ADVANCING NEAREST NEIGHBOR EXPLANATION-BY-EXAMPLE WITH CRITICAL CLASSIFICATION REGIONS

ABSTRACT

There is an increasing body of evidence suggesting that post-hoc explanation-by-example with nearest neighbors is a promising solution for the eXplainable Artificial Intelligence (XAI) problem. However, despite being thoroughly researched for decades, such post-hoc methods have never seriously explored how to enhance these explanations by highlighting specific important *parts* in a classification. Here, we propose the notion of *Critical Classification Regions* (CCRs) to do this, and several possible methods are experimentally compared to determine the best approach for this explanation strategy. CCRs supplement nearest neighbor examples by highlighting similar important *parts* in the image explanation. Experiments across multiple domains show that CCRs represent key features used by the CNN in both the testing and training data. Finally, a suitably-controlled user study (N=163) on ImageNet, shows CCRs improve people's assessments of the correctness of a CNN's predictions for difficult classifications due to ambiguity.

1 INTRODUCTION

The impressive success of deep learning for computer-vision problems has led to proposals that they should be used in high-stakes applications such as diagnostic radiology for Covid-19 (Pham, 2020). However, the interpretability issues for these models raise significant questions about their feasibility for such use-cases. Accordingly, many eXplainable AI (XAI) techniques have been proposed to overcome this interpretability problem, such as saliency maps (Bach et al., 2015) and contrastive methods (Miller, 2019). In this paper, we focus on one of the most long-standing XAI techniques, the use of post-hoc explanation-by-example involving nearest-neighbors (Sørmo et al., 2005), with a view to significantly extending this method's functionality. Recently, explanation-by-example techniques have been increasingly used to interpret deep learning models (Lipton, 2018; Chen et al., 2019; Jeyakumar et al., 2020; Kenny & Keane, 2019; 2021; Papernot & McDaniel, 2018; Kim et al., 2016; Koh & Liang, 2017; Godi et al., 2019), with interest in these techniques being bolstered by their psychological plausibility in human decision-making (Klein, 1989; Cohen et al., 1996), human category-learning (Edwards et al., 2019), and by supportive evidence from several XAI user studies (Borowski et al., 2020; Kenny et al., 2021; Cai et al., 2019; Kim et al., 2014; Yang et al., 2020; Buçinca et al., 2020). However, currently, these techniques do not enhance their explanations by showing very specific important "parts" used in the prediction, we rectify this deficit here.

Hence, this work has two main aims: (1) to extend explanation-by-example's functionality through the use of Critical Classification Regions (CCRs), and (2) to properly test this novel technique in a suitably-controlled user study.[1] *Critical Classification Regions* represent the primary region of importance in a test image and in the nearest-neighbor example used for explanation (e.g., see Fig. 1). CCRs show end-users the main feature used in a Convolutional Neural Network's (CNN's) classification, as well as contextualizing these features in the training data (by also showing them in a nearest neighbor for the test instance). Three experiments are reported testing this novel method (see Sections 3-5). Although many post-hoc XAI techniques for deep learners show salient regions of a test image (Ribeiro et al., 2016; Bach et al., 2015; Zhou et al., 2016), to our knowledge, none have seriously considered relating these regions to nearest neighbors in the training data, to show *what* features were learned by the CNN and (more importantly, our core novelty here) *where* they arose.

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[1]Our method is available to pip install as a Python library at https://after_anon_review.

Figure 1: Difference Between Methods: A misclassification of a "Leopard" as "Cheetah" on ImageNet is explained by four methods: (A) Normal explanation-by-example saying *"I think the test image is a Cheetah because it looks similar to a training image I also think is a Cheetah"*. This explanation is then enhanced by showing the regions used in the classification by (B) FAMs proposed by Kenny & Keane (2019), and our proposed methods of (C) Latent-based CCRs, and (D) pixel-based CCRs. The FAMs highlight multiple regions in both images, and it is difficult to know where a feature begins and ends, in contrast, CCRs highlight a very specific *part* of both images. Note that the CCR explanation methods naturally retrieve a different neighbor due to searching a "pool" of candidates for the closest feature match, whilst FAMs always use the closest NN.

In the XAI literature, few works address the identification of important regions within example-based explanations. The closest work to ours makes use of Feature Activation Maps (FAMs) within the *twin-system framework* to enhance example-based explanations (Kenny & Keane, 2019; 2021). FAMs upsample the most positively contributing convolutional feature kernel (in the last convolutional layer) and, as such, can be thought of as a variant of Class Activation Maps [CAMs by Zhou et al. (2016)], which use a combination of all layers. However, FAMs often fail to isolate a comprehensible "part" of each image, and can be, arguably, hard to contextualize (see Fig. 1B). Moreover, there is no computational experiments to verify any causal role of FAMs in classifications, or psychological user studies to show they make any difference to people. In contrast, we show how CCRs play a causal role in classification, and how they affect users in a study.

From an implementation standpoint, the current latent-based CCR method (see Section 2.2) is partly inspired by Chen et al. (2019), who used a case-based approach to explain a CNN's predictions. However, their approach is a *pre-hoc* method that compresses the training data down into prototypical parts for explanations, integrating them directly into the CNN's calculations in a forward pass. In contrast, the current method is *post-hoc*, using the training data for explanation *after* the prediction is made. Hence, it may be better suited to situations where (i) model accuracy is critical, (ii) it is simply not feasible to train another more interpretable model, or (iii) more diverse explanations (from the full training data) are required (Mothilal et al., 2020). Finally, the current method builds upon the family of activation-mapping techniques for visualising the important regions of an image used by a CNN in its predictions (Zhou et al., 2016; Kenny & Keane, 2021).

This paper has four more sections. Section 2 describes how to compute CCRs in explanation-by-example. As CCRs can be generated from the latent space (i.e., Latent-based CCRs), or the pixel space (i.e., Pixel-based CCRs), Section 3 determines which option works best for the *test image* Section 4 performs additional checks on CCRs to help validate their causal role in classification, and determines the best way to identifying CCRs in nearest-neighbor explanations (henceforth the NN-CCR) in the *training image*. Section 5 reports a user study that tests whether the CCRs found by this method matter to people, before a final discussion (see Section 6). This paper makes three main contributions:

- *Technical Novelty*: A new XAI idea that computes CCRs to augment *post-hoc*, nearest-neighbor explanation-by-example. These CCRs connect critical features used in a classification with *where* they were learned from in the training data.

- *Empirical Novelty*: A novel series of computational experiments that verify the optimal CCR variant to be used in multiple situations (see Expt. 1 and 2).

- *Empirical Novelty*: A heavily-controlled user study showing the conditions under which this explanation strategy works best (see Expt. 3).

2   ALGORITHM: FINDING CCRS IN EXPLANATIONS

The core novelty of this paper is CCRs, but to generate these the first crucial step is to locate a pool of "good" nearest neighbors (NNs) to avoid searching the entire training data. Rather than proposing a novel method, we found four candidate explanation-by-example methods that could deliver such pools (Jeyakumar et al., 2020; Papernot & McDaniel, 2018; Hanawa et al., 2021; Kenny & Keane, 2019). As an aside contribution, we competitively tested these four methods, and found the twin-systems method to be best (n.b., these were never compared before). Concisely, twin-systems are the only method that (1) use all parameters in the network to give explanations [i.e., they passed the sanity checks of Adebayo et al. (2018)], and (2) do not require human-labels (see Appendix A for full experimental details). The *Twin-Systems* approach to post-hoc explanation-by-example analyses the feature-weights of CNNs and maps these into a more transparent k-NN to find explanatory nearest-neighbors (Kenny & Keane, 2019). Specifically, the gradient of the output classification neuron is taken w.r.t. the latent representation of an image, and an element-wise product of the two is taken for a final representation of the image. Following Kenny & Keane (2021), we use ResNets and the image representation in the CNN's penultimate layer for this calculation. These new representations are derived for the entirety of the training data and used to fit a k-NN classifier. When a new test image is presented, its new representation is derived, and the most similar cases (measured by the L_2 norm) are presented for explanations.

Speeding-up Twin-Systems. As an additional aside contribution, our tests found all current explanation-by-example methods too slow in large-scale computational experiments using ImageNet, so we had to speed-up the algorithm. The solution uses a collection of k-NN models, namely, one for each class, instead of a single k-NN for all classes, as is usually done. Formally, consider a training dataset D of images I, with K output classes, K subdivisions of the datasets D_k can be made to fit K separate k-NN classifiers with:

$$D_k = \{I_i\}_{i=1}^n \in D \qquad \text{s.t.} \quad f(I_i) = \hat{y}_k \tag{1}$$

where $\hat{y}_k$ is the node in the CNN output layer corresponding to the *prediction* of some class k (n.b., *not* the label, meaning it also works for self-supervised learning), n the number of images in D_k, and f the CNN in question. This modification to twin-systems was tested on CIFAR-10/ImageNet, in both cases all testing data was used to find 50 NNs for each image, and the retrieved examples were compared to the original twin-system's NNs. The tests showed they were in agreement regarding the NN indexes in D, and their distance ordering to the test image 99.99%+ of the time, meaning there is a negligible difference between them. This reduced the run-time for retrieving NNs on ImageNet from ≈15 sec to ≈0.03 sec using a "brute force" search algorithm (n.b., "faster" k-NN search algorithms like KD-Tree/Ball-Tree resulted in *no* speedup). Note this variation to explanation-by-example will only work for twin-systems, the other methods cannot use this speedup.

2.1   COMPUTING LATENT-BASED CCRS (CAM-CCRS, FAM-CCRS, RAND-CCRS)

This CCR Method we propose uses the latent representations of an image in a CNN to gauge similarity. Assume for a given test image I, a final representation $C \in \mathbb{R}^{(h,w,d)}$ is extracted after all convolutional layers, were h and w represent the height and width of the convolutional output, respectively, and d the number of kernels (in all current experiments $h = w = 7$). This may be broken down into regions shaped as $h_1 \times w_1 \times d$, were $h_1 < h$ and $w_1 < w$. These regions may be upsampled to the size of the original image to visualize them as a "box" (e.g., see Fig. 1), which is the region in pixel-space that corresponds to this region in C. Here, we want to select the region in C which is critical to the classification, and use it to elaborate the explanation further.

Following Chen et al. (2019), we set $h_1 = w_1 = 1$ to represent the smallest part of the image possible and give more granular detail in the explanation. To select which regions of C are CCRs, we assume the presence of some activation map giving a saliency value to each region in C (e.g., FAMs). Such a technique gives a 7×7 saliency map corresponding to C we refer to as $M_{test} \in \mathbb{R}^{(7,7)}$, which gives the importance of each spatial region. Next, by selecting the most positive salient region, we can isolate the test image CCR $\omega_{test} \in \mathbb{R}^{(1,1,d)}$.

Then, with the test-image CCR isolated, the task is to find a similar region from the training data ω_{nn}, giving an example of where this feature was "learned" from. Using some nearest neighbor algorithm, a pool of n training-instances are found that are candidate explanations-by-example. In this pool, let $C_{(n,i,j)}$ represent some potential region $\omega \in \mathbb{R}^{(1,1,d)}$ in the final convolutional layer, with the neighbor indexed by n, and its spatial position in C_n indexed by i and j. These n images have their C representation searched to find the closest match to ω_{test} using the L_2 norm to find ω_{nn}. Importantly however, this region in the NNs is constrained to its relative importance within the instance. Specifically, considering each NN's activation map M_n, only those regions which satisfy the constraint of being higher than $max(M_n) \times \alpha^{-1}$ are considered to find ω_{nn} by minimizing:

$$\arg\min_{n,i,j} \quad \|\omega_{test} - C_{(n,i,j)}\|_2 \qquad \text{s.t.} \quad M_{(n,i,j)} > max(M_n) \times \alpha^{-1}. \tag{2}$$

The alpha constraint is to help ensure ω_{nn} is highly critical to the classification and causally related. For the activation map M, we experiment using CAM, FAM, and Random activation maps (see Expts. 1 and 2). So three variants of latent-based CCRs are tested – CAM-CCRs, FAM-CCRs, and Rand-CCRs – although many other options exist for retrieving M. One of the important points to note about these CCR methods is the regions found are contingent, to some degree, on the pool of NNs over which they are computed (hence, the need for the test of alternative k-NN methods reported in Appendix A – omitted from the main paper due to size constraints).

2.2 Computing Pixel-based CCRs (SP-CCRs)

Another variant of CCRs we propose uses pixel representations, this option is better in domains were spatial relations between the latent layers (e.g., C in the previous section) and the pixel input are not reliable, or convolutions themselves are not used [e.g., vision transformers (Dosovitskiy et al., 2020)]. Specifically, a test image can be broken down into superpixel segments, each segment can be passed into the network one-by-one (with the rest of the image occluded), and the CNN's logit value for the class in question can be recorded to find the most important region used in a classification [similar to LIME by Ribeiro et al. (2016)]. Once the test image CCR is isolated, we upsample it to the CNN input-size, and acquire its representation from taking the penultimate layer activations after a forward pass in the network. This process is repeated in the pool of NNs, to find the segment (i.e., the NN-CCR) most similar to the test image CCR with the L_2 norm.

More formally, consider the test image CCR representation $\omega_{test} \in \mathbb{R}^{(d)}$, were d is the number of extracted features in the penultimate layer. We again want to isolate a comprehensible example from the training data ω_{nn} where this feature was "learned". Let $S_{(n,i)}$ be the representation $\omega \in \mathbb{R}^{(d)}$ of some superpixel segment i in the NN n. Additionally, let $M_{(n,i)}$ represent each region's saliency. These n images have their S representations searched to find the closest match to ω_{test} using the L_2 norm to find ω_{nn}. Importantly however, this closest region in the NNs is again constrained to its relative importance within the instance. Specifically, only those regions which satisfy the constraint of being higher than $max(M_n) \times \beta^{-1}$ are considered to find ω_{nn} by minimizing:

$$\arg\min_{n,i} \quad \|\omega_{test} - S_{(n,i)}\|_2 \qquad \text{s.t.} \quad M_{(n,i)} > max(M_n) \times \beta^{-1}. \tag{3}$$

The beta constraint again helps ensure ω_{nn} is highly critical to the classification and causally-related. For pixel-based CCRs, we consider this single superpixel method (called SP-CCRs). So, including the three latent-based CCR methods, there are four methods tested in our experimental evaluations.

3 Experiment 1: Finding Test Image CCRs

In this experiment, the performance of the latent- and pixel-based CCR methods in isolating an important part of the *test image* was evaluated. This worked by keeping the CCR region in the pixel

Figure 2: Expt. 1 Results: (A) The class logit for each method's CCRs across all the testing data in CUB-200 and all the segmentation options, with (B) showing the same for ImageNet. (C) A detailed regression is shown for CUB-200 when 30 superpixel regions are used, and (D) 20 for ImageNet. Overall, the results show superpixels perform better, and when investigating further with the regressions, particularly when smaller regions of the image are used for the CCRs (i.e., approximately 5-15%), but then for larger regions CAM-based CCRs tend to do the best. Standard error bars are shown.

image, whilst occluding the rest, and then passing the image through the CNN. So, the method that produces the highest logit in the test-image's predicted class reflects the best performance. To do this, the test image SP-CCR is located, then the latent-based CCRs are found by (1) up-sampling their activation maps to the pixel-space, and (2) isolating an equally sized region to the SP-CCR from the pixel space taken from the parts of highest saliency activation (so all methods have their CCR the same size to ensure a fair test). Two datasets CUB-200 and ImageNet were used, with the former having ResNet18 fine-tuned to it and the latter a pre-trained ResNet50. The experiment is repeated with five different segmentation options for the superpixels, dividing the images up into roughly 10, 20, 30, 40, and 50 segments, to understand it's effect on explanations when considering progressively smaller CCRs. All statistical comparisons use a 2-tailed, independent t-test.

3.1 RESULTS

Fig. 2(A) displays results for CUB-200 across all superpixel segmentation options up to 50, and Fig. 2(B) does the same for ImageNet. In general, logit values drop as segments become smaller (i.e., closer to 50), showing a feature's size in the image does matter. Additionally, superpixels perform best with *high significance* after 30 segmentations in CUB-200, and 20 for ImageNet (i.e., all ps < 0.0001). We assume that larger CCRs are generally better, as they will tend to form more interpretable features; hence, we plotted a regression line at these points for a more nuanced examination, Fig. 2(C) shows superpixels will generally only perform best if the region they occupy is roughly $<$ 5%, whilst Fig. 2(D) shows this point for ImageNet is larger at $<$ 15%. This disparity likely occurs because there are far more varied features the model can learn in ImageNet, so segmenting larger regions is more beneficial, but CUB-200 is quite focused by comparison.

4 EXPERIMENT 2: EXPLANATION FIDELITY WITH NN-CCRs

Now we need to know how to find important regions in the training data for an explanation that is of high-fidelity and causally-related to the classification. Eq. (2) and (3) cannot be directly compared because the alpha and beta constraints are relative measures. However, we can discard those hyperparameters temporarily and compare all methods directly (and fairly) by simply adding more superpixel regions one-by-one and then adjusting the size of the latent CCR methods accordingly (adding more of the highest salient regions to match the progressively growing SP-CCR method's size), until the entire image is included. First, we fine-tuned a given CNN by only showing it the most salient CCR region, and then we repeated the process until all of the image is present (so, 30 segmentations on CUB-200 will equal 30 times the CNN must be fine-tuned, for each of the 4 methods, totaling 120 training runs). This procedure gives us an indication of how much of the training data images are actually responsible for test predictions [similar to Hooker et al. (2019)]. Note this experiment requires a constant value for segmentation, so we choose 30 for CUB-200, and 20 for ImageNet, as they performed well in Expt. 1.

Then, when this direct comparison is done, we evaluated each CCR method separately. However, this time, instead of manually increasing the number of CCR regions used during fine-tuning, we manipulate α and β to control the amount of regions shown *relative* to each image (which is required in practice). Finally, with these results in hand guiding our hyperparameter choices, we can finally test each method's performance in retrieving a "similar looking" NN-CCR to the test-image's CCR by passing the upsampled CCRs though the CNN, and comparing their latent representations with the L_2 norm. As before, all statistical comparisons use a 2-tailed, independent t-test. In all fine-tuning tests, CUB-200 was fine-tuned for 5000 iterations, and ImageNet for 1000, with testing data accuracy samples being taken every 50 iterations, the first 200 iterations were discarded as the networks stabilised.

4.1 RESULTS

Fig. 3(A) shows the results of the direct comparative tests which fine-tuned the CNNs using only the most salient CCR to start, and then progressively adding in more of the most salient regions in order. Results on CUB-200 show superpixels become no different to random selections after 10 segments (roughly 33% of the image is used; $p > 0.05$), and the same happens to CAM/FAM at around 15 segments (roughly 50%; $p > 0.05$). Superpixels are significantly better than the other methods when using just one segment (or up to two on ImageNet; $p < 0.01$), but become slightly worse thereafter compared to CAM/FAM-CCRs (n.b., but still better than random). This is likely because each superpixel region is not "context aware" of the rest of the image, unlike the activation maps, so they are not progressively added to the image in an order which is considering the image as a whole. Fig. 3(B) shows overall, that higher alpha values are better for ImageNet than CUB-200, with 1.25 getting a good balance between searching a lot of the NN, and staying very causally linked (mean diff=49.83 between CAM/Random), whilst a smaller value of 1.1 appears close to optimal for CUB-200 (mean diff CAM/Random=22.67; p's < 0.0001). Fig. 3(C) shows similar thresholds for the beta parameter are around 1.1 for CUB-200 (mean diff=14.34) and lower for ImageNet at 1.1 (mean diff=4.93; $p < 0.001$; although interestingly the latter still stays statistically significant until beta=3.0). Lastly, using these hyperparamters, we can optimize the search for NN-CCRs with Eq. (2) and Eq. (3), and measure the latent similarity between them and the test-image's CCR. Fig. 3(D) shows these results for both datasets, illustrating hugely significant differences in favor of SP-CCRs once the number of superpixel segments goes over 20.

Interim Conclusions. Firstly, CAM-CCRs offer the most exploration possible of the NN pool to search for a NN-CCR whilst staying highly causally faithful to the CNN, but SP-CCRs are better when only considering 1-2 CCRs in the NN. Secondly, it is noteworthy that SP-CCRs are less rigid compared to latent-based CCRs (which are confined to 49 "box" regions in NN image), and the latter seem to lose some spatial correlation with the input pixels. Lastly, latent-based CCRs are faster to

Figure 3: Expt. 2 Results: (A) Direct comparative tests of all methods by fine-tuning the networks on just the most salient regions first, then with the rest progressively added in. (B) Finding the optimal alpha parameter for latent-based CCRs in both datasets. (C) Finding the optimal beta parameter for pixel-based CCRs across both datasets. (D) Measuring the visual similarity between test image CCRs, and their NN-CCRs found for explanations. Standard error bars are shown across all plots.

compute, taking 2 sec to generate ImageNet explanations on average, compared to 45 sec for their SP-CCR alternative (using 10 NNs and a CPU). Overall however, all methods are better than the random baseline (except for the beta hyperparamter being set to 3 or higher on ImageNet), so any CCR explanation should always have fidelity.

5 EXPERIMENT 3: USER STUDY

The previous computational experiments showed that the current explanation-by-example method with critical regions bears a high fidelity to what the CNN classifier has learned. However, we do not know whether these critical regions matter to people; whether the provision of example-plus-CCR explanations impact a user's perception of the CNN more than example-only explanations. Hence, a user study (N=163) was run to test example-plus-CCR versus example-only explanations, using latent-based CAM-CCRs. Previous user studies have shown that example-based explanations (i.e., based on 3 nearest neighbours to a test-image) changed people's perceptions of the *correctness* of misclassifications by a CNN on MNIST (Kenny et al., 2021). Specifically, they found that people rated misclassifications as less incorrect (i.e., correctness was rated higher). Here, we examine whether the provision of similar explanatory examples with or without CCRs (i.e., a NoBox v Box manipulation) changes people's perceptions of misclassifications made by a CNN on ImageNet.

The XAI literature has few user studies attempting to test *specific* explanation strategies, and most of these are inadequately designed [e.g., poor test-item selection and low Ns are common deficits (Anjomshoae et al., 2019; Keane et al., 2021)]. For instance, typically, studies use only a handful of test items and these materials are not properly counterbalanced over explanation conditions. Here, we try to rectify these deficits (indeed, we explicitly demonstrate how material-sets can matter).

So, the study presented participants with 32 test-images from the ImageNet dataset (i.e., 24 misclassifications, with 8 "fillers" that were correct classifications for attention checks) and were asked to make classification-correctness and explanation-helpfulness judgements of these items presented alongside one of the two explanation-types (NoBox or Box; i.e., no CCR or CCR). The 24 misclassifications were randomly divided into two material sets (A-set and B-set) to counterbalance the experiment; so, (a) one group (N=82) received the A-set with example-only explanations (NoBox) and the B-set with example-plus-CCR explanations (Box) and (b) the other group (N=81) received the A-set with example-plus-CCR explanations (Box) and the B-set with example-only explanations (NoBox; see Fig. 4 for examples). The statistical analysis then collapsed across these counterbalanced groups controlling for the effects of the material-set. This consideration of material-sets is not just a "statistical nicety", as any given user will only see a sample of these images, a good explanation strategy needs to operate successfully over different image-samples. Hence, user studies need to control for this issue by using different, reasonably-sized and randomly-sampled material-sets.

In summary, the study examined people's responses to the two post-hoc explanation-types, example-based explanation-only v example-based explanation-plus-CCR (i.e., NoBox v Box) over 24 image-misclassifications (i.e., 12 items for each type). The counterbalanced groups allowed us to test both explanation-types used for the same given image. As we shall see, that design also allowed us to examine material-set effects within the counterbalanced group (i.e., A-set v B-set)

5.1 METHOD

Participants. Participants (N=163) were recruited on the Prolific crowdsourcing site (www.prolific.co). All were aged over 18, native English speakers and lived in the USA, UK, or Ireland. Participants were paid £7.50/hr for their participation, which totalled £319.8. This N was chosen based on a power analysis for a low effect-size; this size was chosen because we anticipated the addition of CCR boxes would have a quite nuanced effect over just explanation-by-example due to it already being heavily preferred by users (Jeyakumar et al., 2020). This study passed ethics review of the institution (ref. after anonymous review).

Materials. Twenty-four misclassifications were randomly sampled from the CNN using ImageNet. These were actual test-image errors when the classification label differed from the ground truth. The twin-system method was applied to each prediction to find a nearest-neighbor example-explanation, and the CCR in the item (shown as a Box; see Fig. 5). The materials were randomly

assigned to two different sets (A-set and B-set) and counterbalanced (as described earlier). Importantly, the sampling constrained the images to be both varied and those involving classes people could easily understand (e.g., snail, lemon, etc.).

Procedure & Measures. After being told the system was a program that "learned" to classify objects in images, people were told they would be shown several examples of its classifications (see Appendix E for user study questionnaire). Their task was to rate the correctness (i.e., the question was "The program's labelling of the image is correct.") and helpfulness (i.e., the question was "The explanation helps me understand the program's labelling of the object in the picture.") of the presented classification on a 5-point Likert-scale from "I disagree strongly" (1) to "I agree strongly" (5). Each participant was shown 24 misclassifications (12 NoBox and 12 Box explanations) along with 8 filler items that were all correct classifications appearing every fourth question for attention checks. The 24 incorrect items were randomly re-ordered for each person. A debriefing on the rationale and background to the study was provided after testing.

5.2 Results and Discussion

Correctness & Helpfulness. On average, people perceived the misclassifications as being equally incorrect/correct for both explanation types; overall, the mean correctness ratings for both explanation-types were the same, NoBox (M=1.85) and Box (M=1.85) and not significantly different (using a paired t-test, $t(162)$ = -0.018, 1-tailed, $p > 0.05$). So, people's perception of the correctness of misclassifications when given either of the explanation-types appear to be essentially identical. However, this analysis masks an important difference when ratings are broken out into the two material-sets. The items in the B-set that received the example-plus-CCR explanation (Box; M=1.93) were rated as less-incorrect (more correct) than their equivalent items in Set-A (M=1.77); this difference between B-set-Box and A-set-Box was statistically reliable, $t(161)$ = 2.15, p = 0.03, 2-tailed using a two-sample t-test. No other pairwise comparisons were statistically significant. This result suggests that image-explanations showing CCRs (as a boxed outline) impact people's perception of correctness of the misclassification, but only for certain items. We return to a more detailed analysis of this effect below. On helpfulness, both explanation-types were rated positively and equivalent, NoBox (M=3.16) and Box (M=3.11); using a paired t-test, $t(161)$ = -1.60, 1-tailed, p = 0.06. So, the two explanation options are equally helpful to users. Interestingly, for this measure, both material-sets produced almost identical ratings for both explanation-types and no other pair-wise comparisons are statistically different.

Right* & Wrong Misclassifications. We were puzzled by the difference in correctness ratings for the example-plus-CCR (Box) conditions found in the B-set relative to the A-set. What is it about the B-set that produces this effect? In a follow-up analysis, we discovered that, in both material-sets there were ambiguous materials that people consistently rated as more correct (i.e., mean >2) even though the ground-truth identified these items as incorrect (3/12 in the A-set and 4/12 in the B-set). So, we partitioned the items into two new categories, namely "Right*"-items (that people rated

Figure 4: Expt. 3 results: Correctness ratings for two material-sets (A and B) broken out by "Right*" and Wrong classifications for the two explanation-types, NoBox (example-only) and Box (example-plus-CCR). In the B-Set, the Right*-Box ratings (M=3.04) are reliably different to the Right*-NoBox ratings (NoBox, M=2.83), reflecting people's performance on ambiguous items in that material-set.

Figure 5: Expt. 3 Material Examples: (a) A "Pot Pie" is misclassified as "Lemon". The explanation shows the CCR in the image identified by the CNN. The explanation represents the training data and feature "used" in the CNN's classification. Glossed, the explanation says "I think this is a lemon, because it has a similar part to an image I saw before which I learned should be a lemon". (b) Another misclassification of a "Barbell" as a "Prison" in which the CNN picks up on the bars in the background reflecting the jail bars in a previous training image. Although anecdotal, an analysis of these two items shows that both have significantly higher helpfulness ratings when the CCR is given; t-tests show (a) NoBox 2.37 v Box 3.09, $p < 0.001$ and (b) NoBox 4.19 v Box 4.48, $p < 0.05$.

as more "correct", even though they were incorrect classifications) and Wrong-items (that people confidently rated as incorrect, when they were incorrect) and then re-analyzed the data for each material-set (n.b., we add an asterisk to "Right*" on purpose to signal they are not really "Right"). We also verified this partitioning by clustering the material means (using k-means) and found that the data consistently forms these two groups across 500 iterations. Figures 4(A) and 4(B) show that the "Right*" misclassifications are rated significantly higher than the Wrong ones, irrespective of the material-set (A or B) or the presented explanations (NoBox or Box; all $p < 0.05$ using t-tests). No other differences between conditions are statistically different, except for one involving the B-set; namely, the correctness rating for the Right*-misclassifications with example-plus-CCR explanation (Box, M=3.04) is reliably higher than that for the example-only explanation (NoBox, M=2.83), $t(162) = 1.8$, $p = 0.036$, using 1-tailed, two-sample t-test. Note that while this difference appears small on a Likert scale, overall it constitutes a 5.25% difference in responses, which is a larger effect than that found in other studies (Goyal et al., 2019). What does this mean? This finding suggests that some ambiguous material items (that people think may be correct, though they are incorrect) are affected by being given an explanation showing CCRs. Fig. 5(a) shows one such example, a picture of a "Pot Pie" (which is decorated with lemons), which the CNN labelled as a "Lemon"; here, the Box explanation shows the NN (an image of a lemon) and a boxed region showing the "pulp of the lemon" as the feature that influenced the classification. Clearly, when people see this CCR explanation, it provides more information about the classification, leading them to rate it as more correct (which does not occur for the NoBox version). Though this account makes sense, because this analysis is ad-hoc, it should be treated with some care. Nonetheless, it does show that there are specific image-items that are influenced by the provision of CCR information (presumably, when there is confusion over whether the AI really got the prediction right or wrong). Notably, and more generally, these findings give us a sense of the psychological complexities of XAI; namely, that there can be interactions between specific image-items, the predictions about those items made by the model, and the explanation-type used to justify those predictions.

6 GENERAL DISCUSSION AND CONCLUSIONS

Post-hoc explanation-by-example is one of the most popular and successful explanation strategies in both user testing (Kenny et al., 2021; Jeyakumar et al., 2020), and computational experiments (Kim et al., 2014). This paper has reported comparative tests of several ways to augment this popular explanation method by showing the most important *parts* of the image used, what we call *Critical Classification Regions* (CCRs). Initially, computational tests demonstrated the optimal way to isolate these regions in the test image and training data. Subsequently, a carefully designed user study showed that explanations with and without CCRs are both equally helpful for understanding, but that for certain ambiguous images the provision of CCRs influence people's perception of correctness.

ETHICS STATEMENT

It is clear that XAI has made considerable progress in "opening the black box" to begin to reflect the internal workings of these successful, but complex, deep learning models. Here, we have seen that an explanation-by-example strategy shows some promise in supporting this effort (Jeyakumar et al., 2020; Kenny et al., 2021; Chen et al., 2019). However, we should also not loose sight of the potentially negative societal impacts that may arise from these XAI solutions. Perhaps the main concern being that, any data which is presented for explanation may need to be anonymized to ensure privacy and ethical concerns (Jeyakumar et al., 2020), particularly in sensitive domains such as medicine and law.

There are also wider issues to be considered around ensuring that these automated explanations inform without misleading end-users about the systems. Since CCRs gives users the impression that "incorrect" classification's seem more correct, a concern could be put forth that they may actively mislead end-users. However, since ImageNet has "real world" images which inevitably contain several classes (e.g., the pot pie in Fig. 4 could be a "lemon" or "pot pie"), many different possible classifications are arguably correct. So, the CCR is not necessarily "misleading" users, but rather pointing more precisely to where the CNN is looking, and (thanks to the nearest neighbour CCR explanation), "why" it is looking there (our main contribution). When users see the CNN is looking at the "lemon" when it classifies the "pot pie" as a "lemon", although some may see this as incorrect, it is nevertheless acting in a way which is objectively "correct", so people's feelings of "correctness" increased compared to the "nobox" version (or put another way, they see it as "less incorrect"). In terms of use-cases for CCRs, they appear to be most useful at convincing people a CNN's classification is correct, when there are several possible classifications a CNN could make. This would likely be useful in domains with many possible outcomes for which humans are not totally expert – a multi-class classification problem – (e.g., radiology diagnosis, see Fig. 11).

REPRODUCIBILITY STATEMENT

Much effort has been invested to ensure this work is reproducible. For instance, we are providing a code library which can be installed to use the CCR method easily. This includes the twin-ensemble method from Section 2. Moreover, to reproduce the experiments, we have provided all the code used in the supplementary materials, and all the data pre-processing used in the Appendix sections. The user study is given in full detail also, which shows exactly what we showed users, should anyone wish to recreate the results of this paper.

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A An Evaluation Of Explanation-by-Example Methods

The CCR algorithms proposed in this paper rely on obtaining a "good" pool of nearest neighbors. That is, the pool obtained via some nearest neighbor algorithm should be causally linked to the CNN/test image in question we are explaining, easily applied to any dataset/domain (regardless of the dataset size or complexity), and practical in the "real world". This experiment compares four explanation-by-example techniques: namely, ExMatchina by Jeyakumar et al. (2020), DkNN by Papernot & McDaniel (2018), Grad-Cos-x [inspired by Hanawa et al. (2021)], and twin-systems by Kenny & Keane (2019). Following Hanawa et al. (2021), we use the sanity checks proposed by Adebayo et al. (2018) to determine which method is most sensitive to random changes in the network's parameters. If a given method is not sensitive to this, it is reasonable to assume that the model's parameters are not being used to generate the explanation, and hence the explanation (i.e., the NN pool) is not causally linked to the CNN. Recent similar tests found Grad-Cos to be a good technique (Hanawa et al., 2021), but it does not scale to larger datasets, and their tests did not consider the three other methods tested here. Our modified Grad-Cos, called Grad-Cos-x, uses the loss gradients for similarity comparison at the final feature extraction layer in a given instance, rather than the entire CNN's parameters as described by Hanawa et al. (2021). Other techniques [e.g., Influence functions by Koh & Liang (2017)] were omitted due to them being computationally infeasible on larger datasets.

A.1 SETUP, DATASETS, AND EVALUATION METRICS

Here, a pre-trained CNN f is considered alongside four different randomized variants f_{rand} (see Fig. 2). These variants randomized (1) the CNN's first layer, (2) half the convolutional layers, (3) the output linear layer, and (4) the entire CNN. The evaluation uses the first 500 instances from the test set of CIFAR-10 Krizhevsky et al. (2014) and FashionMNIST Xiao et al. (2017). An overlap set metric called the Szymkiewicz–Simpson coefficient is used to evaluate the NN pool. Specifically, a score of 0 means all the NNs are different, and 1 means the are all the same (i.e., the worst score). For each test image, a set of NNs ranging from 1-1000 is iteratively considered. Due to the complexity of ExMatchina (as the original paper suggested assessing similarity in the final convolutional layer rather than the penultimate linear layer, which increases the size of vectors for comparison $\times 49$), the evaluation is limited to relatively simple datasets. Furthermore, as the randomization of weights is susceptible to erroneous results, experiments are repeated five times with aggregated results shown in Fig. 2 along with standard error bars.

In addition, we also consider the "Agreement" metric proposed by Kenny & Keane (2021) to evaluate the methods. The method adjusts the training data labels to be what the CNN predicted them to be post-training, and then fits a k-NN classifier to the training data. The k-NN is then used to predict the test data and the amount these predictions overlap with the black-box CNN's predictions, is the final score. So, if all predictions are identical, an agreement score of 1.0 is recorded (which is the best score), if both systems disagree on every test prediction, a score of 0.0 is recorded (the worst score). Note this k-NN classifier uses L_2 distance for twin systems, but cosine similarity for the other three methods (as was proposed by the original authors). The intuition behind this evaluation metric is that the k-NN being used to explain the black box CNN should exactly match the CNN's predictions on test data, otherwise the NNs are not a faithful abstraction of the CNN function we are explaining.

Lastly, we wre also inspired to use Spearman's Rank correlation to evaluate the NN pool found as suggested by Hanawa et al. (2021). The distance of the query to all NNs is recorded, and this is evaluated against the new randomized NNs. A score close to 0 means the NN pool is very different after weight randomization (as we want), divergent scores mean the opposite.

A.2 RESULTS

Fig. 6 reports the results of the supplementary experiment. Overall, the results show that twin-systems are the best method across all tests.Fig. 6(C) shows results of the Spearman's Rank test, with twin-systems and Grad-Cos-x being the best methods, with less divergence in the former than the latter. Fig. 6(B) shows the agreement metric with a perfect score of 1.0 for twin-systems, with DkNN, ExMatchina, and Grad-Cos-x doing worse in that order. Lastly, Fig. 6(A) shows the Szymkiewicz–Simpson coefficient, with twin-systems again to be the best method, with most of its NNs changing distance after the weight randomization, compared to the other three methods.

Why does this happen? As DkNN and ExMatchina do not use weights in the output linear layer, their weight randomization in the f_{rand} variant which randomized the weights in the last linear layer produced no difference. So aggregating the results of all tests showed DkNN and ExMatchina to perform much worse overall. Given the better performance of twin-systems and its claimed psychological validity Kenny et al. (2021), Expt. 1-3 focused on this method. Lastly, it is also worth noting that Grad-Cox-x requires testing labels to derived NNs, a constraint twin-systems do not have. Hence, although Grad-Cos-x also performed well in these tests, we did not consider it, as we wanted a method which didn't require testing labels to be know pre-hoc, partly so it could also be used for self-supervised learning in future research.

A.3 ARCHITECTURES

The architecture used in the Appendix A experiments is show in table 1. For CIFAR-10, the model's first Conv layer expected 3 dimensions (for color) rather than 1 on FashionMNIST.

A.4 TRAINING HYPERPARAMTERS

Both models for CIFAR-10 and FashionMNIST were trained the same way.

Figure 6: Experimental Results: The different layers of CNNs trained on CIFAR-10 and Fashion-MNIST are randomized to determine the sensitivity of the method to model parameters. (A) The agreement metric shows twins get a perfect score of 1.0, with DkNN performing second best. (B) The Szymkiewicz–Simpson coefficient overlap set score shows how many NNs retrieved by the randomized CNN overlap with those from the non-randomized CNN, and the fully aggregated results from all tests are shown for both datasets in a bar plot. (A) Spearman's Rank shows twins to be the best method, with concentrated scores close to zero. Results show that overall twin-systems and Grad-Cos-x are the most sensitive across all layers (note the varying scales on the y-axis).

Adam optimizer was used with a learning rate of 0.01. Learning rate was decreased to 90% of it's previous value every epoch. The networks were trained for 20 epochs.

FashionMNIST used data augmentation by padding with 4, random resized cropping 28, random horizontal flips (p=0.5), color jitter (0.1 for brightness, contrast, saturation, and hue) in Pytorch. The network accuracy on the test data was 90.39%.

CIFAR-10 was the same except that random resized cropping was done at 32 pixels. It's accuracy on the testing data was 74.3%.

B EXPERIMENT 2: TRAINING HYPERPARAMTERS

For the training ablation studies ResNet50 and ResNet34 was used. ImageNet experiments used the pre-trained ResNet50 model available on Pytorch. CUB-200 fine tuned ResNet34 with the following hyperparamters.

CUB-200. Epochs 500. 1 GPU used. Number of workers was 2. Batch size 12. Data transformations during training were done with Pytorch transforms: RandomResizedCrop(224), RandomRotation(45), RandomHorizontalFlip(0.5), ColorJitter(brightness=0.126, saturation=0.5). A multi-

Table 1: The CNN architecture used to train models in Appendix A.

Expt 1. CNN	
Layer	Layer Parameters
Conv2d
BatchNorm2d
ReLU	8 filters, (5x5), (1x1), padding=2
Conv2d
BatchNorm2d
ReLU	16 filters, (5x5), (2x2), padding=2
Conv2d
BatchNorm2d
ReLU	32 filters, (5x5), (1x1), padding=2
Conv2d
BatchNorm2d
ReLU	64 filters, (3x3), (2x2), padding=2
Conv2d
BatchNorm2d
ReLU	128 filters, (3x3), (1x1), padding=1
GAP	
Linear
SoftMax	128, 10

plicitive learning rate decay of 0.999 was used. The epoch with best test accuracy was used for the model, which was epoch 41.

ImageNet. This was a pre-trained model from PyTorch.

Standard training and testing splits were used for ImageNet, and CUB-200. However, as is standard practice, the validation data was used for ImageNet, since the test data labels are unavailable.

Fine-Tuning. When finetuning the CNNs, the exact same hyperparamters were used (and the same ones from the original ResNet paper for ImageNet), except that the learning rate was decreased by 10^{-1} from each methods initial learning rate when training the initial CNN model.

C COMPUTATIONAL COSTS

C.1 HARDWARE

Appendix A experiment had both the FashionMNIST and CIFAR-10 models trained on a single Nvidia K80 GPU, 2vCPU @ 2.2GHz, and 13GB RAM. The experiments were subsequently run on MacBook Pro, processor 2.9 GHz Intel Core i5, memory 16 GB 2133 MHz LPDDR3.

Experiments 1-2 were run on a Dell R740XD with an Nvidia V100 (32GB) GPU: 256GB RAM. Storage of the dataset was on scratch storage 220TiB.

Computational time for experiments. The Appendix A experiment took $\approx$8hrs to run each dataset. Expt. 1 took approximately 48hrs and 6hrs to run for ImageNet and CUB-200, respectively, presuming the use of a single Nvidia V100 (32GB) GPU. Expt. 3 took 2 weeks to run the beta experiment on ImageNet, one day for the alpha, and 7 days for the comparative tests. CUB-200 by comparison took less than 2 days for all tests.

D   EXAMPLE EXPLANATIONS

Here more example explanations are showcased with correct classifications, and incorrect classifications. In addition, a misclassification with three CCRs and multiple NNs (rather than just one) to illustrate this explanation option is shown.

Fig. 7 shows six correct classifications on ImageNet by ResNet50, alongside an explanation for them. Firstly, the explanation comprises of a nearest neighbor from a pool of n candidate cases retrieved (50 in our experiments), which alone is already considered a "good" explanation by non-experts (Jeyakumar et al., 2020; Kenny et al., 2021). However, the explanations go further by pinpointing a CCR in the test image which was "learned" from the NN. This type of explanation not only informs the user of what important feature was used in the explanation, but also from *where* it arose in the first place so it may be further contextualized.

Fig. 8 shows two incorrect classifications in ImageNet from our user study. The first image is a "Kimono" misclassified as a "Violin", were the CNN confused the pipe in the test image with a violin bow. Fig. 8b shows a "Hammer" misclassified as a "Shovel". Here the CNN saw similarity in the test image's wooden handle to a previous training image of a "Shovel", and hence classified the image as a shovel.

Fig. 9 shows another two incorrect classification in ImageNet from our user study. Fig. 9a shows an "Acoustic Guitar" which is misclassified as an "Electric Guitar". The CNN conflates the fretboard as being indicative to an electric guitar, but it is also important to an acoustic guitar, and hence the misclassificaiton arises. Fig. 9b shows a misclassificaiton of a "Flute" as a "Horizontal Bar". The visual similarity of the horizontal bar in the NN image is confused with the wooden flute in the test image.

Fig. 10 shows another way of visualizing CCRs with multiple NNs shown. Specifically, the three most salient CCRs are shown alongside the three closest representations of them in the pool of NNs retrieved. Interestingly, in Fig. 10, the third CCR seems to be confused between a Leopard's tail and leg, possibly contributing to the misclassification.

Fig. 11 shows another example of using three latent-based CCRs for the correct diagnosis of Covid-19 in a patient's x-ray.

Fig. 12 shows another example of using SP-CCRs to explain misclassifications on ImageNet. (A) A "Knot" and (B) "Rifle" are misclassified by ResNet50 apparently due to bias in the CNN by associating, what could be called, "wooden background", and "snowy background" with the respective classes.

E   USER STUDY SCREENSHOTS

For complete transparency on the user study design, we include screenshots (anonymous during review) for the reviewer's convenience. In this section exactly what all users of our study saw is shown, page by page, in the exact order. The bulk of the questions are omitted for space and clarity, but all original images used in the study may be acquired from our supplementary folder for this paper.

Or, if you prefer, you may sample your own materials to recreate the study.

Figure 7: Correct examples: Starting from the top left (and going in reading order), we see correct classifications and a NN explanation showing the CCR used in the classification. Namely, the images show correct classifications of a "Castle", "Traffic Light", "iPod", "Cello", "Park Bench", and "Jack O Lantern"

Figure 8: Incorrect examples: (a) A "Kimono" is misclassified as a "Violin", the CCR shows the CNN confused the pipe in the test image as the violinist's bow. (b) A "Hammer" is misclassified as a "Shovel", the CCR shows the CNN learned to focus on the wooden handle of shovels when classifying them, which it partly learned from the training image shown.

Figure 9: More Incorrect examples: (a) An "Acoustic Guitar" is misclassified as an "Electric Guitar", the CCR shows the CNN has learned to associate the guitar's fretboard with electric guitars, and neglected the rest of the image when classifying the test image. (b) A "Flute" is misclassified as a "Horizontal Bar", the CCR shows the CNN seems to have focused on the qualitative similarity between the horizontal bamboo bar in the training image, and the bamboo flute in the test image.

Figure 10: Multiple CCRs: An incorrect classification of a "Leopard" as a "Cheetah". Three of the most salient CCRs are shown for the test image, alongside their three closest representations in the pool of NNs.

Figure 11: Multiple CCRs: A correct classification of "Covid-19". Three of the most salient CCRs are shown for the test image, alongside their three closest representations in the pool of NNs.

Figure 12: Incorrect ImageNet Classifications: SP-CCRs are used to explain two misclassifcations (A) A "Knot" is misclassified as a "Padlock", were the CNN has learned to associate a "wooden background" feature with the predicted class, causing a bias. (B) A "Rifle" is misclassified as a "Shovel", were another bias in the CNN has learned to associate a "snowy background" feature with the class "Shovel".

Evaluating Explanations of a Computer Program

Instructions: Task 4

Finally, on the same page you are asked to do a fourth task.

*In this task you will be asked to **rate the explanation** (in Task 2).*

*That is, to evaluate whether the explanation helps you to **understand** the program's labelling*

*Here, you should assess whether the explanation helps you **understand** the program's labelling, by picking one of the numbers on the rating scale.*

Continue for 32 Questions…. See main paper for study layout.

All original materials may be sampled from ImageNet in the supplement.

Recall there are two versions of the study, one were material Set-A has a CCR explanation, and Set-B does not, and then the other study which does the opposite. All incorrect classifications are randomized.

Correctly classified (e.g., the snail above) materials were spaced out every 4 questions and were not randomized (i.e., question 4, 8, 12… 32)

Debrief Page

This study is being conducted to determine the effect of the use of explanations for the outputs of computer programs. Your responses will be used to compare the perceived usefulness of computer program explanations such as this used here.

Annonymized

Thank you for taking our survey. Your response is very important to us.

If you have any further questions about the study, or would like to access a summary of the findings, please contact:

Annonymized

You must enter this code on the Prolific site.

If after 30 seconds you are not automatically redirected to the Prolific completion page, please click the link below. You must be redirected or click the link to prove that you have completed this survey.

Annonymized