Interpreting Neural Networks Using Flip Points

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Abstract

Neural networks have been criticized for their lack of easy interpretation, which undermines confidence in their use for important applications. Here, we introduce a novel technique, interpreting a trained neural network by investigating its flip points. A flip point is any point that lies on the boundary between two output classes: e.g. for a neural network with a binary yes/no output, a flip point is any input that generates equal scores for “yes” and “no”. The flip point closest to a given input is of particular importance, and this point is the solution to a well-posed optimization problem. This paper gives an overview of the uses of flip points and how they are computed. Through results on standard datasets, we demonstrate how flip points can be used to provide detailed interpretation of the output produced by a neural network. Moreover, for a given input, flip points enable us to measure confidence in the correctness of outputs much more effectively than softmax score. They also identify influential features of the inputs, identify bias, and find changes in the input that change the output of the model. We show that distance between an input and the closest flip point identifies the most influential points in the training data. Using principal component analysis (PCA) and rank-revealing QR factorization (RR-QR), the set of directions from each training input to its closest flip point provides explanations of how a trained neural network processes an entire dataset: what features are most important for classification into a given class, which features are most responsible for particular misclassifications, how an adversary might fool the network, etc. Although we investigate flip points for neural networks, their usefulness is actually model-agnostic.

1. Introduction

In real-world applications, neural networks are usually trained for a specific task and then used as a tool to perform that task, for example to make decisions or to make predictions. Despite their unprecedented success in performing machine learning tasks accurately and fast, these trained models are often described as black-boxes because they are so complex that one cannot interpret their output in terms of their inputs.

When a trained network is used as a black-box, users cannot be sure how confident they can be in the correctness of each individual output. Furthermore, when an output is produced, it would be desirable to know the answer to questions such as, what changes in the input could have made the output different? A black-box cannot provide answers to such questions. This inexplicability becomes problematic in many ways, especially when the network is utilized in tasks consequential to human lives, such as in criminal justice, medicine, and business. Because of these interpretation issues, there have been calls for avoiding neural networks in high-stakes decision making (Rudin, 2018). Alternatives include Markov decision processes (Lakkaraju & Rudin, 2017), scoring systems (Rudin & Ustun, 2018; Chen et al., 2018b), binary decision trees (Bertsimas & Dunn, 2017), and Bayesian rule sets (Wang et al., 2016).

There have been several approaches for interpreting neural networks and general black-box models. We have space here to mention only a few papers representative of the field.

Some studies have taken a model-agnostic approach to interpreting black box models such as neural networks. For example, the approach taken by Ribeiro et al. (2016) builds an explanation for an output via a linear model in the vicinity of a specific input. Similarly, Ribeiro et al. (2018) derive if-then rule explanations about the local behavior of black box models.

Methods based on perturbing each input feature individually have severe computational limitations. First, they can be prohibitively expensive when dealing with a complex high-dimensional nonlinear function such as that represented by a neural network. Second, the output of a neural network can be constant over vast areas of its domain, while it might
be very volatile in other regions. Therefore, it can be hard to find a suitable vicinity that gives sensible results when perturbing high-dimensional inputs. Third, the features may have incompatible scalings, so determining meaningful perturbations is difficult. Finally, the features of the inputs can be highly correlated; therefore, perturbing the inputs one by one will be inefficient and possibly misleading. Koh & Liang (2017) have used influence functions to guide the perturbation and interpret black-box models with emphasis on finding the importance of individual points in the training data.

Pursuing the interpretation of neural networks from an adversarial point of view, Ghorbani et al. (2017) generate adversarial perturbations that produce perceptively indistinguishable inputs that are assigned the same label, yet have very different interpretations. They further show that interpretations based on exemplars (e.g. influence functions) are similarly susceptible to adversarial attack.

Another line of research focuses on performing insightful pre-processing to make the inputs to the neural network more interpretable. One promising approach uses prototypes to represent each output class (Li et al., 2018; Chen et al., 2018a; Snell et al., 2017). Individual inputs are compared to the prototypes (e.g., by measuring the 2-norm distance between each input and all the prototypes), and that information is the input to the neural network. In the context of text analysis, Lei et al. (2016) has introduced a model that first specifies distributions over text fragments as candidate rationales and then uses the rationales to make predictions.

Taking a different approach, Lakkaraju et al. (2017) have used decision rules to emulate a neural network in a subdomain of the inputs. Although the emulated model in their numerical example is interpretable, its outputs are different than the outputs of neural network for about 15% of the data.

Most recently, (Spangher et al., 2018) have proposed the idea of using flip sets to study linear classifiers (logistic regression models, linear support vector machines, etc.). They define a flip set as the set of changes in the input that can flip the prediction of a classifier. This approach has similarities to ours, however their algorithm is only applicable to linear classifiers and does not handle the nonlinearities in neural networks.

Many alternative models such as decision trees and rule lists have been in competition and co-existence with neural networks for decades, but in many applications have not been very appealing with respect to accuracy, scalability, and complexity, particularly with high-dimensional data. Our goal is to improve the interpretability of neural networks and other black-box models so that in cases where they have computational or accuracy advantages over alternative models, they can be used without hesitation. Through the use of flip points we are able to make neural networks interpretable, improve their training, and indicate the reliability of the output classification.

2. Interpreting neural networks using flip points

In this section, we first study the interpretation of a neural network that has two outputs and then extend the results to neural networks with an arbitrary number of outputs.

We consider a general neural network with multiple layers. We assume that the activation function at each node is a continuous function of its inputs, a condition satisfied by all commonly used activation functions. For notation, we use $x$ for the vector of inputs to the neural network and $z$ for the vector of outputs.

Here we define the optimization problems used to compute flip points. Algorithms for the numerical solution of the problems are discussed in Appendix A.

2.1. Neural networks with two outputs: a binary prediction

First, consider a neural network with two output nodes. For definiteness, we refer to the output of the neural network as a prediction of “cancerous” or “noncancerous”, but our results are equally applicable to other types of output, such as decisions. We assume that the output $z(x)$ is normalized (perhaps using softmax) so that the two elements of the output sum to one. Since $z_1(x) + z_2(x) = 1$, we can specify the prediction by a single output: $z_1(x) > \frac{1}{2}$ is a prediction of “cancerous”, and $z_1(x) < \frac{1}{2}$ is a prediction of “noncancerous". If $z_1(x) = \frac{1}{2}$, then the prediction is undefined.

Now, given a prediction $z_1(x) \neq \frac{1}{2}$ for a particular input $x$, we want to investigate how changes in $x$ can change the prediction, for example, from “cancerous” to “noncancerous”. In particular, it would be very useful to find the least change in $x$ that makes the prediction change.

Since the output of the neural network is continuous, $x$ lies in a region of points whose output $z_1$ is greater than $\frac{1}{2}$, and the boundary of this region is continuous. So what we really seek is a nearby point on that boundary, and we call points on the boundary flip points. So given $x$ with $z_1(x) > \frac{1}{2}$, we seek a nearby point $\tilde{x}$ with $z_1(\tilde{x}) = \frac{1}{2}$.

\footnote{One technical point: Because $z_1$ is continuous, there will be a point arbitrarily close to $\tilde{x}$ for which $z_1$ is less than $\frac{1}{2}$ and the prediction becomes “noncancerous” unless $\tilde{x}$ is a local minimizer of the function $z_1$. In this extremely unlikely event, we will have the gradient $\nabla z_1(\tilde{x}) = 0$ and the second derivative matrix positive semidefinite, and $\tilde{x}$ will not be a boundary point. In practice, this is not likely to occur.}
The closest flip point \( \hat{x}^c \) is the solution to an optimization problem

\[
\min_{\hat{x}} \| \hat{x} - x \|,
\]

where \( \| \cdot \| \) is a norm appropriate to the data. Our only constraint is

\[
z_1(\hat{x}) = \frac{1}{2}.
\]

Specific problems might require additional constraints; e.g., if \( x \) is an image, upper and lower bounds might be imposed on \( \hat{x} \), and discrete inputs will require binary or integer constraints. It is possible that the solution \( \hat{x}^c \) is not unique, but the minimal distance is always unique.

### 2.2. Interpreting neural networks with multi-class outputs

For neural networks with multi-class outputs, we can use this same approach to define flip points between any pair of classes and to find the closest flip points for a given input. Suppose our neural network has \( n_z \) outputs and, for \( x \), \( z_i(x) \) is the largest component of \( z(x) \). If we want to find a flip point between classes \( i \) and \( j \), then the objective function (1) remains the same, and the constraints become

\[
z_i(\hat{x}) = z_j(\hat{x}),
\]

and, for \( k \neq i, j \),

\[
z_i(\hat{x}) > z_k(\hat{x}).
\]

Thus, for each individual input, we can compute \( n_z - 1 \) closest flip points \( \hat{x}^c(i, j) \) between the class for that input and each of the other classes.

### 2.3. Interpreting neural networks with a quantified output

Neural networks can also be used to specify a quantity. For example, a neural network can be trained to determine the appropriate dosage of a medicine. In such applications, flip points have a different meaning. For example, we can ask for the least change in the input that changes the dose by a given amount. Again, we can formulate and answer these questions as optimization problems. This will be the subject of future work.

### 3. How flip points provide valuable information to the user

We now explain how flip points can be used to improve the performance and interpretation of neural networks.

#### 3.1. Determine the least change in \( x \) that alters the prediction of the model

The vector \( \hat{x}^c - x \) is an accurate and clear explanation of the minimum change in the input that can make the outcome different. This is insightful information that can be provided along with the output. For example, in a bond court, a judge could be told what changes in the features of a particular arrestee could produce a “detain” recommendation instead of a “release” recommendation.

#### 3.2. Assess the trustworthiness of the classification for \( x \)

In our numerical examples we show that the numerical value of the output of a neural network, when the last layer is defined by the softmax function, does not indicate how sure we should be of the correctness of the output. In fact, many mis-predictions correspond to very high softmax values. This has been previously observed (Nguyen et al., 2015; Guo et al., 2017). Gal & Ghahramani (2016) propose using information from training using dropout to assess the uncertainty in predictions. Their method is restricted to this particular training method, does not provide the likely correct prediction, and is more expensive than the method we propose. Another approach, proposed by Guo et al. (2017) constructs a calibration model, trained separately on a validation set, and appends it as a post-processing component to the network. Also, Lakshminarayanan et al. (2017) used ensembles of neural networks, trained adversarially with pre-calculated scoring rules, in order to estimate the uncertainty in predictions. Using flip points to assess the trustworthiness of predictions is a novel idea that has certain advantages compared to other approaches in the literature, as we explain.

The distances of incorrectly classified points to their flip points tend to be very small compared to the distances for correct predictions, implying that closeness to a flip point is indicative of how sure we can be of the correctness of a prediction. Small distance to the closest flip point means that small perturbations in the input can change the prediction of the model, while large distance to the flip point means that a larger change is necessary. It is important, of course, that distance be measured in a meaningful way, with input features normalized and weighted in a way that emphasizes their importance. Furthermore, in multi-class predictions, our numerical results indicate that when the model makes an incorrect classification, the class with the closest flip point is actually the correct class.

Using flip points can be viewed as a direct method to assess the trustworthiness of predictions, even when models are calibrated or trained adversarially. Therefore, flip point assessment is not necessarily in competition with other methods in the literature; rather it is a simple and straightforward method that can be used for any model. Flip points also provide clear explanations for their assessment in terms of input features and can point out to the possible correct prediction when there is low confidence.
3.3. Identify uncertainty in the classification of $x$

Often, some of the inputs to a neural network are measured quantities which have associated uncertainties. When the difference between $x$ and its closest flip point is less than the uncertainty in the measurements, then the prediction made by the model is quite possibly incorrect, and this information should be communicated to the user.

3.4. Use PCA analysis of the flip points to gain insight about the dataset

In Section 3.1 we discussed using the direction from a single data point to the closest flip point to provide sensitivity information. Using PCA analysis, we can extend this insight to an entire dataset or to subsets within a dataset.

We form a matrix with one row $\hat{x} - x$ for each data point. PCA analysis of this matrix identifies the most influential directions for flipping the outputs in the dataset and thus the most influential features. This procedure provides clear and accurate interpretations of the neural network model. One can use nonlinear PCA or auto-encoders to enhance this approach.

Alternatively, for a given data point, PCA analysis of the directions from the data point to a collection of boundary points can give insight about the shape of the decision boundary.

4. How flip points can improve the training and security of the neural network

Flip points also provide valuable information that can improve the quality and efficiency of the training process.

4.1. Identify the most and least influential points in the training data in order to reduce training time

Points that are correctly classified and far from their flip points have little influence on setting the decision boundaries for a neural network. Points that are close to their flip points are much more influential in defining the boundaries between the output classes.

Therefore, in online learning and real-time applications, where we have to retrain a neural network using streaming data, we can retrain the network more quickly using only the influential data points, those with small distance from their flip points.

As mentioned earlier, Koh & Liang (2017) use influence functions to relate individual predictions of a trained model to training points that are most influential for that prediction. They are not able to draw conclusions about the decision boundaries of the model because they use small perturbations of training data and local gradient information for the loss function, which can be misleading for nonlinear non-convex functions in high dimensional space. Our approach does not just rely on local information but it seeks the closest point that flips the decision of the network. Therefore, the insight we provide goes well beyond their method without adding prohibitive expense.

4.2. Identify out-of-distribution points in the data and investigate overfitting

Out-of-distribution points in the training set appear as incorrectly classified points with large distance to the closest flip point. Finding such points can identify errors in the input or subgroups in the data that do not have adequate representation in the training set (e.g., faces of people from a certain race in a facial recognition dataset (Buolamwini & Gebru, 2018)).

Additionally, after we compute the closest flip points for all the points in the training set, we can further cluster the flip points and study each cluster in relation to its nearby data points. This will potentially enable us to investigate whether the model has overfitted to the data points or not.

We have not investigated these two opportunities in our numerical results, but believe that they are promising directions for study.

4.3. Generate synthetic data to improve accuracy and to shape the decision boundaries

We can use flip points as synthetic data, adding them to the training set to move the output boundaries of a neural network insightfully and effectively.

Suppose that our trained neural network correctly classifies a training point $x$ but that there is a nearby flip point $\hat{x}$. We generate a synthetic data point by adding $\hat{x}$ to the training set, using the same classification as that for $x$. Retraining the network will then tend to push the classification boundary further away from $x$.

Similarly, if our trained neural network makes a mistake on a given training point $x$, then we can add the flip point $\hat{x}$ to the training set, giving it the same classification as $x$. This reinforces the importance of the mistake and tends to correct it.

Using flip points to alter the decision boundaries can be performed not just to improve the accuracy of a model but also to change certain traits adopted by the trained network. For example, if a model is biased for or against certain features of the inputs, we could alter that bias using synthetic data. We will demonstrate this later in our numerical results on the Adult Income dataset.

There are studies in the literature that have used synthetic data (other than flip points) to improve the accuracy, e.g.,
Interpreting Neural Networks Using Flip Points (Jaderberg et al., 2014). There is also a line of research that has used perturbations of the inputs in order to make the trained models robust, Tsipras et al. (2018) for example. However, the idea of using the flip points as synthetic data is novel and would benefit the studies on robustness of networks, too.

4.4. Understand adversarial influence

Flip points also provide insight for anyone with adversarial intentions. First, these points can be used to understand and exploit possible flaws in a trained model. Second, adding flip points with incorrect labels to the training data will distort the class boundaries in the trained model and can diminish its accuracy or bias its results. Our methods could be helpful in studying adversarial attacks such as the problems studied by Schmidt et al. (2018), Sinha et al. (2018), Madry et al. (2017), and Katz et al. (2017).

5. Results

In our numerical results, we use feed-forward neural networks with 12 layers and softmax on the output layer. We use a tunable error function as the activation function and use Tensorflow for training the networks, with Adam optimizer and learning rate of 0.001. Keep in mind that one can compute the flip points for trained models and interpret them, regardless of the architecture of the model (number of layers, activation function, etc.), the training set, and the training regime (regularization, etc.).

When calculating flip points, we measure the distance in equation (1) using the 2-norm. Calculating the closest flip points is quite fast, under 1 second for the MNIST, CIFAR-10, and Wisconsin Breast Cancer datasets using a 2017 MacBook. Calculating the closest flip point for the Adult Income dataset takes about 5 seconds, because it has both discrete and continuous variables.

5.1. Image classification

5.1.1. MNIST

The MNIST dataset has 10 output classes, corresponding to the digits 0 through 9. We could use pixel data as input to the networks, but, for efficiency, we choose to represent each data point as a vector of length 100, using the Haar wavelet basis. The 100 most significant wavelets are chosen by rank-revealing QR decomposition (Chan, 1987) of the matrix formed from the wavelet coefficients of all images in the training set. The wavelet transformation is a systematic way of applying convolutions of various widths to the input data, and the reduction applied by using rank-revealing QR decomposition leads to significant compression of the input data, from 784 features to 100, allowing us to use smaller networks. This idea, independent of flip points, is valuable whenever working with image data. Using pixel input instead of wavelet coefficients would yield interpretation traits similar to those that we present here.

We train two networks, NET1 and NET2, using half of the training data (30,000 images) for each. Table 1 shows the accuracy of each network in the 2-fold cross validation. Accuracy could be improved using techniques such as skip architecture, but these networks are adequate for our purposes.

| Trained network | Accuracy on 1st half of training set | Accuracy on 2nd half of training set | Accuracy on testing set |
|-----------------|-------------------------------------|-------------------------------------|-------------------------|
| NET1            | 100%                                | 97.62%                              | 97.98%                  |
| NET2            | 97.56%                              | 100%                                | 97.64%                  |

For each of the images in the training set, we calculate the flip points between the class predicted by the trained neural networks and each of the other 9 classes.

Flip points identify alternate classifications. Some images are misclassified and close to at least one flip point. For all of these points, the correct label is identified by the closest of the 9 flip points (or one of those tied for closest after rounding to 4 decimal digits). For example, the image shown in Figure 1, from the second half of the MNIST training set, is an “8” mistakenly classified as “3” by NET1 with softmax score of 98%. Its distances to the closest flip points are shown in Table 2. Assuming that we do not know the correct label for this image, we would report the label as “3”, with the additional explanation that there is low confidence in this prediction (because of closeness to the flip point), and the correct label might be “8”.

Figure 1. MNIST image mistakenly classified as “3” by NET1.

Flip points provide better measure of confidence than softmax. Many practitioners use the softmax output as a measure of confidence in the correctness of the output. As illustrated in Figure 2, the softmax scores range between 31% and 100% for the mistakes by NET1 and NET2, and
Table 2. Distance to closest flip points between class “3” and other classes, for image in Figure 1.

| CLASS | 0 | 1 | 2 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------|---|---|---|---|---|---|---|---|---|
| DISTANCE | 1.27 | 1.32 | 0.58 | 2.16 | 0.56 | 1.45 | 1.51 | 0.16 | 0.90 |

range between 37% and 100% for correct classifications, providing no separation between the groups. If softmax were a good proxy for distance, then the data would lie close to a straight line. Instead, most of the mistakes have small distance but large softmax score: more than 73% of the mistakes have 80% or more softmax score. Hence, softmax cannot identify mistakes. Fortunately, the figure shows that the distance to the closest flip point is a much more reliable indicator of mistakes: mistakes almost always correspond to small distances. This is further demonstrated in Figure 3 which shows the distinct difference between the distribution of distances for the mistakes and the distribution of distances for the correct classifications.

Figure 2. For the MNIST data, a large softmax score says nothing about the reliability of the classification. In contrast, distance to the closest flip point is a much more reliable indicator.

Figure 3. Distribution of distance to closest flip point among the images in the MNIST training set for mistakes (orange) and correctly classified points (blue).

Flip points identify influential training points. Images that are correctly classified but are relatively close to a flip point are the most influential ones in the training process. To verify this, consider the first half of the MNIST training set, and order the images by their distances to their nearest \( \hat{x}^c \) for NET1. We then consider using neural networks trained using a subset of this data.

Data points at most 0.75 from a flip point form a subset of 9,463 images, about 15% of the training set. A model trained on this subset achieves 97.9% accuracy on the testing set. When we train with a subset of 9,463 images randomly chosen from the training set, on average (50 trials) we achieve 96.2% accuracy on the testing set. A subset of same size from the images farthest from their flip points achieves only 90.6% accuracy on the testing set.

These trends hold for all distance thresholds, as shown in Figure 4. This confirms that distance to the flip point is in fact related to influence in the training process.

Figure 4. Accuracy of models trained on MNIST subsets.

We note that the model learns the entire training set with 100% accuracy when trained on about 16,000 images chosen by the distance measure. In contrast, it only achieves 98.8% accuracy when trained on a randomly chosen subset of the same size.

Also note that flip points are computed by solving a non-convex optimization problem, so we cannot guarantee that we have indeed found the closest flip point. Nevertheless, in practice, the computation seems to provide very useful flip points, validated by the small distances achieved by some flip points and by the results shown in Figures 2 – 4.

Flip points improve the training of the network. Finally, we append to the entire training set a flip point for each mistake in the training set, labeled with the correct label for the mistake. The resulting neural network achieves 100% accuracy on the appended training set and 98.6% on the testing set, an improvement over the 98.2% accuracy of the original network. We expect that this technique of appending synthetic images to the training set will be much more helpful for datasets that have a limited amount of training data.

5.1.2. CIFAR-10

We now consider two classes of airplanes and ships in the CIFAR-10 data set. This time we perform 3D wavelet de-
composition on images using the Haar wavelet basis and
use all of the wavelet coefficients to train a neural network,
achieving 100% and 84.2% accuracy on the training and
testing sets. We then calculate the flip points for all the
images in both sets.

Observations that we reported for MNIST on CIFAR-10
apply here, too. So, we focus our discussion on the directions
to flip points and PCA analysis of them.

Figure 5 shows an image in the testing set that is mistakenly
classified as an airplane, along with its closest flip point. We
have computed the closest flip point in the wavelet space. It
is interesting that the 1-norm distance between the image
and its closest flip point in the pixel space is 210, and the
differences are hard to detect by eye.

![Figure 5. A ship image misclassified as airplane (left), its flip point
(right).](image)

The matrix of directions between the misclassified images
and their closest flip points is highly rank deficient. While
we have 2,304 features for each image, the rank of directions
for flipping an airplane to a ship is 162, and it is 170 for
flipping a ship to an airplane. Therefore, we can investigate
the mistakes by looking at very small subset of wavelet
features out of the 2304 features.

Moreover, the matrix of directions that flip a misclassified
ship to its correct class has 53% sparsity. The first principal
component of the directions has the pattern shown in
Figure 6.

![Figure 6. First principal component of directions that flip a misclassified ship to its correct class.](image)

We threshold the principal coefficients in Figure 6, retaining
pixels with coefficient greater than 0.05. Then we plot the
corresponding pixels of the misclassified images of ships.

Some of those images are plotted in Figure 7. One can
see that for many of the mistakes, those pixels actually
contain the prow of the ship in the image. This points to one
vulnerability of our trained neural network, which we could
then investigate further.

![Figure 7. Pixels with large principal coefficients for misclassified ships.](image)

Finally, we note that great similarity exists between the
directions for the correct classifications in the training and
testing sets. Investigating other principal components can
provide additional insights.

5.2. Adult income dataset

Next, we consider the Adult dataset from the UCI Machine
Learning Repository (Dheeru & Karra Taniskidou, 2017), an
example that has a combination of discrete and continuous
variables. There are 32,561 data points in the training set
and 16,281 in the testing set. Each data point has information
about an individual, and the label is binary, indicating
whether the individual’s income is greater than 50K annually.

Each of the continuous variables (age, fnlwgt, education-
num, capital-gain, capital-loss and hours-per-week) has a
lower bound of 0. We normalize each variable to the range
0 – 100 using upper bounds of 100, 2e6, 20, 2e5, 1e4 and
120, respectively, and we also use these ranges to constrain
the search for flip points.

Moreover, we transform the categorical variables (work-
class, education level, marital status, occupation, relation-
ship, race, sex, native country) into a binary form where
each category type is represented by one binary feature. The
categories that are active for a data point have binary value
of 1 in their corresponding features, while the rest of fea-
tures are set to zero. When searching for a flip point, we
have a constraint that requires exactly one binary element be
equal to 1 for each of the categorical variables. Our trained
neural network achieves accuracy of 87.3% and 86.1% on
the training and testing sets.

Our aim here is to show how a trained neural network can
be interpreted, and our focus is not to draw conclusions
about the dataset itself. Clearly, choosing a different method
for pre-processing the data, choosing different bounds for
continuous variables, or defining other distance measures
between the categories can affect the trained neural network
function and consequently the result of interpretation. Our
interpretation tools allow the user of model to become in-
sightful about how to process the data and train the network
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in order to obtain a trained neural network whose output obeys known relationships between input and output. Our preprocessing and scaling choices are suboptimal but illustrative; clearly, application scientists should always be involved in setting the distance metric in order to ensure meaningful results.

**Flip points provide interpretations and can expose bias.**
To illustrate the interpretation of the output of the neural network, consider the 53rd training data point, corresponding to a person with income greater than 50K. The answer to the question of how features differ between this point and its computed flip point, for this particular neural network, is shown in Table 3. We can see that the race of this individual is influential in the decision of model, as are other features such as “working hours” and “work class”. These two latter features seem to have an obvious causal relationship with the income, but influence of race should be questioned.

| Table 3. Difference in features for Adult dataset training point #53 and its closest flip point. |
|-----------------------------------------------|
| **Data** | **INPUT #53 IN TRAINING SET** | **CLOSEST FLIP POINT** |
| Capital-gain | 0 | 625 |
| Capital-loss | 1,902 | 1,862 |
| Hours-per-week | 60 | 59.8 |
| Race | White | Asian-Pac-Islander |
| Work class | Private | State-gov |
| Marital status | Married-civ-spouse | Married-AF-spouse |

We can also constrain selected features when computing flip points. For example, we can ask for the closest flip point corresponding to a person with the same gender or race, or with a different gender or race. This enables us to investigate gender/racial bias in the output of the neural network.

**Flip points reveal patterns in how the trained model treats the data.** As an example, we consider the effect of gender (Male, Female) in connection with the family relationship (Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried) for individuals that have income “<= 50K”. For this model, 89% of data points in that income category have the same gender as their closest flip points, while 11% have switched from Female to Male, and 0.2% have switched from Male to Female. This shows that being Male is moderately helpful in being labeled “> 50K” by the model. But, as we will see later, education is the most influential feature for flipping to the high income category. For the same income category, we also observe that for 2.5% of the flip points, the family role switches from Husband to Wife, while a third of those have simultaneously switched from Female to Male. This reveals that the trained model considers both the family role of Wife and the gender of Male helpful for having high income. The switch from family role of Wife to Husband is absolutely rare among the flip points.

**PCA on the flip point directions identifies influential features.** Another important interpretation question is which features in the input are most influential in the decisions of the network. To answer this kind of question, we use PCA on the matrix of directions between inputs and their flip points. Here, we discuss some of the insights that are obtained.

Consider the subset of directions that flip a “<= 50K” income to “> 50K”. The first principal component reveals that, for this neural network, the most prominent features with positive impact are having a master’s degree, having capital-gains, and working in the private sector, while the features with most negative impact are having highest education of Preschool, working without-pay, and having capital-loss. Looking more deeply at the data, RR-QR decomposition of the matrix of directions reveals that some features, such as having a Prof-school degree, have no impact on this flip.

PCA on the directions between the mistakes in the training set and their closest flip points shows that native country of United States has the largest coefficient in the first principal component, followed by being a wife and having capital-gain. The most significant features with negative coefficient are being a husband and native countries of Cambodia and Ireland. These features can be considered the most influential in confusing and de-confusing the neural network.

PCA on the direction vectors explains how our neural network is influenced by various features. It thus enables us to calculate inputs that are mistakenly classified, for adversarial purposes.

**Flip points can deal with flaws and can reshape the model.** Here as an example, we try to change the behavior of the trained model towards the individuals with country of origin “Mexico”. We observed that among various countries of origin, data points labeled “Mexico” had the highest likelihood of a different country in their flip points. We consider all the data points with that country of origin that have a flip point with a different country. 82% of those points have income “<= 50K”. We generate closest flip points for all those inputs while constraining the country of origin to remain “Mexico”. We then add each generated flip point to the training set, using the same label as the data point, and train a new model using the appended set. After
performing PCA analysis on the directions to the new flip points, we observe that Mexico does not appear in any of the first 10 principal components, whereas it had a large value in the first principal component obtained for the original model. The accuracy of the trained model has remained almost the same (slightly increased by 0.05%), confirming that we have achieved our goal. Using this kind of analysis, we can reshape the behavior of the model as needed.

5.3. Wisconsin Breast Cancer Dataset

Neural networks have shown promising results in identifying cancer (Agrawal & Agrawal, 2015). As a simple example, we use the Wisconsin breast cancer database from the UCI repository which has 30 features extracted from digitized images of fine needle aspirate of 569 breast masses. We divide standard error features by their corresponding mean feature, and then normalize the mean and worst features between 0 and 1. The label is binary: “malignant” or “benign”.

We randomly divide the dataset into a training set and testing set, consisting of 80% and 20% of data respectively. We achieve 100% and 94.7% accuracy on the training and testing sets, respectively. The average distance to the closest flip point is 0.022 for the mistakes in the testing set and 0.103 for the correct classifications in the testing set. The average distance is 0.106 for correct classifications in the training set, very similar to the average distance in testing set. All of the mistakes have softmax score of at least 97.4%. In fact, the average softmax for all the correct and wrong classifications are both more than 99%. Again, the distance to the closest flip point is a reliable measure to identify classifications that are possibly wrong, while softmax score is not.

Flip points can be used to improve the model. What features in the input are most important? As an example, consider the first data point which is classified correctly as “malignant” by the trained neural network. Its closest flip point differs mostly in features “standard error of texture” and “standard error of fractal dimension”.

We perform PCA on the matrix of directions between each “benign” input and its closest flip point, and look at the first principal component. The most prominent features that can flip the decision of the network to “malignant” are “standard error of radius” and “standard error of texture”. Similarly, the most prominent features to flip a “malignant” decision to “benign” are “standard error of texture” and “worst area”.

A clinician can use this information to validate the trained neural network as a computational tool. The information also enables the designer of the neural network to work with a clinician to rescale the data to emphasize features believed to be over- or under-emphasized by the current model and to provide better classifications.

6. Conclusion

We studied the problem of neural network interpretation and proposed methods that can interpret a trained neural network.

1. We used flip points to investigate the boundaries between the output classes of any trained neural network. For any input to a neural network, we defined and solved optimization problems in order to find the closest flip point to each of the output boundaries. This provided accurate explanations about changes in the input that can flip the output from one class to another.

2. The distance of an input to the closest flip point proved to be a very effective measure of the confidence we should have in the correctness of the output, much more reliable than softmax score. Moreover, this distance enables us to identify most and least influential points in the training data.

3. PCA analysis identified the most influential features in the inputs. Also, for each output class, PCA identified the directions and magnitudes of change in each of the features that can change the output.

4. By computing relevant flip points, we created synthetic data and used it to boost the accuracy of a neural network. We also demonstrated how the synthetic data can be designed to adversarially affect a trained neural network by altering the output boundaries of the network. Our approach can be effective in identifying corrupt data, and also in generating corrupt data to attack a deep learning model.

5. The distance and direction to the nearest flip point, coupled with a practitioner’s knowledge of the measurement uncertainty in each of the features, can provide insight into whether the classification is unique or ambiguous.

The computation and use of flip points greatly improves the interpretability of neural networks and enhances their use in applications where they have proven to be highly useful. However, we note that flip points exist for any model, not just neural networks, and can be defined in a model-agnostic way as the closest point to a particular input that changes the model’s decision or classification. We expect that flip points can be useful in providing insight and interpretation of a variety of types of models.
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Appendix A: How flip points are computed

General approach. If the activation function is differentiable (e.g., erf), we can make use of its gradient in solving the optimization problems we have introduced. Otherwise, subgradients can be used, but this can make the optimization algorithms more costly.

The gradient of the outputs of the network with respect to its inputs is a Jacobian matrix when the network has more than one input feature and more than one output class. We compute this gradient analytically, which is generally more efficient and reliable than using finite differences. Analytic computation of the gradients is possible for many different kinds of network architectures, including feed-forward, convolutional, and residual networks, assuming that the network does not contain non-differentiable elements such as non-differentiable activation functions or max pooling.

For the feed-forward networks used in this work, the computation of the gradient is analogous to the back-propagation approach commonly used to compute the gradients with respect to the training parameters of the networks (Rumelhart et al., 1988).

Using the gradients, we minimize (1) subject to the constraints mentioned in Section 2 in order to find the closest flip point. The problem is non-convex, so standard optimization software generally computes a local minimizer but not necessarily a global minimizer. In the case of inputs with discrete features, we can add the discrete constraints to the problem or add regularization terms to the objective function using the techniques described by Nocedal & Wright (2006).

Our optimization problem can be considered a generally solvable problem using off-the-shelf methods available in the literature. However, difficulties sometimes arise in solving nonlinear non-convex optimization problems, and therefore it is beneficial to design an optimization method tailored to our particular problem. To illustrate this, we first specify our network and then our optimization algorithm.

In our notation, vectors and scalars are in lower case and matrices are in upper case. Bold characters are used for vectors and matrices, and the relevant layer in the network is shown as a superscript in parenthesis. Subscripts denote the index for a particular element of a matrix or vector. Iterations of the algorithm are denoted by superscripts.

Our neural network. We specify the neural network \( \mathcal{N} \) shown in Figure 8 by weight matrices \( W^{(k)} \) and bias vectors \( b^{(k)} \) for each layer \( k = 1, \ldots, m \). The output of layer \( k \) in the network is denoted by \( y^{(k)} \).

The activation function used in the nodes is the error function

\[
y = \text{activation}(c|\sigma) = \text{erf}(\frac{c}{\sigma}) = \frac{1}{\sqrt{\pi}} \int_{-c/\sigma}^{+c/\sigma} e^{-t^2} dt,
\]

where \( c \) is the result of applying the weights and bias to the node's inputs. The tuning parameter \( \sigma \) is constant among the nodes on each layer and is optimized during the training process. Hence, for the whole network, we have a vector of tuning parameters, \( \sigma \), where each element of it corresponds to one hidden layer in the network. While erf is not a very common choice for activation function, it has been shown that its performance in terms of accuracy is comparable to other activation functions (Ramachandran et al., 2018). We note that when \( \sigma \) is small, then the activation function resembles a step function, while when \( \sigma \) is large, it resembles a linear function, as shown in Figure 6, so erf captures the behavior of popular activation functions while preserving differentiability.

![Figure 8. Sketch of a prototype feed-forward neural network \( \mathcal{N} \) with \( n_x \) inputs, \( m \) layers, and \( n_m \) outputs.](image)

![Figure 9. Shape of erf function as \( \sigma \) varies.](image)

Using the erf activation function, the output of the first inner layer for input \( x \) is

\[
y^{(1)} = \text{erf} \left( \frac{xW^{(1)} + b^{(1)}}{\sigma_1} \right).
\]
For the hidden layers,
\[ y^{(i)} = \text{erf} \left( \frac{y^{(i-1)} W^{(i)} + b^{(i)}}{\sigma_t} \right). \]
Finally,
\[ y^{(m)} = y^{(m-1)} W^{(m)} + b^{(m)}, \]
and the output of the network is
\[ z(x) = \text{softmax}(y^{(m)}). \]

Optimization framework. We recommend a homotopy method for calculating the closest flip points. Here, we briefly explain its framework in the context of our network. Our method can be easily generalized to neural networks with different architectures, such as convolutional and residual networks. The homotopy algorithm applies an optimization module to a series of networks.

Optimization module. We define the numerical process of computing the closest flip point \( \hat{x} \) to an input \( x \) between classes \( i \) and \( j \) by the function \( F \):
\[ \hat{x}^{c(i, j)} = F(x, N, x_0, C, i, j), \]
The inputs include the trained neural network \( N \), the starting point \( x_0 \), and the constraints \( C \). As a general practice and based on our numerical experiments, an interior-point algorithm can be considered a good choice, as it is known to be successful in solving constrained, nonlinear, non-convex optimization problems with high dimensional variables (Nocedal & Wright, 2006). This can be used in conjunction with a branch-and-bound algorithm for discrete variables.

Ideally, \( F \) efficiently finds the closest flip point for our network, possibly using the input \( x \) as the starting point. If this fails, then we use a homotopy method, starting by applying \( F \) to an easier network and gradually transforming it to the desired network, each time using the previously determined flip point as our starting point for \( F \). We now discuss the family of networks used in the homotopy.

Homotopy algorithms. Our homotopy method, defined by Algorithm A1, begins with a neural network for which \( x \) is a flip point, and then computes flip points for a series of networks, gradually transforming to the original network, using the closest flip point found at each iteration as the starting point for the next iteration. This way, the algorithm follows a path of flip points starting from \( x \), until it finds the closest flip point to \( x \) for the original network.

The initial neural network used in the algorithm is the same as the original network except that it has parameters \( \sigma^h \) for the \( \text{erf} \) and \( \hat{b}^{h(m)} \) for the bias on the last layer. These are computed in Algorithm A2, discussed below.

The parameter \( \eta \) defines the number of iterations that Algorithm A1 uses to transform the network back to its original form. A large \( \eta \) means that each neural network is a small change from the previous one, so the starting point is close to the solution. A small \( \eta \) means that only a few optimization problems are solved, but each starting point may be far from the solution. We want to perform enough iterations so that the global minimizer is found, but we also want to keep the computational cost low. We have achieved best results with \( \eta \) ranging between 1 and 10. Choosing \( \eta = 1 \) is equivalent to not using the homotopy algorithm and directly applying \( F \) to the original network with starting point \( x \).

The initial transformation of the network is performed by Algorithm A2, pursuing two goals, first, bounding the flow of gradients through the layers of the network by changing the value of tuning parameters (lines 1 through 12), and second, changing the bias parameters in the last layer of the network so that \( x \) is a flip point for the transformed network (line 13).

The tuning parameters for the original network are \( \sigma^{N^c} \), and \( \sigma^h \) denotes the transformed parameters computed by Algorithm A2. Similarly, \( b^{N^c(m)} \) and \( b^{h(m)} \) denote the original and transformed bias in the last layer of the network.

By changing \( \sigma^{N^c} \) to \( \sigma^h \), we try to control the magnitudes of the gradients of output with respect to inputs. The hierarchy of neural networks can cause the gradients to vanish and/or explode through its layers, which could lead to a badly scaled gradient matrix and eventually an ill-conditioned optimization problem, and we would like to avoid this. For flip point computation, we are concerned about the gradients of outputs with respect to inputs, while in neural network literature, this issue of “vanishing and exploding gradients” usually concerns the training process and the gradient of the loss function with respect to the training parameters (Bengio et al., 1994; Hanin, 2018). In both cases, the “vanishing and exploding gradients” phenomenon can be studied by investigating individual matrices in the chain rule formulation of

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**Algorithm A1** Homotopy algorithm for calculating closest flip point

**Inputs:** \( N, x, \eta, \tau, C, i, j \)

**Output:** Closest flip point to \( x \)

1: Compute \( \sigma^h \) and \( b^{h(m)} \) using Algorithm A2 with inputs \( (N, x, \tau, i, j) \)
2: \( \hat{x}^{c,0} = x \)
3: for \( k = 1 \) to \( \eta \) do
4: \( \sigma^k = \sigma^h + k(\frac{\sigma^{N^c} - \sigma^h}{\eta}) \)
5: \( b^{k(m)} = b^{h(m)} + k(\frac{b^{N^c(m)} - b^{h(m)}}{\eta}) \)
6: Replace \( \sigma^k \) and \( b^{k(m)} \) in \( N \), to obtain \( N^k \)
7: \( \hat{x}^{c,k} = F(x, N^k, \hat{x}^{c,k-1}, C, i, j) \)
8: end for
9: return \( \hat{x}^{c,\eta} \) as the closest flip point to \( x \)
Algorithm A2 Algorithm to transform the network for the Homotopy algorithm

Inputs: $N, x, \tau, i, j$
Output: $\sigma^h$ and $b^{h(m)}$

1: $\gamma = \sqrt{\log\left(\frac{2}{\sqrt{\pi}}\right)}$
2: $y^{(0)} = x$
3: for $k = 1$ to $m - 1$ do
4:  $\sigma^h_k = \max\left(\frac{2}{\sqrt{\pi}}, \frac{1}{\gamma} \|y^{(k-1)}W^{(k)} + b^{(k)}\|_\infty\right)$
5:  if $\sigma^h_k > \frac{2}{\sqrt{\pi}}$ then
6:    $c = y^{(k-1)}W^{(k)} + b^{(k)}$
7:    for $t = 1$ to $n_k$ do
8:      $\sigma^h_{k,t} = \max\left(\frac{2}{\sqrt{\pi}}, \frac{1}{\gamma} c_t\right)$
9:  end for
10: end if
11: $y^{(k)} = \text{erf}\left(\frac{y^{(k-1)}W^{(k)} + b^{(k)}}{\sigma^h_k}\right)$
12: end for
13: $\min_{b^{h(m)}} \|b^{h(m)} - b^{N(m)}\|_2$, subject to:
   1. $y_i^{(m)} = y_i^{(m-1)}W^{(m)} + b^{h(m)}$
   2. $y_i^{(m)} = y_j^{(m)}$
   3. $\forall i \neq j \mid y_i^{(m)} > y_j^{(m)}$
14: return $\sigma^h, b^{h(m)}$

the gradient matrix.

To compute the $\sigma^h$, we trace the $x$ as it flows through the layers of the network. As the input reaches each hidden layer, before applying the activation function, we tune the corresponding element of $\sigma^h$, so that the absolute values of the gradients of the output of each neuron, with respect to neuron’s input, is greater than or equal to $\tau$, and less than or equal to 1. In our numerical experiments, we have used different values of $\tau$ ranging between $10^{-5}$ and $10^{-9}$.

In Algorithm A2, line 1 computes a scalar $\gamma$ such that the derivative of the erf is equal to $\tau$. Lines 3 through 12, tune the $\sigma$, layer by layer, starting from the first layer and ending at the last hidden layer. Line 4 bounds the individual gradient between $\tau$ and 1. Choosing the $\sigma^h_k > \frac{2}{\sqrt{\pi}}$ ensures the gradients of neurons are upper bounded by 1. This relationship can be easily derived by setting the maximum derivative of erf equal to $\tau$.

Choosing $\sigma^h_k \geq \frac{1}{\tau} \|y^{(k-1)}W^{(k)} + b^{(k)}\|_\infty$ can potentially make the gradients of all the neurons in layer $k$ lower bounded by $\tau$. Sometimes, this might not be possible to achieve for all the neurons in a layer, if we obtain $\sigma^h_k > \frac{2}{\sqrt{\pi}}$.

In such situations, we calculate the $\sigma^h_k$ separately for each neuron on that layer (lines 5 through 10), and use a non-uniform $\sigma^h_k$ in the homotopy algorithm. Line 11, computes the output of each layer after the $\sigma$ is tuned for that layer.

Since our activation function is erf, we can effectively control the gradients and make them bounded. The maximum gradient of erf is at point zero, and by moving away from zero, its gradient decreases monotonically, until it asymptotically reaches zero. This boundedness and the monotonicity of both the erf and its gradient are helpful features that we leverage in our homotopy method. When using activation functions other than erf, we have to avoid exploding and vanishing gradients, depending on the properties of the activation function in use.

By changing $b^{N(m)}$ to $b^{h(m)}$, computed at line 13 of Algorithm A2, the input $x$ actually becomes a flip point for the transformed network. Having a starting point that is feasible with respect to flip point constraints considerably facilitates the optimization process. The optimization problem on line 13 of the algorithm is a convex quadratic programming problem and can be solved by standard algorithms.

Interpreting Neural Networks Using Flip Points
Appendix B: Information about neural networks used in our numerical examples

Here, we provide more information about the models we have trained and used in Section 5.

We have used fully connected feed-forward neural networks with 12 hidden layers. The number of nodes for the models used for each data set is shown in Table B1. The activation function we have used in the nodes is the error function, as defined in Appendix A. We have also used softmax on the output layer, and cross entropy for the loss function.

Table B1. Number of nodes in neural network used for each data set.

| DATA SET | MNIST | CIFAR-10 | ADULT | CANCER (WBCD) |
|----------|-------|----------|-------|----------------|
| INPUT LAYER | 100   | 2304     | 107   | 30             |
| LAYER 1    | 500   | 400      | 100   | 40             |
| LAYER 2    | 500   | 400      | 100   | 20             |
| LAYER 3    | 500   | 400      | 100   | 15             |
| LAYER 4    | 400   | 350      | 80    | 10             |
| LAYER 5    | 300   | 300      | 60    | 5              |
| LAYER 6    | 250   | 250      | 50    | 5              |
| LAYER 7    | 250   | 250      | 50    | 5              |
| LAYER 8    | 250   | 250      | 50    | 5              |
| LAYER 9    | 200   | 200      | 40    | 5              |
| LAYER 10   | 150   | 150      | 30    | 5              |
| LAYER 11   | 150   | 150      | 30    | 5              |
| LAYER 12   | 100   | 100      | 20    | 5              |
| OUTPUT LAYER | 10   | 2        | 2     | 2              |