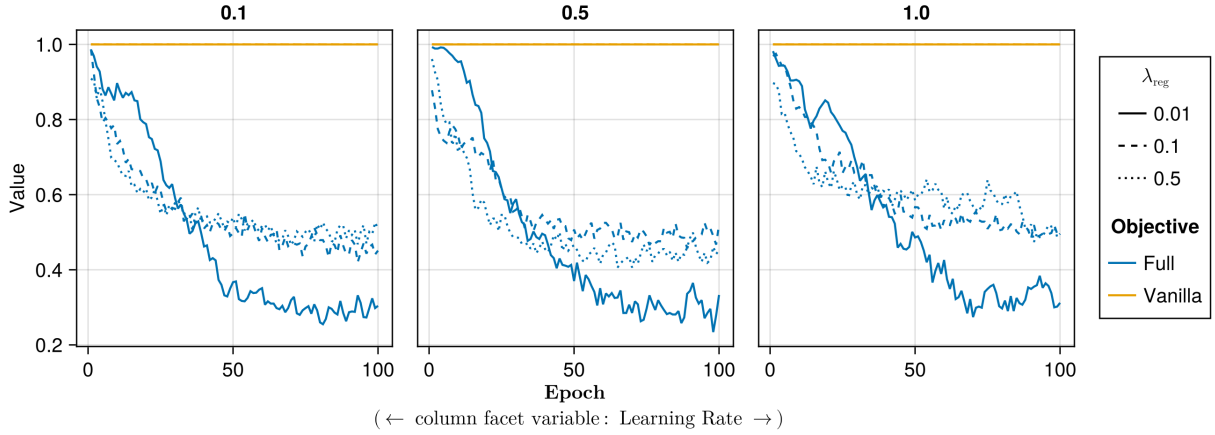

Figure A53: Proportion of mature counterfactuals in each epoch. Data: GMSC.

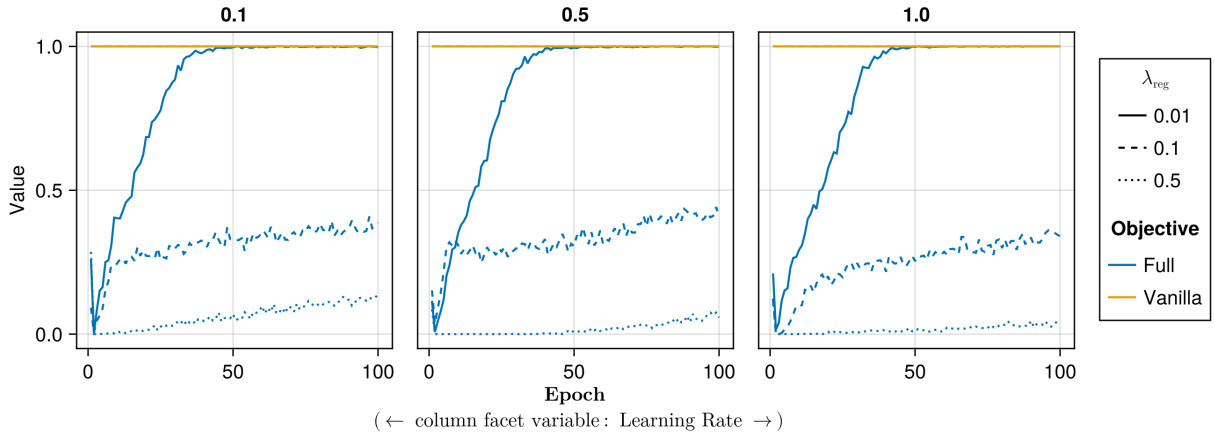

Figure A54: Proportion of mature counterfactuals in each epoch. Data: MNIST.

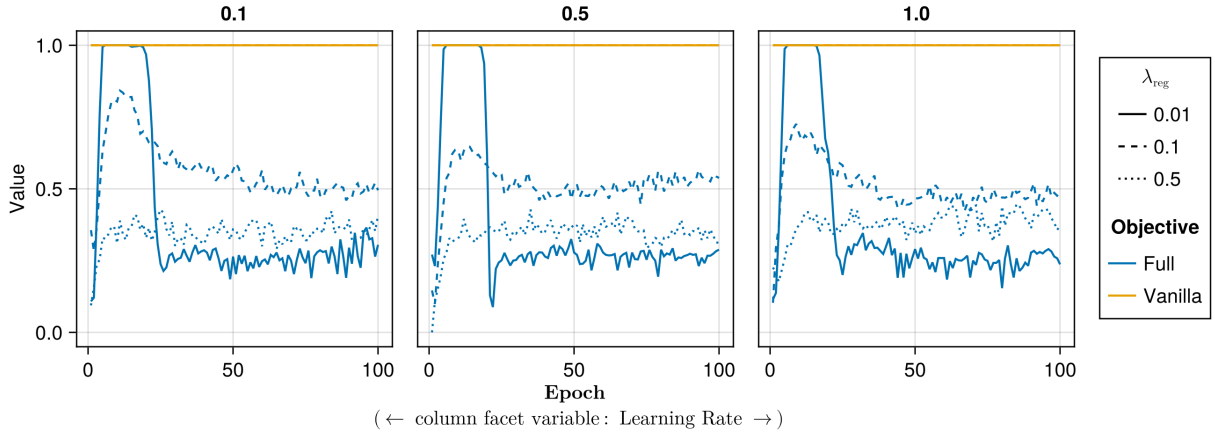

Figure A55: Proportion of mature counterfactuals in each epoch. Data: Overlapping.

J Computation Details

J.1 Hardware

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

J.1.1 Grid Searches

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

J.1.2 Tuning

For tuning of selected hyperparameters, we distributed the task of generating counterfactuals during training across 40 CPUs with 2GB memory each for all tabular datasets. Except for the *Adult* dataset, all training runs were completed in less that half an hour (<0h30m). The *Adult* dataset took around 0h35m to complete. Evaluations across 20 CPUs with 3GB memory each generally took less than 0h30m to complete. For *MNIST*, we relied on 100 CPUs with 2GB memory each. For the *MLP*, training of all models could be completed in 1h30m, while the evaluation across 20 CPUs

(6GB memory) took 4h12m. For the *CNN*, training of all models took ~8h, with conventionally trained models taking ~0h15m each and model with CT taking ~0h30m-0h45m each.

J.2 Software

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