Neural Belief Reasoner

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Abstract

This paper proposes a new generative model called neural belief reasoner (NBR). It differs from previous models in that it specifies a belief function rather than a probability distribution. Its implementation consists of neural networks, fuzzy-set operations and belief-function operations, and query-answering, sample-generation and training algorithms are presented. This paper studies NBR in two tasks. The first is a synthetic unsupervised-learning task, which demonstrates NBR’s ability to perform multi-hop reasoning, reasoning with uncertainty and reasoning about conflicting information. The second is supervised learning: a robust MNIST classifier. Without any adversarial training, this classifier exceeds the state of the art in adversarial robustness as measured by the $L_2$ metric, and at the same time maintains 99% accuracy on natural images. A proof is presented that, as capacity increases, NBR classifiers can asymptotically approach the best possible robustness.

1 Introduction

It is a widely held hypothesis that bridging the gap between machine learning and reasoning would bring benefits to both domains. For reasoning systems, this could provide an elegant solution to automatically discover rules from observations, and could provide new approaches to reasoning with uncertainty. On the other hand, despite the phenomenal successes of deep learning, neural networks tend to have poor robustness and interpretability, both of which are nonissue in reasoning systems. The robustness issue has recently been highlighted by the existence of adversarial examples in many systems. For example, even for the well-studied MNIST task, the state of the art in $L_2$ robustness is far from satisfactory and comes at a cost of accuracy on natural images. More discussions are in Section 5.

There are numerous works at the intersection of machine learning and reasoning, some of which will be reviewed in Section 5. A prominent one is Boltzmann machine and its variants (Salakhutdinov and Hinton 2009), which combine neural networks and Markov random field that is a form of reasoning with uncertainty. A recent example is differentiable inductive logic programming (Evans and Grefenstette 2018), which combines neural networks and logic programs.

This paper presents a new approach called neural belief reasoner (NBR), which combines neural networks and belief functions. Belief function is a generalization of probability function (Shafer 1976), and has the advantage of modeling epistemic uncertainty, i.e., the lack of knowledge, and an elegant way of combining multiple sources of information. Despite these advantages, belief function has seen much less adoption than mainstream methods like Bayesian network and Markov random field. NBR is built on two innovations: 1) using neural networks to represent fuzzy sets, and 2) using fuzzy sets to specify a belief function. From the machine-learning perspective, NBR is a new generative model that specifies a belief function rather than a probability distribution. From the reasoning perspective, NBR is a new system of reasoning with uncertainty that enables automatic discovery of non-symbolic rules from observations and that uses belief functions to model uncertainty.

The next section will define the model and present query-answering, sample-generation and training algorithms. Then Sections 3 and 4 demonstrate NBR’s capabilities through two tasks. The first task is unsupervised learning: in a synthetic 11-bit world where only partial observations are available, an NBR model is trained and then answers queries. The queries involve calculating belief and plausibility of a proposition conditioned on another, and demonstrate multi-hop reasoning, reasoning with uncertainty and reasoning about conflicting information. The second task is supervised learning: a robust MNIST classifier. Techniques to adapt NBR for classification and techniques specific for robustness will be presented. The resulting classifier sets a new state of the art in adversarial robustness as measured by the $L_2$ metric, and at the same time maintains 99% accuracy on natural images. A proof is presented that, with more capacity, NBR classifiers can asymptotically approach the best possible robustness on the training set. This is the first such proof in literature.

2 Neural Belief Reasoner

Let’s start with a restricted framework of reasoning in Section 2.1 which serves as a stepping stone towards NBR’s definitions in Section 2.2 and algorithms after that.
2.1 Prototype with classical sets

Let $U$ denote the sample space, i.e., the set of all possibilities. Consider a reasoning framework where a model is composed of $K$ sets, $R_1, \cdots, R_K \subseteq U$, and each $R_i$ is annotated with a scalar $0 \leq b_i \leq 1$. Let’s interpret each $R_i$ as a logic rule: an outcome $x \in U$ is said to satisfy $R_i$ if and only if $x \in R_i$. Let’s interpret $b_i$ as the belief in $R_i$.

Define vector $y \triangleq (y_1, \cdots, y_K)$ where entries are 0 or 1. Define intersection sets $S_y \triangleq \bigcap_{1 \leq i \leq K} y_i$, and define $S_{(0,\ldots,0)} \triangleq U$. Intuitively each $S_y$ contains outcomes that satisfy a subset of the $K$ rules as selected by $y$. Define scalar function $p(y) \triangleq \prod_{i=1}^K (b_i \cdot y_i + (1 - b_i) \cdot (1 - y_i))$.

Let $2^U$ denote the power set of $U$. Define the following function from $2^U$ to $\mathbb{R}$:

$$m(A) \triangleq \frac{\sum_{y|S_y=A} p(y)}{1 - \sum_{y|S_y=\emptyset} p(y)}$$

(1)

It is straightforward to verify that $\sum_{A \subseteq U} m(A) = 1$. Therefore this function $m(\cdot)$ uniquely specifies a belief function over $U$ (Shafer 1976). Hence this function $m(\cdot)$ uniquely specifies a belief function over $U$ (Shafer 1976): $Bel(A) = \sum_{B \subseteq A} m(B), \forall A \subseteq U$.

Intuitively this framework considers $2^K$ possible worlds: each world corresponds to each $y$, and in each world a subset of the $K$ rules, as selected by $y$, exist. Each satisfiable world, i.e., where $S_y \neq \emptyset$, is assigned a mass that is proportional to $p(y)$, the product of $b_i$’s for rules that are present and $(1 - b_i)$’s for rules that are absent. Each unsatisfiable world, i.e., where $S_y = \emptyset$, is assigned a mass of zero. The total mass is one, which is achieved through the denominator in (1) that is essentially Dempster’s rule of combination (Shafer 1976).

With a belief function defined, this framework is able to answer queries. Similar to conditional probabilities in traditional models, it answers with conditional belief functions. Given a condition $C \subseteq U$ and a proposition $Q \subseteq U$, the conditional belief and conditional plausibility are

$$Bel(Q \mid C) = \frac{Bel(Q \cup C) - Bel(C)}{1 - Bel(C)}$$

$$= \frac{\sum_{y|S_y \cap C \cap Q \neq \emptyset} p(y)}{\sum_{y|S_y \cap C \cap Q \neq \emptyset} p(y)}$$

$$= \frac{\sum_{y|S_y \cap Q \neq \emptyset} p(y)}{\sum_{y|S_y \cap C \neq \emptyset} p(y)}$$

$$\text{Pl}(Q \mid C) = 1 - Bel(\overline{Q} \mid C)$$

$$= \frac{\sum_{y|S_y \cap C \cap \overline{Q} \neq \emptyset} p(y)}{\sum_{y|S_y \cap C \neq \emptyset} p(y)}$$

2.2 Model definitions

I now define the full form of NBR by generalizing the previous section in a number of ways: $R$’s are replaced by fuzzy sets represented by neural networks; $U$ becomes the latent space which is separated from observation space.

An NBR model has the following components and Figure 1 illustrates the architecture.

- Function $x = F(z)$ where vector $x$ is the observation variables and vector $z$ is the latent variables.
- Function $r = R(z)$ with output values in range $[0,1]$.
- Bernoulli variables $Y = (Y_1, Y_2, \cdots, Y_K)$, where $K$ is the dimension of $r$.

The $F$ and $R$ functions can be implemented by neural networks. The parameters of an NBR model are the parameters of functions $F$ and $R$, and $b_i = P_{Y_i}(1)$ for $i = 1, 2, \cdots, K$.

Each $R_i(x)$ is interpreted as the membership function of a fuzzy set over $z$ space [Zadeh 1965]. I consider the same $2^K$ possible worlds as in Section 2.1, but the intersection set $S_y$ for each world now becomes the intersection of fuzzy sets and has the following membership function:

$$\mu_y(z) = \min_{i=1}^K (y_i \cdot R_i(z) + 1 - y_i)$$

(3)

Consequently, the satisfiability of each world is no longer a binary property, but a degree in $[0,1]$: $\max_x \mu_y(z)$. Therefore, the mass assigned to each world should be proportional to $p(y) \cdot \max_x \mu_y(z)$. I still need to ensure that the total mass is one, and that leads to the following formula which replaces (1) as the new basic probability assignment.

$$m(S_y) \triangleq \frac{p(y) \cdot \max_x \mu_y(z)}{\sum_{y'} (p(y') \cdot \max_x \mu_{y'}(z))}$$

(4)

Considering that $p(\cdot)$ is exactly the probability function of the Bernoulli vector $Y$, the above has a more concise form:

$$m(S_y) \triangleq \frac{p(y) \cdot \max_x \mu_y(z)}{E[\max_x \mu_y(z) \mid z]}$$

(5)

With this new $m(\cdot)$ function, a belief function is specified over the $z$ space. The mapping from $m(\cdot)$ to $Bel(\cdot)$ is also generalized to handle fuzzy sets and is in Appendix A.2. Since $x$ is a deterministic function of $z$, a belief function over the $x$ space is also implicitly specified.

2.3 Query answering

The most general form of a query is a conditional belief function given a condition function $C(z)$ which outputs a scalar in range $[0,1]$. In an application, the condition likely comes as a function of $x$, and since $x$ is a deterministic function of $z$, $C(z)$ is the general form. The condition is classical.
if $C(z)$ is Boolean, otherwise it is fuzzy and $C(z)$ is essentially the membership function of a fuzzy set over $z$ space.

To answer a general query, I simply add $C(z)$ as an extra entry to $r$, and add a constant 1 as an extra entry to vector $Y$. Intuitively, the NBR now has an additional rule that always exist. After such additions, the same formula \ref{eq:condbelief} specifies a conditional belief function.

Let us now consider a special type of queries that are perhaps the most common in practice: given a Boolean function $C(z)$ as condition, compute the conditional belief and plausibility of a classical proposition, i.e., another Boolean function $Q(z)$. In other words, I will derive the replacement of \ref{eq:condbelief} in a general NBR. Because $S_y$ is a fuzzy set specified by \ref{eq:condbelief} while $C(z)$ is a classical set, the constraint of $S_y \cap C \neq \emptyset$ is no longer binary but a degree in $[0, 1]$ and can be written as $\max_{x | C(x) = 1} \mu_y(z)$. Therefore, the denominator in both formulas in \ref{eq:condbelief} becomes $\sum_y (p(y) \cdot \max_{x | C(x) = 1} \mu_y(z))$. Applying the same to other terms in \ref{eq:condbelief}, and again utilizing the fact that $p(\cdot)$ is the probability function of $Y$, I have the following formulas for conditional belief and plausibility for classical condition and proposition in a general NBR:

\begin{align}
\text{Bel} \left( Q(\cdot) \mid C(\cdot) \right) &= 1 - \frac{E \left[ \max_{x | C(x) = 1, Q(x) = 0} \mu_y(z) \right]}{E \left[ \max_{x | C(x) = 1} \mu_y(z) \right]} \tag{6} \\
\text{Pl} \left( Q(\cdot) \mid C(\cdot) \right) &= \frac{E \left[ \max_{x | C(x) = 1, Q(x) = 1} \mu_y(z) \right]}{E \left[ \max_{x | C(x) = 1} \mu_y(z) \right]} \tag{7}
\end{align}

\subsection{2.4 Sample generation}

A belief function allows sample generation only if it is also a probability function. – recall that probability functions are a special case of belief functions \cite{shafer1976}. When combining two belief functions where one of the two is a probability function, by Dempster’s rule of combination \cite{shafer1976}, the resulting belief function is always a probability function. Therefore, to generate observation samples like traditional generative models, I combine the belief function of an NBR with a probability function over the $x$ space. This probability function is referred to as the prior-knowledge distribution. Intuitively, the prior-knowledge distribution represents assumptions or knowledge that are not included in this NBR. For example, if one only knows the range of $x$, a uniform prior-knowledge distribution could be used; if one knows the mean and variance of $x$, a Gaussian distribution could be used. As will become evident later, I only require the ability to draw samples from it. The flexibility to combine an NBR with various prior-knowledge distributions is analogous to applying the same knowledge in multiple environments. Section \ref{2.5} will discuss more on the role of prior-knowledge distributions.

For clarity of presentation, let us focus on the scenario where the $x$ space is discrete. For a sample value $	ilde{x}$, let $P_0(\tilde{x})$ denote its probability in the prior-knowledge distribution. Its probability after combining with an NBR is \cite{proof}

\begin{equation}
P(x = \tilde{x}) = \frac{P_0(\tilde{x}) \cdot \text{Pl}(x = \tilde{x})}{\sum_{x'} (P_0(x') \cdot \text{Pl}(x = x'))} \tag{8}
\end{equation}

where the plausibilities are given by \ref{eq:plausibility} with $C$ being always true. To generate samples according to \ref{eq:plausibility}. I simply draw samples from the prior-knowledge distribution and randomly keep or discard a sample, such that the probability to keep sample $\tilde{x}$ is proportional to $\text{Pl}(x = \tilde{x})$. Note that the denominator in \ref{eq:plausibility} does not change with $Q$ and hence is the same for all $\tilde{x}$ values; therefore I can simply use the numerator. In summary, the probability to keep a sample $\tilde{x}$ drawn from the prior-knowledge distribution is:

\begin{equation}
P_{\text{keep}}(\tilde{x}) = E \left[ \max_{x \in \mathbb{S}_y} \mu_y(z) \right] \tag{9}
\end{equation}

When the $x$ space is continuous, the generation procedure is the same: draw samples from a continuous prior-knowledge distribution and randomly keep or discard a sample according to the keep probability of \ref{eq:plausibility}.

\subsection{2.5 Training}

For unsupervised learning, an NBR is trained by maximizing the likelihood of observations in the sample generation process of the previous section. Therefore I need to choose a prior-knowledge distribution for training. This choice defines what should be learned by the NBR: information that is present in the observations yet that is beyond what is already encoded in the prior-knowledge distribution. For example, samples generated by an existing NBR can be used as the prior-knowledge distribution, and then the new NBR would be trained to learn and only learn knowledge that is beyond that existing NBR. Note that, after an NBR is trained, the query-answering process of Section \ref{2.3} is independent of the prior-knowledge distribution used in training. In other words, an NBR’s answers are based on only the knowledge contained in itself, and this allows knowledge learned in one environment to be used in a different environment.

Given observations $x_1, \ldots, x_n$, the likelihood loss is:

\begin{equation}
\mathcal{L} = - \frac{1}{n} \sum_{i=1}^{n} \log P(x = x_i) = - \frac{1}{n} \sum_{i=1}^{n} \log P_0(x_i) \cdot P_{\text{keep}}(x_i) = - \frac{1}{n} \log P_0(x_i) - \frac{1}{n} \sum_{i=1}^{n} \log P_{\text{keep}}(x_i) + \log \sum_{x'} (P_0(x') \cdot P_{\text{keep}}(x')) \tag{10}
\end{equation}

The first term is a constant and can be removed; the last term can be shortened by letting $X$ denote a vector of random variables that has the prior-knowledge distribution. The loss function becomes:

\begin{equation}
\mathcal{L} = - \frac{1}{n} \sum_{i=1}^{n} \log P_{\text{keep}}(x_i) + \log E [P_{\text{keep}}(X)] \tag{11}
\end{equation}

\footnote{Proof is in Appendix A.3}
Each training iteration uses a batch of observations to approximate the first term and a batch of samples from the prior-knowledge distribution to approximate the second term. There is an implementation issue with the second term: the expectation is before log, and with small batch size there is bias in gradient estimation. In practice, I use the following loss instead:

\[
\mathcal{L} = -\frac{1}{n} \sum_{i=1}^{n} \log P_{\text{keep}}(x_i) + \mathbb{E}[P_{\text{keep}}(X)] / \alpha
\]

where \( \alpha \) is a constant that gets updated once every certain number of batches, and its value is an estimate of \( \mathbb{E}[P_{\text{keep}}(X)] \) on a large number of samples. It is straightforward to verify that, with a large batch size, \ref{eq:loss_eq} and \ref{eq:loss_eq} result in asymptotically the same gradients with respect to model parameters. The benefit of \ref{eq:loss_eq} is that the expectation in the second term is exposed and now small batch size can be used without causing bias in in gradient estimation.

3 Unsupervised Learning: a Synthetic Task

This section gives a first demonstration of NBR on an unsupervised-learning task. Source code for training and inference is available at http://researcher.watson.ibm.com/group/10228

Consider a world with 11 bits. Partial observations are available that observe either the first 10 bits or the last 10 bits. In observations of the first 10 bits, the first bit is the majority function of the middle 9 bits for 90% of the cases, and the inverse for 10% of the cases. In observations of the last 10 bits, the last bit is the majority function of the middle 9 bits for 20% of the cases, and the inverse for 80%.

An NBR is trained on these observations: \( K = 2 \); \( F(\cdot) \) is identity function; \( R(\cdot) \) is two three-layer ReLU networks, where each network is followed by a sigmoid unit, and where one network takes the first 10 bits as input and the other takes the last 10 bits. The loss function \ref{eq:loss_eq} is used, and the prior-knowledge distribution is uniform distribution over the \( 2^{11} \) possibilities. For a partial observation \( x_i \), let \( x_{i,0} \) and \( x_{i,1} \) be the two possible full observations. Substituting \( P(x = x_i) = P(x = x_{i,0}) + P(x = x_{i,1}) \) into \ref{eq:loss_eq} and following the same derivation to \ref{eq:loss_eq}, it is straightforward to see that I simply need to compute \( P_{\text{keep}}(x_i) \) in \ref{eq:loss_eq} as \( P_{\text{keep}}(x_{i,0}) + P_{\text{keep}}(x_{i,1}) \).

Table 1 lists NBR’s answers to five sample queries. The belief values are computed by \ref{eq:belief_plausibility} and the plausibility values are by \ref{eq:belief_plausibility}. In the first query, the condition is the first bit being 1 and the query is on the last bit. NBR answers with belief zero and plausibility 0.33, which means that it has some evidence to support \( x_{10} \) being 0 but no evidence to support \( x_{10} \) being 1. This answer is intuitive: with \( x_0 = 0 \), it is likely that the majority of the middle 9 bits is 1, and consequently it is likely that \( x_{10} \) is 0. Recall that during training the NBR has never seen an observation that simultaneously shows \( x_0 \) and \( x_{10} \), and it answers the query by performing multi-hop reasoning with uncertainty. The second query is the opposite: with \( x_0 = 0 \), NBR has some evidence to support \( x_{10} \) being 1 but no evidence to support \( x_{10} \) being 0. There is an interesting comparison between the third and fourth queries: NBR’s belief decreases when \( x_{10} = 1 \) is added to the condition.

4 Supervised Learning: a Robust MNIST Classifier

This section demonstrates NBR for supervised learning, and specifically discusses a robust MNIST classifier.

4.1 Using NBR for classification

It is possible to convert a classification task to unsupervised learning by treating training labels as part of the observation. However that is not the most efficient way to use NBR for classification, and this section presents a better approach. The discussion is on MNIST but most techniques are applicable to classification in general.

Given an MNIST image, let’s consider a world with 10 possibilities, – one of the ten labels is true. Recall from Section 2.2 that, in an NBR, the role of each entry in \( r \) is to specify a fuzzy set. In a world with 10 possibilities, a fuzzy set is defined by 10 grades of membership, i.e., simply 10 numbers between 0 and 1. Therefore, each entry in \( r \) can be implemented by an arbitrary NBR classifier, and I simply add 10 sigmoid units at the end to convert logits to output
values in $[0, 1]$. Function $F(\cdot)$ is identity function and in fact will not be used. In summary, an NBR classifier is composed of $r$, which is $K$ classifiers with sigmoids added, and Bernoulli variables $Y$.

Now let’s define its outputs. With $\hat{\beta}_r$, the belief and plausibility of each label can be computed, let them be $\text{Bel}_j$, $\text{Pl}_j$, $j \in \{0, \ldots, 9\}$. I use this output vector:

$$o = (\log \text{Pl}_0, \ldots, \log \text{Pl}_9) \quad (13)$$

and its argmax is NBR’s output label. The values in $\{13\}$ are the negative of weights of evidence against each label (Shafer 1976). There are other choices: I could use $-\log (1 - \text{Bel}_j)$ which is the weight of evidence for label $j$ (Shafer 1976), or use $\log \text{Pl}_j - \log (1 - \text{Bel}_j)$ which combines weights of evidence for and against label $j$. I choose $\{13\}$ for computational efficiency.

Given an MNIST image, consider the fuzzy set specified by one entry in $r$. It is possible, in fact often, that all grades of membership are below 1. In such a scenario, intuitively there is conflicting information within this rule itself: none of the possibilities is a full member of this fuzzy set. Although the NBR formulas can handle such rules as they are, it’s beneficial to resolve such conflicts before computing $\{13\}$ via $\{7\}$. For a given image, let $\max (r_1)$ denote the largest grade of membership from the $i$th rule; I simply divide all grades of membership from the $i$th rule by $\max (r_1)$ and multiply $b_i$ with $\max (r_1)$. Intuitively, if a rule is conflicted on an image, the belief in it is reduced accordingly. Note that this scaling is different per image, and hence the now scaled $b_i$ values vary by image. This operation is in a similar vein to the scaling step in Dempster’s rule of combination, and I refer to it as Dempster-style scaling. Section 4.4 discusses its role in robustness.

4.2 Frames of discernment

Dempster’s rule of combination assumes that sources represent entirely distinct bodies of evidence (Shafer 1976). Hence the $K$ classifiers that constitute $r$ ought to learn different knowledge than each other. I achieve this by using different frames of discernment on them, and training those that share the same frame of discernment on different data.

Our implementation uses $K = 46$ rules, and Table 2 lists the 46 frames of discernment. To explain by example, let us consider the rule that has this frame of discernment: $\{0\} \{5, 6\} \{7\}$. It is built as a classifier with 3 classes; for an image, let its three outputs after sigmoid be $v_1$, $v_2$ and $v_3$, and let $\hat{v} = \max (v_1, v_2, v_3)$. Then it specifies a fuzzy set with the following grades of membership for the 10 labels:

$$v_1 \in \hat{v}, 1, 1, 1, v_2 \in \hat{v}, v_3 \in \hat{v}, \hat{v}, 1, 1,$$

Note that the grades of membership for labels outside its frame of discernment, $\{1, 2, 3, 4, 8, 9\}$, are always 1; intuitively this rule makes no judgment about them and considers those labels perfectly plausible. Also note that the grades of membership for 5 and 6 are always the same; intuitively this rule does not distinguish between them. In the above, I have applied Dempster-style scaling, and the $b_i$ value for this rule for this image is multiplied with $\hat{v}$.

| Table 2: Frames of discernment in NBR MNIST classifier. |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| $\{4\} \{9\}$ | $\{5\} \{8\}$ | $\{2\} \{8\}$ | $\{2\} \{6\}$ | $\{3, 5\} \{4\}$ |
| $\{4\} \{9\}$ | $\{5\} \{8\}$ | $\{8\} \{9\}$ | $\{5\} \{6\}$ | $\{0, 2, 6\} \{9\}$ |
| $\{4\} \{9\}$ | $\{3\} \{5\}$ | $\{8\} \{9\}$ | $\{4\} \{6\}$ | $\{0, 6\} \{1\} \{3\}$ |
| $\{4\} \{9\}$ | $\{3\} \{5\}$ | $\{0\} \{2\}$ | $\{2\} \{4\}$ | $\{0\} \{5, 6\} \{7\}$ |
| $\{4\} \{9\}$ | $\{3\} \{5\}$ | $\{0\} \{2\}$ | $\{3\} \{9\}$ | $\{0\} \{1\} \{4\}$ |
| $\{7\} \{9\}$ | $\{3\} \{8\}$ | $\{0\} \{6\}$ | $\{1\} \{7\}$ | $\{1\} \{5\} \{9\}$ |
| $\{4\} \{9\}$ | $\{7\} \{3\} \{8\}$ | $\{0\} \{6\}$ | $\{2\} \{7\}$ | $\{0, 6\} \{8\}$ |
| $\{4\} \{9\}$ | $\{7\} \{3\} \{8\}$ | $\{1\} \{6\}$ | $\{3\} \{7\}$ | $\{1, 4, 7\} \{8\}$ |

Frames of discernment specify what knowledge each entry in $r$ learns from the training data. An obvious way to choose them is letting them be all pairs of labels, and the reason for those in the last column of Table 2 is to reduce $K$ and reduce computational cost.

The reason for duplicates in Table 2 is that those frames of discernment are difficult to learn robustly and hence multiple rules are needed to do the job. For example, 4 and 9 are perhaps the most difficult pair to distinguish and three rules are used on this pair. For rules that share the same frame, training data are split among them so that they learn different knowledge, and this will be discussed in the next section.

4.3 Loss functions for robustness

Each of the 46 classifiers that constitute $r$ is implemented as sigmoid ($s_i \cdot G_i(\text{image})$), where $s_i$ is a scalar trainable parameter and $G_i(\cdot)$ is an $L_2$-nonexpansive neural network (L2NNN) (Qian and Wegman 2019). Hence the overall trainable parameters are the parameters of $G_i(\cdot)$, $s_i$ and $b_i$, for $i = 1, \ldots, 46$. The training process has two steps. First, all $G_i(\cdot)$’s are trained: ones that share the same frame of discernment are trained jointly, while others are trained individually. Second, the NBR is trained as a whole but with only $s_i$’s and $b_i$’s being trainable; the reason for freezing $G_i(\cdot)$’s is to maintain them as distinct bodies of evidence. I present loss functions used in the two steps.

For the first step, when multiple $G_i(\cdot)$’s are trained jointly, they only influence each other through training data splitting which gets updated once every certain number of batches, and the loss function is independent for each individual $G_i(\cdot)$. Let the $i$th frame of discernment be $\Lambda_{i,1}, \ldots, \Lambda_{i,J_i}$, where each $\Lambda_{i,j}$ is a set of labels. Let $T_{i,j}$ denote the set of training data with labels in $\Lambda_{i,j}$, and that are assigned to $G_i(\cdot)$; note that $T_{i,j} \cap T_{i,j'} = \emptyset$ if the $i$th and $i'$th frames of discernment are identical. Let $\bar{T}_{i,j}$ denote all training data with labels in $\bigcup_{1 \leq j' \leq J_i, j' \neq j} \Lambda_{i,j'}$. The loss function for training $G_i(\cdot)$ is:

$$L_i = \sum_{j=1}^{J_i} \text{avg}_{t \in T_{i,j}} l \left( \text{ReLU} \left( \beta - G_i(t)_j \right) \right)$$

$$+ \gamma \cdot \sum_{j=1}^{J_i} \text{avg}_{t \in \bar{T}_{i,j}} l \left( \text{ReLU} \left( \beta + G_i(t)_j \right) \right) \quad (14)$$

where $l(\cdot)$ is a scalar penalty function; $\beta > 0$ and $\gamma \geq 1$ are hyperparameters. Intuitively, $G_i(\cdot)$ is penalized if its logit
for the correct \( \Lambda_{i,j} \) is less than \( \beta \) or if the logits for the incorrect \( \Lambda_{i,j} \)'s are greater than \( -\beta \), \( \beta \) controls the robustness-accuracy trade-off. \( \gamma \) controls the balance between the two types of penalties. Our implementation uses

\[
l(a) = \min \left( \frac{a^2}{2} - \frac{\eta}{2} \right) + \text{ReLU} (a - \eta) + \omega \cdot \text{ReLU} (a - \xi)
\]

where \( \eta, \omega \) and \( \xi \) are hyperparameters. (15) is a heuristic and can be replaced by any increasing and convex function.

Once every certain number of batches, \( T_{i,j} \)'s are updated: among \( G_i(\cdot) \)'s that share the same frame of discernment, training images are re-assigned such that they incur less penalty in (14), subject to size lower bound for \( T_{i,j} \)'s which is imposed for training stability. Intuitively, a training image \( t \) tends to be assigned to a \( G_i(\cdot) \) that classifies \( t \) the most robustly. Note that \( T_{i,j} \)'s are constant and never updated.

In the second step, I train \( s_i \)'s and \( b_i \)'s through a technique called poor man’s adversarial training. It is a cheap operation of decreasing the logit of each \( G_i(\cdot) \) for the correct \( \Lambda_{i,j} \) by \( \tau \) while increasing the logits for the incorrect \( \Lambda_{i,j} \)'s by \( \tau \), where \( \tau \) is a hyperparameter. Intuitively, because \( G_i(\cdot) \)'s are L2NNNs, this operation is assuming the worst case scenario of an adversarial attack of \( L_2 \) distortion of \( \tau \). Let \( o_{adv} \) denote the NBR output vector (13) under this assumption. For a training image \( t \), let \( g_{adv}(t) \) denote the difference between the entry in \( o_{adv} \) that corresponds to the correct label and its greatest entry for an incorrect label, and let \( g_{ori}(t) \) denote the same for the original (13); classification is correct when \( g \) is positive. The loss function for the second step is:

\[
L = \text{avg}_t \left( \text{sigmoid} \left( -g_{adv}(t) \cdot \chi \right) \right) + \nu \cdot \text{avg}_t \left( \text{sigmoid} \left( -g_{ori}(t) \cdot \chi \right) \right)
\]

where \( \chi, \nu \) are hyperparameters. (16) is a heuristic and one can derive other loss functions based on \( o_{adv} \) and (13).

### 4.4 Proof of asymptotic robustness

For a training image \( t \), let \( d(t) \) denote the distance from \( t \) to the nearest training image with a different label. There exists a classifier that has 100% accuracy on the training set, and, for each \( t \), outputs the same label within a ball of radius \( d(t)/2 \) around \( t \). I refer to this as the oracle robustness as it is the best achievable on a given training set. For the MNIST training set and for \( L_2 \) distance, the oracle robustness radius is above 3 for 51% of images, above 2.5 for 79% of images, and above 2 for 96% of images. Consequently, it is arguable that \( \epsilon = 2 \) is the meaningful \( L_2 \) threshold when quantifying robustness of MNIST classifiers, because measuring with a higher \( \epsilon \) could introduce the possibility of a biased classifier that favors a subset of images.

This section uses the \( L_2 \) metric. Although the same argument applies to other metrics, there is only practical significance in \( L_2 \) because there are not yet known efficient ways to build nonexpansive neural networks for other metrics.

**Theorem 1.** For any constant \( \delta > 0 \), there exists an NBR classifier that classifies each training datum \( t \) correctly within a ball of \( L_2 \) radius \( d(t)/2 - \delta \).

**Proof.** Without loss of generality, let us consider a task with two classes, A and B. For all \( G_i(\cdot) \)'s, the frame of discernment is the same: \( \{A\} \{B\} \). Consider the extreme case that each \( T_{i,j} \) contains exactly one training datum. Then \( G_i(\cdot) \) has a trivial implementation: the first logit is \( G_i(t) = d(\hat{t}_i)/2 - \|t - \hat{t}_i\|_2 \) where \( \hat{t}_i \) is the only member of \( T_{i,1} \), and the second logit is similar.

Consider a training datum \( t \) with label A, and let \( T_{i,1} \) be the subset that contains it. I have \( G_i(t) = d(t) \) and \( G_i(t) = \|t - \hat{t}_i\|_2 \), proof in Appendix A.4.

Hence for any \( t' \) such that \( \|t' - t\|_2 \leq d(t)/2 - \delta \), it must be true that \( G_i(t')_1 \geq d(t)/2 \) and \( G_i(t')_2 \leq d(t)/2 \), \forall t. Obviously \( G_i(\cdot) \) classifies correctly. Some others could misclassify: in such a rule, it must be true that \( G_i(t')_1 < G_i(t')_2 \leq \|t - \hat{t}_i\|_2 \). Therefore the grades of membership before Dempster-style scaling are \( \text{sigmoid}(s_i \cdot G_i(t')_1) < \text{sigmoid}(s_i \cdot G_i(t')_2) \leq \text{sigmoid}(-s_i \cdot \delta) \). Therefore Dempster-style scaling multiplies \( b_i \) with the grade of membership for B, which is no greater than \( \text{sigmoid}(-s_i \cdot \delta) \). \( s_i \) can be arbitrarily large in this NBR, and hence the scaled \( b_i \) can be arbitrarily small for \( t' \) and this rule has little effect in (7). This argument applies to any \( G_i(\cdot') \) that misclassifies. Therefore, with sufficiently large \( s_i \)'s, this NBR always classifies \( t' \) as label A.

The NBR in the proof is neither practical, due to an extremely large \( K \), nor desirable because it memorizes training data. However, there is a continuous spectrum of NBRs as \( K \) varies, and the sweet spot is likely in the middle: when the \( T_{i,j} \)'s are meaningful subsets of data, an NBR might reach the best combination of robustness and generalization.

### 4.5 Results

The NBR MNIST classifier is available at [http://researcher.watson.ibm.com/group/10228](http://researcher.watson.ibm.com/group/10228).

Table 3 compares the NBR MNIST classifier against those in [Madry et al. 2018] [Wong and Kolter 2018] [Qian and Wegman 2019], all of which are publicly available. Among them, the L2NNN classifier from [Qian and Wegman 2019] is the state of the art in robustness as measured by \( L_2 \) metric.

The robust accuracies are measured on the first 1000 images in the MNIST test set by running four attacks: projected gradient descent (PGD) [Madry et al. 2018], boundary attack [Brendel, Rauber, and Bethge 2018], Carlini & Wagner (CW) attack [Carlini and Wagner 2017b] and seeded CW. Foolbox [Rauber, Brendel, and Bethge 2017] is used for PGD and boundary attacks; CW is original code from [Carlini and Wagner 2017b]; seeded CW is a CW search with a starting point that is provided by a transfer attack, and is a straightforward variation of the CW code. Iteration limit is 100 for PGD, 50K for boundary attack, and 10K for CW and seeded CW. More details are in Appendix B. As discussed in Section 4.4, \( \epsilon = 2 \) is a meaningful \( L_2 \) threshold for MNIST. A classifier is considered robust on an image if it remains correct under all four attacks.

Table 3 shows that the NBR classifier has the best robustness, and at the same time the best natural accuracy among all but the non-robust vanilla model. I do not have access to the model in [Schott et al. 2019] and can only compare with
icism in literature, e.g., (Pearl 1990). I disagree with much of
reported numbers: their natural accuracy is 99% and robust
accuracy is 80% for $L_2$ threshold of 1.5. For 1.5, the NBR
classifier has a robust accuracy of 83.5%. It’s worth noting
that the NBR model is end-to-end differentiable while the
model of (Schott et al. 2019) is not, and hence our 83.5% is
likely after more scrutiny from attacks than their 80%.
Ablation studies are in Appendix C and include classifiers
in which belief-function arithmetic is replaced by Markov
random field and Gaussian naive Bayes.
Another hypothesis is that a model with reasoning ought
to generalize better on out-of-distribution data points. I de-
ferred two data sets from the MNIST test set: thin-MNIST,
in which many pixels are set to zero based on each pixel’s
neighborhood information, and framed-MNIST, in which
the boundary pixels are set to one. Generation scripts are
available at the link at the beginning of this section. Sam-
ple images are shown in Figure 2. Table 4 compares various
models on these out-of-distribution images, and NBR out-
performs the rest.

5 Related Work

As a formalism for reasoning with uncertainty, belief func-
tions (Shafer 1976) have two distinct advantages: explicit
modeling of the lack of knowledge and an elegant mech-
anism of combining multiple sources of information. Con-
sequently reasoning frameworks based on belief functions
have been proposed (Gordon and Shortliffe 1985; Baldwin
1986; Lowrance, Garvey, and Strat 1986; Laskey and Lehner
1988; D’Ambrosio 1988; Wan and Kifer 2009), and they
have varying degrees of similarity to the restricted frame-
work of Section 2.1. These early works share some com-
mon weaknesses in practice: where do rules come from,
where do uncertainty quantifications on the rules come from.
Relying on manual inputs is clearly not scalable.

Table 3: Accuracies on natural images and on adversarial
images where the $L_2$-norm limit of distortion is 2.
|            | natural | robust |
|------------|---------|--------|
| Vanilla    | 99.1%   | 0%     |
| Madry et al. | 98.5%  | 3.3%   |
| Wong&Koller | 98.8%   | 8.9%   |
| L2NNN      | 98.2%   | 61.2%  |
| NBR        | 99.0%   | 61.6%  |

Table 4: Accuracies on out-of-distribution images.
|            | thin     | framed  |
|------------|----------|---------|
| Vanilla    | 88.5%    | 85.3%   |
| Madry et al.| 97.3%   | 82.7%   |
| Wong&Koller| 97.1%    | 91.6%   |
| L2NNN      | 95.7%    | 98.3%   |
| NBR        | 97.6%    | 98.8%   |

Another reason for limited adoption of belief function is crit-
icism in literature, e.g., (Pearl 1990). I disagree with much of

fair, mainstream methods based on Bayesian network (Pearl
1988) or Markov random field (Kindermann and Snell 1980)
often have the same weaknesses. Some have addressed
the second weakness: for example, Markov logic networks
(Richardson and Domingos 2006) learn the weights on
clauses. Attempts to address the first weakness, e.g., by in-
ductive logic programming (Muggleton and De Raedt 1994;
De Raedt and Kersting 2008), are often limited.

Progresses in addressing the first weakness via automatic
discovery of rules have emerged from the machine learn-
ing field. In (Hinton 2002; Salakhutdinov and Hinton 2009).
Markov-random-field models, which can be viewed as com-
positions of non-symbolic rules, are learned from data. In
(França, Zaverucha, and Garcez 2013; Evans and Grefen-
stette 2018), symbolic logic programs are learned from ex-
amples by neural networks. Another example is (Serafini
and Garcez 2016) which defines a formalism of real-valued
logic and thereby enables learning non-symbolic rules.

Adversarial robustness is a well-known difficult prob-
lem (Szegedy et al. 2013; Goodfellow, Shlens, and Szegedy
2015; Carlini and Wagner 2017b), and many remedies have
been tried and failed (Carlini and Wagner 2017a; Athalye,
Carlini, and Wagner 2018). For MNIST, if distortion is mea-
sured by the $L_∞$ distance, there are a number of approaches
(Wong and Kolter 2018; Raghunathan, Steinhardt, and Liang
2018; Schott et al. 2019) and in particular (Madry et al.
2018) achieves good $L_∞$ robustness by adversarial train-
ing. For $L_2$ robustness which is less understood and per-
haps more difficult, before this work the state of the art is
an L2NNN from (Qian and Wegman 2019) with adversar-
ial training. It’s worth noting that adversarial training alone
does not work well for $L_2$ robustness (Schott et al. 2019;
Qian and Wegman 2019; Tsipras et al. 2019). One hypothe-
sis in this paper is that reasoning is a missing piece in previ-
ous works on robustness.

6 Conclusions and Future Work

This paper presents neural belief reasoner, which is a new
generative model and a new approach to combine learning
and reasoning. Its properties are studied through two tasks:
an unsupervised-learning task of reasoning with uncertainty,
and a supervised-learning task of robust classification. In
particular, the MNIST classifier sets a new state of the art
in $L_2$ robustness while maintaining 99% nominal accuracy.
This paper only scratches the surface. As discussed in the
text, both tasks use NBRs with certain restrictions, e.g., $F(\cdot)$
the criticism. A comparative study between belief function and
Bayesian inference is beyond the scope of this paper; ablation stud-
ies in Appendix C do offer some empirical results.
being identity function. To unlock its full potential, innovations would be needed for efficient inference and training algorithms, including but not limited to Monte Carlo methods, as well as efficient constraint-programming solvers. There are also open questions from the application perspective, e.g., how to take advantage of NBR’s sample-generation capability and how to leverage NBR for interpretability.

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A Proofs

A.1 Proof of equation (2)

Proof. According to (Shafer 1976), conditional belief is

$$\text{Bel} (Q \mid C) = \frac{\text{Bel} (Q \cup \overline{C}) - \text{Bel} (\overline{C})}{1 - \text{Bel} (\overline{C})} \quad (A.1)$$

Substituting the mapping formula from $m (\cdot)$ to Bel $(\cdot)$, the formula becomes

$$\text{Bel} (Q \mid C) = 1 - \frac{\sum_{B \subseteq Q \cap \overline{C}} m (B)}{1 - \sum_{B \subseteq \overline{C}} m (B)} \quad (A.2)$$

Substituting (1) into the above, since the denominator in (1) is a constant, I can then multiply both the numerator and the denominator in (A.2) with it, and the formula becomes

$$\text{Bel} (Q \mid C) = 1 - \frac{\sum_{y: S_y \neq 0} p (y) \cdot \sum_{y: S_y \neq 0, S_y \subseteq Q \cap \overline{C}} p (y)}{1 - \sum_{y: S_y \neq 0} p (y) \cdot \sum_{y: S_y \neq 0, S_y \subseteq \overline{C}} p (y)} \quad (A.3)$$

It’s straightforward to verify that $\sum_{y} p (y) = 1$. Substituting this in both the numerator and the denominator in (A.3) with this sum, the formula becomes

$$\text{Bel} (Q \mid C) = 1 - \frac{\sum_{y: S_y \neq 0, S_y \subseteq Q \cap \overline{C}} p (y)}{\sum_{y: S_y \neq 0} p (y)} \quad (A.4)$$

By now I have proved the first half of (2). The second half can be easily derived from the first half, by utilizing the relation between belief and plausibility (Shafer 1976):

$$\text{Pl} (Q \mid C) = 1 - \text{Bel} (\overline{Q} \mid C)$$

$$\text{Pl} (Q \mid C) = 1 - \left( 1 - \frac{\sum_{y: S_y \cap C \neq 0 \neq 0} p (y)}{\sum_{y: S_y \cap C \neq 0} p (y)} \right) \quad (A.5)$$

A.2 Mapping from $m (\cdot)$ to Bel $(\cdot)$ with fuzzy sets

For a classical set $A$, the formula for Bel $(A)$ is given by equation (6), with $C$ being always true and $Q$ being the Boolean membership function of $A$. Hence I only need to derive the equivalent of (6) for a fuzzy set $A$; let $\mu_A (z)$ denote its membership function. With a fuzzy set, I can no longer take the max in the numerator of (6) under a hard condition of $\mu_A (z) = 0$. That needs to be replaced by the max grade of membership in the intersection set between $A$ and each $S_y$. Let $\mu_{S_y \cap A} (z) = \min \{ \mu_y (z), 1 - \mu_A (z) \}$

according to fuzzy set arithmetic (Zadeh 1965), and the belief on a fuzzy set is

$$\text{Bel} (A) = 1 - \frac{\text{E} \left[ \max_z \left( \min \{ \mu_y (z), 1 - \mu_A (z) \} \right) \right]}{\text{E} \left[ \max_z \mu_y (z) \right]} \quad (A.6)$$

Utilizing equation (5) and the fact that total mass assignment is 1, the above equation can be rewritten to the following.

$$\text{Bel} (A) = \sum_y m (S_y) \cdot \left( 1 - \frac{\max_z \mu_{S_y \cap A} (z)}{\max_z \mu_y (z)} \right) \quad (A.7)$$

The above mapping from $m (\cdot)$ to Bel $(\cdot)$ is intuitive: the belief in a fuzzy set is a weighted sum of mass values assigned to each possible world, and each weight is a fraction value that depends on the satisfiability of $S_y \cap A$ as well as $S_y$ itself. It’s straightforward to verify that, if $A$ and $S_y$’s are all classical sets, equation (A.7) is identical to the classical mapping (Shafer 1976): Bel $(A) = \sum_{B \subseteq A} m (B)$.

A.3 Proof of equation (8)

Proof. For clarity of presentation, let us focus on the scenario where the x space is discrete. Because Dempster’s rule of combination is associative (Shafer 1976), combining an NBR and a prior-knowledge distribution is the same as combining $K + 1$ belief functions, where the first $K$ are from the NBR while the last one is the prior-knowledge distribution. Let $m' (\cdot)$ denote the resulting basic probability assignment. By Dempster’s rule of combination, $m' (\cdot)$ assigns mass to sets in the form of $S_y \cdot \Xi \Leftrightarrow S_y \cap \{ z \mid F (z) = \Xi \}$ where $\Xi$ is an element in the x space. Let $\mu_y (\Xi)$ denote the membership function of $S_y \cdot \Xi$. Obviously $\mu_y (\Xi)$ is non-zero only where $F (\Xi) = \Xi$. Therefore, if I consider the implicitly specified belief function over the x space, mass is only assigned to singletons, – sets with one and only one element; this is exactly the condition when a belief function becomes a probability function, and the probability of an outcome is the total mass assigned to the corresponding singleton. If $S_y$’s are classical sets, the resulting probability from combining $K + 1$ sources is

$$P (x = \Xi) = \sum_y m' (S_y \cdot \Xi) \quad (A.8)$$

where $P_0 (\Xi)$ is the probability of $\Xi$ in the prior-knowledge distributions, $\sigma_{S_y \cdot \Xi}$ is the Boolean satisfiability of $S_y \cdot \Xi$, and $\Xi$ is a normalizing constant.

For fuzzy sets, I only need to replace $\sigma_{S_y \cdot \Xi}$ with a degree of satisfiability:

$$\max_z \mu_y (z) = \max_{z \mid F (z) = \Xi} \mu_y (z) \quad (A.9)$$
Therefore the generalized form of (A.8) is

\[
P(x = \tilde{x}) = \sum_{y} \frac{P_0(\tilde{x}) \cdot p(y) \cdot \max_{z | F(z) = \tilde{x}} \mu_y(z)}{\Xi} \]

\[
= \frac{P_0(\tilde{x}) \cdot \sum_{y} \left( p(y) \cdot \max_{z | F(z) = \tilde{x}} \mu_y(z) \right)}{\Xi} \]

\[
= \frac{P_0(\tilde{x}) \cdot E \left[ \max_{z | F(z) = \tilde{x}} \mu_y(z) \right]}{\Xi} \]

(A.10)

Note that the expectation term matches the numerator in (7) with \( C \) being always true and \( Q \) being the Boolean proposition of \( F(z) = \tilde{x} \). After substituting (7) and setting a proper \( \Xi \), (A.10) can be converted to the form of (8).

\[ \square \]

A.4 Proof of logit bounds in Section 4.4

Proof. For the NBR used in the proof in Section 4.4, consider a training datum \( t \) with label A. For any \( i \), let \( \tilde{t}_i \) denote the only member of \( T_{i,2} \), which has label B.

If \( d(\tilde{t}_i) \geq d(t) \), then it must be true that

\[
G_i(t) = d(\tilde{t}_i) - d(t) \leq d(\tilde{t}_i) / 2 \]

\[
= -d(\tilde{t}_i) / 2 \]

(A.11)

If \( d(\tilde{t}_i) < d(t) \), then it must be true that

\[
G_i(t) = d(\tilde{t}_i) - d(t) \leq d(\tilde{t}_i) / 2 - d(t) \]

\[
< d(\tilde{t}_i) / 2 - d(t) \]

\[
= -d(t) / 2 \]

(A.12)

\[ \square \]

B Details of Robustness Evaluation

This section presents a detailed description of the robustness evaluation used for Table 3, as well as results from individual attacks in Table B.1.

Robust accuracies are measured on the first 1000 images in the MNIST test set due to limitation of computing resources.\(^\dagger\) On each image and for each classifier, four attacks are performed:

- Projected gradient descent (PGD) (Madry et al. 2018): the implementation in Foolbox (Rauber, Brendel, and Bethge 2017) is used, with an iteration limit of 100. I observe empirically that, for \( L_2 \) attacks, PGD with 100 iterations outperforms PGD with 1000 iterations.

- Boundary attack (Brendel, Rauber, and Bethge 2018): the implementation in Foolbox (Rauber, Brendel, and Bethge 2017) is used, with an iteration limit of 50,000.

- Carlini & Wagner (CW) attack (Carlini and Wagner 2017b): the original code from (Carlini and Wagner 2017b) is used, with an iteration limit of 10,000.

- Seeded CW attack: a CW attack that starts each search from an image that is provided by a transfer attack. The implementation is a straightforward modification from the code of (Carlini and Wagner 2017b), and an iteration limit of 10,000 is used. The transfer attack is a CW attack on a modified NBR classifier in which all \( s_i \) values are reduced, and I simply save the adversarial images and load them during seeded CW attacks. Theoretically this transfer attack should produce starting points that are the most effective in attacking the NBR classifier. As shown in Table B.1, these starting points are also quite effective in attacking the classifiers from (Madry et al. 2018; Wong and Kolter 2018). I hypothesize that they are close to genuinely ambiguous images and hence are good starting points for CW attacks.

Per discussion in Section 4.4 on oracle robustness, \( \varepsilon = 2 \) is the meaningful \( L_2 \) threshold when quantifying robustness of MNIST classifiers. A classifier is considered robust on an image if it remains correct under all four attacks, i.e., if none of the four attacks is able to find an adversarial example within \( L_2 \) distance of 2.

One observation in Table B.1 is that the boundary attack is particularly powerful in attacking the classifiers from (Madry et al. 2018; Wong and Kolter 2018). Similar results on (Madry et al. 2018) have been reported in (Schott et al. 2019).

C Ablation Studies

The NBR MNIST classifier of Section 4 can be viewed as combining \( K = 46 \) sources of information, each of which is an L2NNN, and NBR is the method to combine them. From this perspective, an important question is: what other methods are there for performing the combination, and how do they compare with NBR? This section presents some empirical answers by building classifiers in which the 46 sources are kept the same while NBR’s combining operations are replaced by various approaches, including Markov random field (MRF) and Gaussian naive Bayes.

Table C.1 lists the natural accuracy and robust accuracy of the ablation-study models, which are measured in the same way as Table 3 and as described in the previous section. The first row is copied from Table 3 as a reference.

\[ \text{Table B.1: Accuracies on adversarial images where the } L_2 \text{-norm limit of distortion is } 2. \text{ BA is boundary attack. SCW is seeded CW attack. Best is picking the best of four attacks for each image.} \]

|                | PGD | BA | CW | SCW | best |
|----------------|-----|----|----|-----|------|
| Vanilla        | 45.7% | 0% | 0% | 0%  | 0%   |
| Madry et al.   | 96.6% | 8.3% | 56.2% | 19.1% | 3.3% |
| Wong & Kolter  | 95.8% | 13.5% | 66.6% | 33.1% | 8.9% |
| L2NNN          | 92.3% | 79.5% | 62.4% | 61.3% | 61.2% |
| NBR            | 89.4% | 78.0% | 72.8% | 62.8% | 61.6% |

\[ \dagger \text{Note that natural accuracies in Table 3 are measured on the whole test set, and so are all measurements in Table 4.} \]
Table C.1: Accuracies of ablation-study models on natural images and on adversarial images where the $L_2$-norm limit of distortion is 2.

|                  | natural | robust |
|------------------|---------|--------|
| NBR              | 99.0%   | 61.6%  |
| No Dempster-style scaling | 97.6%   | 53.2%  |
| Markov random field #1 | 98.6%   | 55.5%  |
| Markov random field #1+ | 98.9%   | 57.2%  |
| Markov random field #2 | 97.2%   | 54.1%  |
| Gaussian naive Bayes #1 | 98.8%   | 54.1%  |
| Gaussian naive Bayes #1+ | 98.0%   | 45.0%  |
| Gaussian naive Bayes #2 | 97.6%   | 42.6%  |

- The second row is an NBR classifier without the step of Dempster-style scaling, which was discussed in Section 4.1; the $s_i$ and $b_i$ parameters are re-trained. Given the role that Dempster-style scaling plays in the robustness proof of Section 4.4, the drop in robustness is not surprising. The results suggest that Dempster-style scaling also contributes to the accuracy on natural images.

- The third, fourth and fifth rows are models that assume a Boltzmann distribution among the ten labels for a given image. I refer to them as MRF models because the formulas for MRF classifiers are used, in which each of the ten outputs is a weighted sum of energy functions, and also because the frames of discernment from Section 4.2 do form a graph structure for MRF. Trainable weight parameters $w_1, \ldots, w_{46}$ replace NBR’s $b_1, \ldots, b_{46}$. For each of the three models, the $s_i$ and $w_i$ parameters are re-trained. There are two choices of energy functions: MRF #1 and MRF #1+ use $-\text{sigmoid}(s_i \cdot G_i(\text{image}))$, $i \in \{1, \ldots, 46\}$, as energy functions, while MRF #2 uses $-\log(\text{sigmoid}(s_i \cdot G_i(\text{image})))$. The difference between MRF #1 and MRF #1+ is that a step is added in MRF #1+ that mimics Dempster-style scaling: the energy values from each energy function are scaled up as discussed in Section 4.1 and the corresponding $w_i$ is scaled down by the same factor; these operations have effects on the weighted sums of energy functions because the energy values within each frame of discernment are scaled while those outside the frames remain at value -1. Although MRF #2 is more intuitive as the log scale gives zero energy to the correct label in an ideal scenario, it performs worse than MRF #1 and MRF #1+.

- The last three rows are classifiers that apply Gaussian naive Bayes on the 46 features from the NBR classifier. There are two choices of features: Gaussian naive Bayes #1 and #1+ use $\text{sigmoid}(s_i \cdot G_i(\text{image}))$, $i \in \{1, \ldots, 46\}$, as features, while Gaussian naive Bayes #2 uses $G_i(\text{image})$. The difference between Gaussian naive Bayes #1 and #1+ is that a step is added in #1+ that mimics Dempster-style scaling: the feature values are scaled up as discussed in Section 4.1; note that there is no corresponding operation to the scaling of $b_i$’s in an NBR classifier or the scaling of $w_i$’s in MRF #1+.

Among the seven ablation-study models, MRF #1+ is the clear winner. In fact, it can be viewed as a poor man’s NBR classifier: it contains the same L2NNNs and a step that mimics Dempster-style scaling, yet it replaces the top-level belief-function operations with weighted sums. The effect is that it reduces computational complexity at the cost of accuracy and robustness.