ECCCos from the Black Box: Faithful Counterfactual Explanations through Energy Based Modeling and Conformal Prediction

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Abstract

Counterfactual Explanations offer an intuitive and straightforward way to explain black-box models but they are not unique. To address the need for plausible explanations, existing work has primarily relied on surrogate models to learn how the input data is distributed. This effectively reallocates the task of learning realistic representations of the data from the model itself to the surrogate. Consequently, the generated explanations may look plausible to humans but not necessarily faithfully describe the behaviour of the black-box model. We formalise this notion of faithfulness through the introduction of a tailored evaluation metric and propose a novel algorithmic framework for generating Energy-Constrained Conformal Counterfactuals that are only as plausible as the model permits. To do so, ECCCo leverages recent advances with respect to energy-based models and conformal inference. Through extensive empirical studies, we demonstrate that ECCCos reconcile the need for plausibility and faithfulness. Our findings also highlight that black-box models that are trained jointly to discriminate outputs and generate inputs yield more plausible explanations than pure discriminative models.

1 Introduction

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Counterfactual Explanations provide a powerful, flexible and intuitive way to not only explain black-box models but also enable affected individuals to challenge them through the means of Algorithmic Recourse. Instead of opening the black box, Counterfactual Explanations work under the premise of strategically perturbing model inputs to understand model behaviour [29]. Intuitively speaking, we generate explanations in this context by asking simple what-if questions of the following nature: 'Our credit risk model currently predicts that this individual's credit profile is too risky to offer them a loan. What if they reduced their monthly expenditures by 10%? Will our model then predict that the individual is credit-worthy'?

This is typically implemented by defining a target outcome $\mathbf{y}^* \in \mathcal{Y}$ for some individual $\mathbf{x} \in \mathcal{X} = \mathbb{R}^D$ described by D attributes, for which the model $M_\theta: \mathcal{X} \mapsto \mathcal{Y}$ initially predicts a different outcome: $M_\theta(\mathbf{x}) \neq \mathbf{y}^*$. Counterfactuals are then searched by minimizing a loss function that compares the predicted model output to the target outcome: $yloss(M_\theta(\mathbf{x}), \mathbf{y}^*)$. Since Counterfactual Explanations (CE) work directly with the black-box model, valid counterfactuals always have full local fidelity by construction [17]. Fidelity is defined as the degree to which explanations approximate the predictions of the black-box model. This is arguably one of the most important evaluation metrics for model explanations, since any explanation that explains a prediction not actually made by the model is useless [16].

In situations where full fidelity is a requirement, CE therefore offers a more appropriate solution to Explainable Artificial Intelligence (XAI) than other popular approaches like LIME [22] and SHAP [12], which involve local surrogate models. But even full fidelity is not a sufficient condition for ensuring that an explanation faithfully describes the behaviour of a model. That is because multiple very distinct explanations can all lead to the same model prediction, especially when dealing with heavily parameterized models like deep neural networks which are typically underspecified by the available data [30].

In the context of CE, the idea that no two explanations are the same arises almost naturally. A key 41 focus in the literature has therefore been to identify those explanations and algorithmic recourses 42 that are deemed most appropriate based on a myriad of desiderata such as sparsity, actionability 43 and plausibility. In this work, we draw closer attention to the insufficiency of model fidelity as an 44 evaluation metric for the faithfulness of counterfactual explanations. Our key contributions are as 45 follows: firstly, we introduce a new notion of faithfulness that is suitable for counterfactuals and 46 propose a novel evaluation measure that draws inspiration from recent advances in Energy-Based Modelling (EBM); secondly, we a novel algorithmic approach for generating Energy-Constrained Conformal Counterfactuals (ECCCo) that explicitly address the need for faithfulness; finally, we 49 provide illustrative examples and extensive empirical evidence demonstrating that ECCCos faithfully 50 explain model behaviour without sacrificing existing desidarata like plausibility and sparsity.

52 **Background and Related Work**

In this section, we provide some background on Counterfactual Explanations and our motivation for this work. To start, we briefly introduce the methodology underlying most state-of-the-art (SOTA) counterfactual generators.

2.1 Gradient-Based Counterfactual Search

While Counterfactual Explanations can be generated for arbitrary regression models [24], existing work has primarily focused on classification problems. Let $\mathcal{Y} = (0,1)^K$ denote the one-hot-encoded output domain with K classes. Then most SOTA counterfactual generators rely on gradient descent to optimize different flavours of the following counterfactual search objective:

Here yloss denotes the primary loss function already introduced above and cost is either a single penalty or a collection of penalties that are used to impose constraints through regularization. Equation 1 restates the baseline approach to gradient-based counterfactual search proposed by Wachter

$$\mathbf{Z}' = \arg\min_{\mathbf{Z}' \in \mathcal{Z}^L} \left\{ y loss(M_{\theta}(f(\mathbf{Z}')), \mathbf{y}^*) + \lambda cost(f(\mathbf{Z}')) \right\}$$
(1)

et al. [29] in general form where $\mathbf{Z}' = \{\mathbf{z}_l\}_L$ denotes an L-dimensional array of counterfactual states [2]. This is to explicitly account for the multiplicity of explanations and the fact that we may 65 choose to generate multiple counterfactuals and traverse a latent encoding ${\mathcal Z}$ of the feature space ${\mathcal X}$ where we denote $f^{-1}: \mathcal{X} \mapsto \mathcal{Z}$. Encodings may involve simple feature transformations or more 67 advanced techniques involving generative models, as we will discuss further below. The baseline 68 approach, which we will simply refer to as Wachter [29], searches a single counterfactual directly in 69 the feature space and penalises its distance between the original factual. 70 Solutions to Equation 1 are considered valid as soon as the predicted label matches the target label. A 71 stripped-down counterfactual explanation is therefore little different from an adversarial example. In 72 Figure 1, for example, we have applied Wachter to MNIST data (centre panel) where the underlying 73 classifier M_{θ} is a simple Multi-Layer Perceptron (MLP) with above 90 percent test accuracy. For the 74 generated counterfactual \mathbf{x}' the model predicts the target label with high confidence (centre panel in Figure 1). The explanation is valid by definition, even though it looks a lot like an Adversarial 76 77 Example [6]. Schut et al. [23] make the connection between Adversarial Examples and Counterfactual Explanations explicit and propose using a Jacobian-Based Saliency Map Attack (JSMA) to solve Equation 1. They demonstrate that this approach yields realistic and sparse counterfactuals for 79 Bayesian, adversarially robust classifiers. Applying their approach to our simple MNIST classifier does not yield a realistic counterfactual but this one, too, is valid (right panel in Figure 1).

2.2 From Adversial Examples to Plausible Explanations

The crucial difference between Adversarial Examples (AE) and Counterfactual Explanations is one of intent. While an AE is intended to go unnoticed, a CE should have certain desirable properties. The literature has made this explicit by introducing various so-called *desiderata* that counterfactuals should meet in order to properly serve both AI practitioners and individuals affected by AI decision-making systems. The list of desiderate includes but is not limited to the following: sparsity, proximity [29], actionability [27], diversity [17], plausibility [9, 21, 23], robustness [26, 20, 2] and causality [11].

Researchers have come up with various ways to meet these desiderata, which have been extensively

Researchers have come up with various ways to meet these desiderata, which have been extensively surveyed and evaluated in various studies [28, 10, 19, 4, 8]. Perhaps unsurprisingly, the different desiderata are often positively correlated. For example, Artelt et al. [4] find that plausibility typically also leads to improved robustness. Similarly, plausibility has also been connected to causality in the sense that plausible counterfactuals respect causal relationships [13].

4 2.2.1 Plausibility through Surrogates

Arguably, the plausibility of counterfactuals has been among the primary concerns and some have focused explicitly on this goal. Joshi et al. [9], for example, were among the first to suggest that 96 instead of searching counterfactuals in the feature space \mathcal{X} , we can instead traverse a latent embedding 97 \mathcal{Z} (Equation 1) that implicitly codifies the data generating process (DGP) of $\mathbf{x} \sim \mathcal{X}$. To learn the 98 latent embedding, they introduce a surrogate model. In particular, they propose to use the latent 99 embedding of a Variational Autoencoder (VAE) trained to generate samples $\mathbf{x}^* \leftarrow \mathcal{G}(\mathbf{z})$ where \mathcal{G} 100 denotes the decoder part of the VAE. Provided the surrogate model is well-trained, their proposed 101 approach —REVISE— can yield compelling counterfactual explanations like the one in the centre 102 panel of Figure 2. 103

Others have proposed similar approaches. Dombrowski et al. [5] traverse the base space of a normalizing flow to solve Equation 1, essentially relying on a different surrogate model for the generative task. Poyiadzi et al. [21] use density estimators $(\hat{p}:\mathcal{X}\mapsto[0,1])$ to constrain the counterfactuals to dense regions in the feature space. Karimi et al. [11] argue that counterfactuals should comply with the causal model that generates the data. All of these different approaches share a common goal: ensuring that the generated counterfactuals comply with the true and unobserved DGP. To summarize this broad objective, we propose the following definition:

Definition 2.1 (Plausible Counterfactuals). Let $\mathcal{X}|\mathbf{y}^*$ denote the true conditional distribution of samples in the target class \mathbf{y}^* . Then for \mathbf{x}' to be considered a plausible counterfactual, we need: $\mathbf{x}' \sim \mathcal{X}|\mathbf{y}^*$.

Surrogate models offer an obvious solution to achieve this objective. Unfortunately, surrogates also 114 introduce a dependency: the generated explanations no longer depend exclusively on the black-box 115 model itself, but also on the surrogate model. This is not necessarily problematic if the primary 116 objective is not to explain the behaviour of the model but to offer recourse to individuals affected by 117 it. It may become problematic even in this context if the dependency turns into a vulnerability. To 118 illustrate this point, we have used REVISE [9] with an underfitted VAE to generate the counterfactual 119 in the right panel of Figure 2: in this case, the decoder step of the VAE fails to yield plausible values 120 $(\{\mathbf{x}' \leftarrow \mathcal{G}(\mathbf{z})\} \not\sim \mathcal{X}|\mathbf{y}^*)$ and hence the counterfactual search in the learned latent space is doomed. 121

2.2.2 Plausibility through Minimal Predictive Uncertainty

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Schut et al. [23] show that to meet the plausibility objective we need not explicitly model the input distribution. Pointing to the undesirable engineering overhead induced by surrogate models, they propose that we rely on the implicit minimisation of predictive uncertainty instead. Their proposed methodology solves Equation 1 by greedily applying JSMA in the feature space with standard crossentropy loss and no penalty at all. They demonstrate theoretically and empirically that their approach yields counterfactuals for which the model M_{θ} predicts the target label \mathbf{y}^* with high confidence. Provided the model is well-specified, these counterfactuals are plausible. Unfortunately, this idea hinges on the assumption that the black-box model provides well-calibrated predictive uncertainty estimates.



Figure 1: Explanations or Adversarial Examples? Counterfactuals for turning an 8 (eight) into a 3 (three): original image (left); counterfactual produced using Wachter et al. [29] (centre); and a counterfactual produced using the approach introduced by [23] that uses Jacobian-Based Saliency Map Attacks to solve Equation 1.



Figure 2: Using surrogates can improve plausibility, but also increases vulnerability. Counterfactuals for turning an 8 (eight) into a 3 (three): original image (left); counterfactual produced using REVISE [9] with a well-specified surrogate (centre); and a counterfactual produced using REVISE [9] with a poorly specified surrogate (right).

2.3 From Fidelity to Model Conformity

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Above we explained that since Counterfactual Explanations work directly with the Black Box model, the fidelity of explanations as we defined it earlier is not a concern. This may explain why research has primarily focused on other desiderata, most notably plausibility (Definition 2.1). Enquiring about the plausibility of a counterfactual essentially boils down to the following question: 'Is this counterfactual consistent with the underlying data'? We posit a related, slightly more nuanced question: 'Is this counterfactual consistent with what the model has learned about the underlying data'? We will argue that fidelity is not a sufficient evaluation measure to answer this question and propose a novel way to assess if Counterfactual Explanations conform with model behaviour.

The word *fidelity* stems from the Latin word 'fidelis', which means 'faithful, loyal, trustworthy' [15].

As we explained in Section 2, model explanations are generally considered faithful if their corresponding predictions coincide with the predictions made by the model itself. Since this definition of faithfulness is not useful in the context of Counterfactual Explanations, we propose an adapted version:

Definition 2.2 (Conformal Counterfactuals). Let $\mathcal{X}_{\theta}|\mathbf{y}^* = p_{\theta}(x|\mathbf{y}^*)$ denote the conditional distribution of \mathbf{x} in the target class \mathbf{y}^* , where θ denotes the parameters of model M_{θ} . Then for \mathbf{x}' to be considered a conformal counterfactual, we need: $\mathbf{x}' \sim \mathcal{X}_{\theta}|\mathbf{y}^*$.

In words, conformal counterfactuals conform with what the predictive model has learned about the input data \mathbf{x} . Since this definition works with distributional properties, it explicitly accounts for the multiplicity of explanations we discussed earlier. To assess counterfactuals with respect to Definition 2.2, we need to be able to quantify the posterior conditional distribution $p_{\theta}(\mathbf{x}|\mathbf{y}^*)$. This is very much at the core of our proposed methodological framework, which reconciles the notions of plausibility and model conformity and which we will introduce next.

3 Methodological Framework

The primary objective of this work has been to develop a methodology for generating maximally plausible counterfactuals under minimal intervention. Our proposed framework is based on the premise that explanations should be plausible but not plausible at all costs. Energy-Constrained Conformal Counterfactuals (ECCCo) achieve this goal in two ways: firstly, they rely on the Black Box itself for the generative task; and, secondly, they involve an approach to predictive uncertainty quantification that is model-agnostic.

3.1 Quantifying the Model's Generative Property

Recent work by Grathwohl et al. [7] on Energy Based Models (EBM) has pointed out that there is a 'generative model hidden within every standard discriminative model'. The authors show that we can draw samples from the posterior conditional distribution $p_{\theta}(\mathbf{x}|\mathbf{y})$ using Stochastic Gradient Langevin Dynamics (SGLD). The authors use this insight to train classifiers jointly for the discriminative task using standard cross-entropy and the generative task using SGLD. They demonstrate empirically that

among other things this improves predictive uncertainty quantification for discriminative models.
Our findings in this work suggest that Joint Energy Models (JEM) also tend to yield more plausible
Counterfactual Explanations. Based on the definition of plausible counterfactuals (Definition 2.1)
this is not surprising.

Crucially for our purpose, one can apply their proposed sampling strategy during inference to essentially any standard discriminative model. Even models that are not explicitly trained for the joint objective learn about the distribution of inputs X by learning to make conditional predictions about the output y. We can leverage this observation to quantify the generative property of the Black Box model itself. In particular, note that if we fix y to our target value y^* , we can sample from $p_{\theta}(\mathbf{x}|\mathbf{y}^*)$ using SGLD as follows,

$$\mathbf{x}_{j+1} \leftarrow \mathbf{x}_j - \frac{\epsilon^2}{2} \mathcal{E}(\mathbf{x}_j | \mathbf{y}^*) + \epsilon \mathbf{r}_j, \quad j = 1, ..., J$$
 (2)

where $\mathbf{r}_j \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ is the stochastic term and the step-size ϵ is typically polynomially decayed. The term $\mathcal{E}(\mathbf{x}_j|\mathbf{y}^*)$ denotes the energy function where we use $\mathcal{E}(\mathbf{x}_j|\mathbf{y}^*) = -M_{\theta}(\mathbf{x}_j)[\mathbf{y}^*]$, that is the negative logit corresponding to the target class label \mathbf{y}^* . Generating multiple samples in this manner yields an empirical distribution $\hat{\mathcal{X}}_{\theta}|\mathbf{y}^*$ that we use in our search for plausible counterfactuals, as discussed in more detail below. Appendix A provides additional implementation details for any tasks related to energy-based modelling.

3.2 Quantifying the Model's Predictive Uncertainty

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To quantify the model's predictive uncertainty we use Conformal Prediction (CP), an approach that has recently gained popularity in the Machine Learning community [3, 14]. Crucially for our intended application, CP is model-agnostic and can be applied during inference without placing any restrictions on model training. Intuitively, CP works under the premise of turning heuristic notions of uncertainty into rigorous uncertainty estimates by repeatedly sifting through the training data or a dedicated calibration dataset. Conformal classifiers produce prediction sets for individual inputs that include all output labels that can be reasonably attributed to the input. These sets tend to be larger for inputs that do not conform with the training data and are therefore characterized by high predictive uncertainty. In order to generate counterfactuals that are associated with low predictive uncertainty, we use a smooth set size penalty introduced by Stutz et al. [25] in the context of conformal training:

$$\Omega(C_{\theta}(\mathbf{x}; \alpha)) = \max \left(0, \sum_{\mathbf{y} \in \mathcal{Y}} C_{\theta, \mathbf{y}}(\mathbf{x}_i; \alpha) - \kappa \right)$$
(3)

Here, $\kappa \in \{0, 1\}$ is a hyper-parameter and $C_{\theta, \mathbf{y}}(\mathbf{x}_i; \alpha)$ can be interpreted as the probability of label y being included in the prediction set.

In order to compute this penalty for any black-box model we merely need to perform a single calibration pass through a holdout set \mathcal{D}_{cal} . Arguably, data is typically abundant and in most applications, practitioners tend to hold out a test data set anyway. Consequently, CP removes the restriction on the family of predictive models, at the small cost of reserving a subset of the available data for calibration. This particular case of conformal prediction is referred to as Split Conformal Prediction (SCP) as it involves splitting the training data into a proper training dataset and a calibration dataset. Details concerning our implementation of Conformal Prediction can be found in Appendix B.

3.3 Energy-Constrained Conformal Counterfactuals (ECCCo)

Our framework for generating ECCCos combines the ideas introduced in the previous two subsections. Formally, we extend Equation 1 as follows,

$$\mathbf{Z}' = \arg\min_{\mathbf{Z}' \in \mathcal{Z}^M} \{ yloss(M_{\theta}(f(\mathbf{Z}')), \mathbf{y}^*) + \lambda_1 dist(f(\mathbf{Z}'), \mathbf{x}) + \lambda_2 dist(f(\mathbf{Z}'), \hat{\mathbf{x}}_{\theta}) + \lambda_3 \Omega(C_{\theta}(f(\mathbf{Z}'); \alpha)) \}$$
(4)

where $\hat{\mathbf{x}}_{\theta}$ denotes samples generated using SGLD (Equation 2) and dist(·) is a generic term for a distance metric. Our default choice for dist(·) is the L1 Norm, or Manhattan distance, since it induces sparsity.

The first two terms in Equation 4 correspond to the counterfactual search objective defined in Wachter 210 et al. [29] which merely penalises the distance of counterfactuals from their factual values. The 211 additional two penalties in ECCCo ensure that counterfactuals conform with the model's generative 212 property and lead to minimally uncertain predictions, respectively. The hyperparameters $\lambda_1, ..., \lambda_3$ 213 can be used to balance the different objectives: for example, we may choose to incur larger deviations 214 from the factual in favour of conformity with the model's generative property by choosing lower 215 values of λ_1 and relatively higher values of λ_2 . Figure 3 illustrates this balancing act for an example 216 involving synthetic data: vector fields indicate the direction of gradients with respect to the different 217 components our proposed objective function (Equation 4). 218

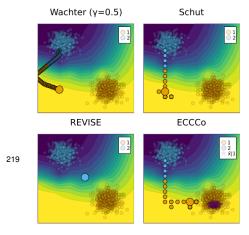


Figure 3: [PLACEHOLDER] Vector fields indicating the direction of gradients with respect to the different components of the ECCCo objective (Equation 4).

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Algorithm 1: Generating ECCCos (For more details, see Appendix C)

Input: $\mathbf{x}, \mathbf{y}^*, M_{\theta}, f, \Lambda, \alpha, \mathcal{D}, T, \eta, n_{\mathcal{B}}, N_{\mathcal{B}}$ where $M_{\theta}(\mathbf{x}) \neq \mathbf{y}^*$

Output: x'

- 1: Înitialize $\mathbf{z}' \leftarrow f^{-1}(\mathbf{x})$
- 2: Generate buffer \mathcal{B} of $N_{\mathcal{B}}$ conditional samples $\hat{\mathbf{x}}_{\theta}|\mathbf{y}^*$ using SGLD (Equation 2)
- 3: Run *SCP* for M_{θ} using \mathcal{D}
- 4: Initialize $t \leftarrow 0$
- 5: while not converged or t < T do
- 6: $\hat{\mathbf{x}}_{\theta,t} \leftarrow \text{rand}(\mathcal{B}, n_{\mathcal{B}})$
- 7: $\mathbf{z}' \leftarrow \mathbf{z}' \eta \overset{\cdot}{\nabla}_{\mathbf{z}'} \overset{\cdot}{\mathcal{L}}(\mathbf{z}', \mathbf{y}^*, \hat{\mathbf{x}}_{\theta, t}; \Lambda, \alpha)$
- 8: $t \leftarrow t+1$
- 9: end while
- 10: $\mathbf{x}' \leftarrow f(\mathbf{z}')$

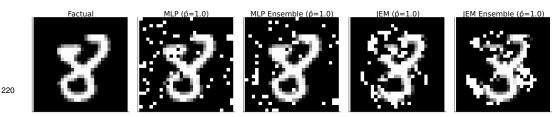


Figure 4: [SUBJECTO TO CHANGE] Original image (left) and ECCCos for turning an 8 (eight) into a 3 (three) for different Black Boxes from left to right: Multi-Layer Perceptron (MLP), Ensemble of MLPs, Joint Energy Model (JEM), Ensemble of JEMs.

The entire procedure for Generating ECCCos is described in Algorithm 1. For the sake of simplicity and without loss of generality, we limit our attention to generating a single counterfactual $\mathbf{x}' = f(\mathbf{z}')$ where in contrast to Equation 4 \mathbf{z}' denotes a 1-dimensional array containing a single counterfactual state. That state is initialized by passing the factual \mathbf{x} through the encoder f^{-1} which in our case corresponds to a simple feature transformer, rather than the encoder part of VAE as in REVISE [9]. Next, we generate a buffer of $N_{\mathcal{B}}$ conditional samples $\hat{\mathbf{x}}_{\theta}|\mathbf{y}^*$ using SGLD (Equation 2) and conformalise the model M_{θ} through Split Conformal Prediction on training data \mathcal{D} .

Finally, we search counterfactuals through gradient descent. Let $\mathcal{L}(\mathbf{z}', \mathbf{y}^*, \hat{\mathbf{x}}_{\theta,t}; \Lambda, \alpha)$ denote our loss function defined in Equation 4. Then in each iteration, we first randomly draw $n_{\mathcal{B}}$ samples from the buffer \mathcal{B} before updating the counterfactual state \mathbf{z}' by moving in the negative direction of that loss function. The search terminates once the convergence criterium is met or the maximum number

of iterations T has been exhausted. Note that the choice of convergence criterium has important implications on the final counterfactual (for more detail on this see Appendix C). 233

Figure 4 presents ECCCos for the MNIST example from Section 2 for various black-box models of 234 increasing complexity from left to right: a simple Multi-Layer Perceptron (MLP); an Ensemble of 235 MLPs, each of the same architecture as the single MLP; a Joint Energy Model (JEM) based on the 236 same MLP architecture; and finally, an Ensemble of these JEMs. Since Deep Ensembles have an 237 improved capacity for predictive uncertainty quantification and JEMs are explicitly trained to learn 238 plausible representations of the input data, it is intuitive to see that the plausibility of counterfactuals 239 visibly improves from left to right. This provides some first anecdotal evidence that ECCCos achieve 240 plausibility while maintaining faithfulness to the Black Box. 241

Empirical Analysis 242

In this section, we bolster our anecdotal findings from the previous section through rigorous empirical analysis. We first briefly describe our evaluation framework and data, before presenting and discussing 244 our results. 245

4.1 Evaluation Measures

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Explanations. In this subsection, we introduce evaluation measures that facilitate a quantitative 248 evaluation of counterfactuals for these objectives. 249 Firstly, in order to assess the plausibility of counterfactuals we adapt the implausibility metric 250 proposed in Guidotti [8]. The authors propose to evaluate plausibility in terms of the distance of the 251 counterfactual \mathbf{x}' from its nearest neighbour in the target class \mathbf{y}^* : the smaller this distance, the more plausible the counterfactual. Instead of focusing only on the nearest neighbour of \mathbf{x}' , we suggest 253

Above we have defined plausibility (Definition 2.1) and conformity (Definition 2.2) for Counterfactual

computing the average over distances from multiple (possibly all) observed instances in the target 254 class. Formally, for a single counterfactual, we have:

$$impl = \frac{1}{|\mathbf{x} \in \mathcal{X}|\mathbf{y}^*|} \sum_{\mathbf{x} \in \mathcal{X}|\mathbf{y}^*} dist(\mathbf{x}', \mathbf{x})$$
(5)

This measure is straightforward to compute and should be less sensitive to outliers in the target class 256 than the one based on the nearest neighbour. It also gives rise to a very similar evaluation measure for 257 conformity. We merely swap out the subsample of individuals in the target class for the empirical distribution of generated conditional samples:

$$conf = \frac{1}{|\mathbf{x} \in \mathcal{X}_{\theta}|\mathbf{y}^*|} \sum_{\mathbf{x} \in \mathcal{X}_{\theta}|\mathbf{y}^*} dist(\mathbf{x}', \mathbf{x})$$
(6)

(5)

As noted by Guidotti [8], these distance-based measures are simplistic and more complex alternative measures may ultimately be more appropriate for the task. For example, we considered using statistical divergence measures instead. This would involve generating not one but many counterfactuals and comparing the generated empirical distribution to the target distributions in Definitions 2.1 and 2.2. While this approach is potentially more rigorous, generating enough counterfactuals is not always practical.

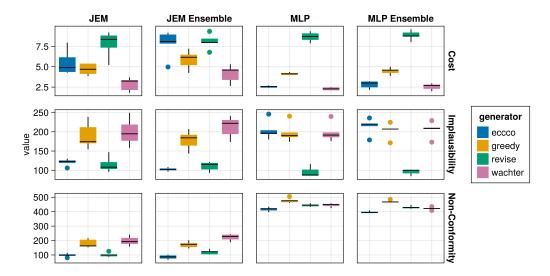


Figure 5: [SUBJECTO TO CHANGE] Original image (left) and ECCCos for turning an 8 (eight) into a 3 (three) for different Black Boxes from left to right: Multi-Layer Perceptron (MLP), Ensemble of MLPs, Joint Energy Model (JEM), Ensemble of JEMs.

Data 4.2

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Results 267

Discussion 5 268

5.1 **Key Insights** 269

Consistent with the findings in Schut et al. [23], we have demonstrated that predictive uncertainty 270 estimates can be leveraged to generate plausible counterfactuals. Interestingly, Schut et al. [23] point out that this finding — as intuitive as it is — may be linked to a positive connection between 272 the generative task and predictive uncertainty quantification. In particular, Grathwohl et al. [7] 273 demonstrate that their proposed method for integrating the generative objective in training yields 274 models that have improved predictive uncertainty quantification. Since neither Schut et al. [23] nor we have employed any surrogate generative models, our findings seem to indicate that the positive connection found in Grathwohl et al. [7] is bidirectional.

5.2 Limitations

- BatchNorm does not seem compatible with JEM
 - Coverage and temperature impacts CCE in somewhat unpredictable ways
 - It seems that models that are not explicitly trained for generative task, still learn it implictly
 - Batch size seems to impact quality of generated samples (at inference, but not so much during JEM training)
 - ECCCo is sensitive to optimizer (Adam works well), learning rate and distance metric (11 currently only one that works)
 - SGLD takes time
 - REVISE has benefit of lower dimensional space
 - For MNIST it seems that ECCCo is better at reducing pixel values than increasing them (better at erasing than writing)
- JEMs are more difficult to train

291 6 Conclusion

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367 Appendices

368 A JEM

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- While \mathbf{x}_J is only guaranteed to distribute as $p_{\theta}(\mathbf{x}|\mathbf{y}^*)$ if $\epsilon \to 0$ and $J \to \infty$, the bias introduced for a small finite ϵ is negligible in practice [18, 7]. While Grathwohl et al. [7] use Equation 2 during
- training, we are interested in applying the conditional sampling procedure in a post-hoc fashion to
- any standard discriminative model.

B Conformal Prediction

- The fact that conformal classifiers produce set-valued predictions introduces a challenge: it is not
- immediately obvious how to use such classifiers in the context of gradient-based counterfactual
- search. Put differently, it is not clear how to use prediction sets in Equation 1. Fortunately, Stutz et al.
- 377 [25] have recently proposed a framework for Conformal Training that also hinges on differentiability.
- 378 Specifically, they show how Stochastic Gradient Descent can be used to train classifiers not only
- for the discriminative task but also for additional objectives related to Conformal Prediction. One
- such objective is *efficiency*: for a given target error rate α , the efficiency of a conformal classifier

improves as its average prediction set size decreases. To this end, the authors introduce a smooth set size penalty defined in Equation 3 in the body of this paper

Formally, it is defined as $C_{\theta, \mathbf{y}}(\mathbf{x}_i; \alpha) := \sigma\left((s(\mathbf{x}_i, \mathbf{y}) - \alpha)T^{-1}\right)$ for $\mathbf{y} \in \mathcal{Y}$, where σ is the sigmoid function and T is a hyper-parameter used for temperature scaling [25].

Intuitively, CP works under the premise of turning heuristic notions of uncertainty into rigorous uncertainty estimates by repeatedly sifting through the data. It can be used to generate prediction intervals for regression models and prediction sets for classification models [1]. Since the literature on CE and AR is typically concerned with classification problems, we focus on the latter. A particular variant of CP called Split Conformal Prediction (SCP) is well-suited for our purposes, because it imposes only minimal restrictions on model training.

Specifically, SCP involves splitting the data $\mathcal{D}_n = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1,...,n}$ into a proper training set $\mathcal{D}_{\text{train}}$ and a calibration set \mathcal{D}_{cal} . The former is used to train the classifier in any conventional fashion. The latter is then used to compute so-called nonconformity scores: $\mathcal{S} = \{s(\mathbf{x}_i, \mathbf{y}_i)\}_{i \in \mathcal{D}_{\text{cal}}}$ where $s: (\mathcal{X}, \mathcal{Y}) \mapsto \mathbb{R}$ is referred to as *score function*. In the context of classification, a common choice for the score function is just $s_i = 1 - M_{\theta}(\mathbf{x}_i)[\mathbf{y}_i]$, that is one minus the softmax output corresponding to the observed label \mathbf{y}_i [3].

³⁹⁷ Finally, classification sets are formed as follows,

$$C_{\theta}(\mathbf{x}_i; \alpha) = \{ \mathbf{y} : s(\mathbf{x}_i, \mathbf{y}) \le \hat{q} \}$$
(7)

calibration set increases, the probability that the classification set $C(\mathbf{x}_{test})$ for a newly arrived sample \mathbf{x}_{test} does not cover the true test label \mathbf{y}_{test} approaches α [3]. 400 Observe from Equation 7 that Conformal Prediction works on an instance-level basis, much like 401 Counterfactual Explanations are local. The prediction set for an individual instance x_i depends only 402 on the characteristics of that sample and the specified error rate. Intuitively, the set is more likely 403 to include multiple labels for samples that are difficult to classify, so the set size is indicative of 404 predictive uncertainty. To see why this effect is exacerbated by small choices for α consider the case 405 of $\alpha = 0$, which requires that the true label is covered by the prediction set with probability equal to 406 1. 407

where \hat{q} denotes the $(1-\alpha)$ -quantile of \mathcal{S} and α is a predetermined error rate. As the size of the

408 C Conformal Prediction

409 A Submission of papers to NeurIPS 2023

Please read the instructions below carefully and follow them faithfully.

411 A Style

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Papers to be submitted to NeurIPS 2023 must be prepared according to the instructions presented here. Papers may only be up to **nine** pages long, including figures. Additional pages *containing only acknowledgments and references* are allowed. Papers that exceed the page limit will not be reviewed, or in any other way considered for presentation at the conference.

The margins in 2023 are the same as those in previous years.

Authors are required to use the NeurIPS LATEX style files obtainable at the NeurIPS website as indicated below. Please make sure you use the current files and not previous versions. Tweaking the style files may be grounds for rejection.

B Retrieval of style files

The style files for NeurIPS and other conference information are available on the website at

The file neurips_2023.pdf contains these instructions and illustrates the various formatting requirements your NeurIPS paper must satisfy.

- The only supported style file for NeurIPS 2023 is neurips_2023.sty, rewritten for LaTeX 2ε .
- 426 Previous style files for LATEX 2.09, Microsoft Word, and RTF are no longer supported!
- The LATEX style file contains three optional arguments: final, which creates a camera-ready copy,
- 428 preprint, which creates a preprint for submission to, e.g., arXiv, and nonatbib, which will not
- load the natbib package for you in case of package clash.
- 430 **Preprint option** If you wish to post a preprint of your work online, e.g., on arXiv, using the
- NeurIPS style, please use the preprint option. This will create a nonanonymized version of your
- work with the text "Preprint. Work in progress." in the footer. This version may be distributed as you
- see fit, as long as you do not say which conference it was submitted to. Please do not use the final
- option, which should **only** be used for papers accepted to NeurIPS.
- 435 At submission time, please omit the final and preprint options. This will anonymize your
- submission and add line numbers to aid review. Please do not refer to these line numbers in your
- paper as they will be removed during generation of camera-ready copies.
- The file neurips_2023.tex may be used as a "shell" for writing your paper. All you have to do is
- replace the author, title, abstract, and text of the paper with your own.
- The formatting instructions contained in these style files are summarized in Sections B, C, and D
- 441 below.

442 B General formatting instructions

- The text must be confined within a rectangle 5.5 inches (33 picas) wide and 9 inches (54 picas) long.
- The left margin is 1.5 inch (9 picas). Use 10 point type with a vertical spacing (leading) of 11 points.
- Times New Roman is the preferred typeface throughout, and will be selected for you by default.
- Paragraphs are separated by ½ line space (5.5 points), with no indentation.
- The paper title should be 17 point, initial caps/lower case, bold, centered between two horizontal
- rules. The top rule should be 4 points thick and the bottom rule should be 1 point thick. Allow 1/4 inch
- space above and below the title to rules. All pages should start at 1 inch (6 picas) from the top of the
- 450 page.
- 451 For the final version, authors' names are set in boldface, and each name is centered above the
- 452 corresponding address. The lead author's name is to be listed first (left-most), and the co-authors'
- names (if different address) are set to follow. If there is only one co-author, list both author and
- 454 co-author side by side.
- Please pay special attention to the instructions in Section D regarding figures, tables, acknowledg-
- 456 ments, and references.

457 C Headings: first level

- 458 All headings should be lower case (except for first word and proper nouns), flush left, and bold.
- First-level headings should be in 12-point type.

460 A Headings: second level

Second-level headings should be in 10-point type.

462 A.1 Headings: third level

- Third-level headings should be in 10-point type.
- 464 **Paragraphs** There is also a \paragraph command available, which sets the heading in bold, flush
- left, and inline with the text, with the heading followed by 1 em of space.

D Citations, figures, tables, references

These instructions apply to everyone.

468 A Citations within the text

- The natbib package will be loaded for you by default. Citations may be author/year or numeric, as
- 470 long as you maintain internal consistency. As to the format of the references themselves, any style is
- acceptable as long as it is used consistently.
- The documentation for natbib may be found at
- http://mirrors.ctan.org/macros/latex/contrib/natbib/natnotes.pdf
- Of note is the command \citet, which produces citations appropriate for use in inline text. For example,
- 476 \citet{hasselmo} investigated\dots
- 477 produces
- Hasselmo, et al. (1995) investigated...
- 479 If you wish to load the natbib package with options, you may add the following before loading the 480 neurips_2023 package:
- 481 \PassOptionsToPackage{options}{natbib}
- 482 If natbib clashes with another package you load, you can add the optional argument nonatbib 483 when loading the style file:
- 484 \usepackage[nonatbib] {neurips_2023}
- As submission is double blind, refer to your own published work in the third person. That is, use "In
- the previous work of Jones et al. [4]," not "In our previous work [4]." If you cite your other papers
- that are not widely available (e.g., a journal paper under review), use anonymous author names in the
- citation, e.g., an author of the form "A. Anonymous" and include a copy of the anonymized paper in
- 489 the supplementary material.

490 B Footnotes

- Footnotes should be used sparingly. If you do require a footnote, indicate footnotes with a number 1
- in the text. Place the footnotes at the bottom of the page on which they appear. Precede the footnote
- with a horizontal rule of 2 inches (12 picas).
- Note that footnotes are properly typeset *after* punctuation marks.²

495 C Figures

- 496 All artwork must be neat, clean, and legible. Lines should be dark enough for purposes of reproduction.
- The figure number and caption always appear after the figure. Place one line space before the figure
- 498 caption and one line space after the figure. The figure caption should be lower case (except for first
- word and proper nouns); figures are numbered consecutively.
- You may use color figures. However, it is best for the figure captions and the paper body to be legible
- if the paper is printed in either black/white or in color.

¹Sample of the first footnote.

²As in this example.

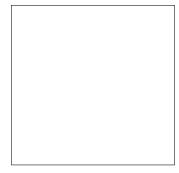


Figure 6: Sample figure caption.

Table 1: Sample table title

	Part	
Name	Description	Size (μm)
Dendrite Axon Soma	Input terminal Output terminal Cell body	$\begin{array}{c} \sim \! 100 \\ \sim \! 10 \\ \text{up to } 10^6 \end{array}$

D Tables

- All tables must be centered, neat, clean and legible. The table number and title always appear before
- the table. See Table 1.
- Place one line space before the table title, one line space after the table title, and one line space after
- the table. The table title must be lower case (except for first word and proper nouns); tables are
- numbered consecutively.
- Note that publication-quality tables *do not contain vertical rules*. We strongly suggest the use of the
- booktabs package, which allows for typesetting high-quality, professional tables:

https://www.ctan.org/pkg/booktabs

This package was used to typeset Table 1.

512 E Math

- Note that display math in bare TeX commands will not create correct line numbers for sub-
- 514 mission. Please use LaTeX (or AMSTeX) commands for unnumbered display math. (You
- really shouldn't be using \$\$ anyway; see https://tex.stackexchange.com/questions/
- 516 503/why-is-preferable-to and https://tex.stackexchange.com/questions/40492/
- what-are-the-differences-between-align-equation-and-displaymath for more infor-
- 518 mation.)

519 F Final instructions

- 520 Do not change any aspects of the formatting parameters in the style files. In particular, do not modify
- 521 the width or length of the rectangle the text should fit into, and do not change font sizes (except
- perhaps in the **References** section; see below). Please note that pages should be numbered.

523 E Preparing PDF files

- Please prepare submission files with paper size "US Letter," and not, for example, "A4."
- Fonts were the main cause of problems in the past years. Your PDF file must only contain Type 1 or
- Embedded TrueType fonts. Here are a few instructions to achieve this.

- You should directly generate PDF files using pdflatex.
 - You can check which fonts a PDF files uses. In Acrobat Reader, select the menu Files>Document Properties>Fonts and select Show All Fonts. You can also use the program pdffonts which comes with xpdf and is available out-of-the-box on most Linux machines.
 - xfig "patterned" shapes are implemented with bitmap fonts. Use "solid" shapes instead.
 - The \bbold package almost always uses bitmap fonts. You should use the equivalent AMS Fonts:

\usepackage{amsfonts}

followed by, e.g., \mathbb{R} , \mathbb{R} , \mathbb{N} or \mathbb{C} . You can also use the following workaround for reals, natural and complex:

```
\newcommand{\RR}{I\!\!R} %real numbers
\newcommand{\Nat}{I\!\!N} %natural numbers
\newcommand{\CC}{I\!\!\!C} %complex numbers
```

Note that amsforts is automatically loaded by the amssymb package.

If your file contains type 3 fonts or non embedded TrueType fonts, we will ask you to fix it.

42 A Margins in LATEX

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- Most of the margin problems come from figures positioned by hand using \special or other
- commands. We suggest using the command \includegraphics from the graphicx package.
- Always specify the figure width as a multiple of the line width as in the example below:

```
546     \usepackage[pdftex]{graphicx} ...
547     \includegraphics[width=0.8\linewidth]{myfile.pdf}
```

- See Section 4.4 in the graphics bundle documentation (http://mirrors.ctan.org/macros/
- 149 latex/required/graphics/grfguide.pdf)
- A number of width problems arise when LATEX cannot properly hyphenate a line. Please give LaTeX
- 551 hyphenation hints using the \- command when necessary.

552 F Supplementary Material

- Authors may wish to optionally include extra information (complete proofs, additional experiments
- and plots) in the appendix. All such materials should be part of the supplemental material (submitted
- separately) and should NOT be included in the main submission.

556 References

- 557 References follow the acknowledgments in the camera-ready paper. Use unnumbered first-level
- beading for the references. Any choice of citation style is acceptable as long as you are consistent. It
- is permissible to reduce the font size to small (9 point) when listing the references. Note that the
- Reference section does not count towards the page limit.
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- 563 609–616. Cambridge, MA: MIT Press.
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