Improving Certified Robustness via Statistical Learning with Logical Reasoning

Abstract

Intensive algorithmic efforts have been made to enable the rapid improvements of certificated robustness for complex ML models recently. However, current robustness certification methods are only able to certify under a limited perturbation radius. Given that existing *pure data-driven* statistical approaches have reached a bottleneck, in this paper, we propose to integrate statistical ML models with knowledge (expressed as logical rules) as a *reasoning* component using Markov logic networks (MLN), so as to further improve the overall certified robustness. This opens new research questions about certifying the robustness of such a paradigm, especially the reasoning component (e.g., MLN). As the first step towards understanding these questions, we first prove that the computational complexity of certifying the robustness of MLN is #P-hard. Guided by this hardness result, we then derive the first certified robustness bound for MLN by carefully analyzing different model regimes. Finally, we conduct extensive experiments on five datasets including both high-dimensional images and natural language texts, and we show that the certified robustness with knowledge-based logical reasoning indeed significantly outperforms that of the state-of-the-arts.

1 Introduction

Given extensive studies on adversarial attacks against ML models recently [3, 13, 38, 24, 59, 23, 51], building models that are robust against such attacks is an important and emerging topic. Thus, a plethora of *empirical defenses* have been proposed to improve the ML robustness [29, 56, 22, 42]; however, most of these are attacked again by stronger adaptive attacks [3, 1, 45]. To end such repeated security cat-and-mouse games, there is a line of research focusing on developing *certified defenses* for DNNs under certain adversarial constraints [8, 26, 25, 52, 27].

Though promising, existing *certified defenses* are restricted to certifying the model robustness within a limited ℓ_p norm bounded perturbation radius [54, 8]. One potential reason for such limitations for existing robust learning approaches is inherent in the fact that most of them have been treating machine learning as a "pure data-driven" technique that solely depends on a given training set, without interacting with the rich exogenous information such as domain knowledge (e.g., *a stop sign should be of the octagon shape*); while we know human, who has knowledge and inference abilities, is resilient to such attacks. Indeed, a recent seminal work [17] illustrates that integrating knowledge rules can significantly improve the *empirical* robustness of ML models, while leaving the *certified robustness* completely unexplored.

In this paper, we follow this promising `Learning+Reasoning` paradigm [17] and conduct, to our best knowledge, the first study on certified robustness for it. Actually, such a `Learning+Reasoning` paradigm has enabled a diverse range of applications [37, 57, 2, 36, 31, 53, 17] including the ECCV'14 best paper [10] that encodes label relationships as a probabilistic graphical model and improves the *empirical* performance of deep neural networks on ImageNet. In this work, we first provide a concrete

Sensing-reasoning pipeline following such paradigm to integrate statistical learning with logical reasoning as illustrated in Figure 1. In particular, the *Sensing Component* contains a set of statistical ML models such as deep neural networks (DNNs) that output their predictions as a set of Boolean random variables; and the *Reasoning Component* takes this set of Boolean random variables as inputs for logical inference models such as Markov logic networks (MLN) [39] or Bayesian networks (BN) [35] to produce the final output. We then prove the hardness of certifying the robustness of such a pipeline with MLN as the reasoning component. Finally, we provide an effective algorithm to certify the robustness of sensing-reasoning pipeline and we evaluate it on five datasets including both image and text data.

However, certifying the robustness of sensing-reasoning pipeline is challenging, especially given the inference complexity of the reasoning component. Our goal is to take the first step in tackling this challenge. In particular, the robustness certification of sensing-reasoning pipeline can be expressed as the confidence interval of the marginal probability for the final output of *reasoning component*. That is to say, we can use existing state-of-the-art methods to certify the robustness of the sensing component that contains DNNs or ensem-

Figure 1: The sensing-reasoning pipeline, i.e., a *sensing component* consists of DNNs and a *reasoning component* is constructed as MLN. The goal of this paper is to provide certified robustness for such a pipeline, especially the reasoning component.

bles [8, 41, 55]. Thus, to provide the end-to-end certification for the whole pipeline, what is left is to understand *how to certify the reasoning component*, which is the focus of this work.

Compared with previous efforts focusing on certified robustness of neural networks, the reasoning component brings its own challenges and opportunities. Different from a neural network whose inference can be executed in polynomial time, many reasoning models such as MLN can be #P-complete for inference. However, as many reasoning models define a probability distribution in the exponential family, we have more functional structures that could potentially make the robustness optimization (which essentially solves a min-max problem) easier. *In this paper, we provide the first treatment to this problem characterized by these unique challenges and opportunities.*

We focus on MLN as the *reasoning component*, and explored three technical questions, each of which corresponds to a technical contribution of this work.

1. Is certifying robustness for the reasoning component feasible when the inference of the reasoning component is #P-hard? (Section 3) Before any concrete algorithm can be proposed, it is important to understand the computational complexity of the robustness certification. We first prove that the famous problem of counting in statistical inference [48] can be reduced to the problem of checking the certified robustness of general reasoning components and MLN. Therefore, checking certified robustness is no easier than counting on the same family of distribution. In other words, when the reasoning component is a graphical model such as MLN, checking certified robustness is no easier than calculating the partition function of the underlying graphical model, which is #P-hard.

2. Can we efficiently reason about the certified robustness for the reasoning component when given an oracle for statistical inference? (Section 4.2) Given the above hardness result, we focus on certifying the robustness given an inference oracle. However, even when statistical inference can be done by a given oracle [21, 18], it is still challenging to certify the robustness of MLN. Our second technical contribution is to develop such an algorithm for MLN as the reasoning component. We prove that providing certified robustness for MLN is possible because of the structure inherent in the probabilistic graphical models and distributions in the exponential family, which could lead to monotonicity and convexity properties under certain conditions for solving the certification optimization.

3. Can a reasoning component improve the certified robustness compared with the state-of-the-art certification methods? (Section 5) We test our algorithms on multiple sensing-reasoning pipelines, in which the sensing components contain the state-of-the-art *deep neural networks*. We construct these pipelines to cover a range of applications including image classification and natural language processing tasks. We show that based on our certification method on the reasoning component, the

knowledge-enriched sensing-reasoning pipelines achieves significantly higher certified robustness
than the state-of-the-art certification methods for DNNs.

2 Robust Statistical Learning with Logical Reasoning

In this section, we first provide a sensing-reasoning pipeline and then formally defined its certified
robustness, and particularly links it to certifying the robustness for the reasoning component.

2.1 Sensing-Reasoning Pipeline

A sensing-reasoning pipeline contains a set of n
sensors $\{S_i\}_{i\in[n]}$ and a reasoning component R.
Each sensor is a binary classifier (for multi-class
classifier it corresponds to a group of sensors) —
given an input data example X, each of the sen-
sor S_i outputs a probability $p_i(X)$ (i.e., if S_i is a
neural network, $p_i(X)$ represents its output after
the final softmax layer). The reasoning compo-
nent takes the outputs of all sensing models as
its inputs, and outputs a new Boolean random
variable $R(\{p_i(X)\}_{i\in[n]})$.

Figure 2: A sensing-reasoning pipeline with MLN as
the reasoning component.

One natural choice of the reasoning component is to use a probabilistic graphical model (PGM). In
the following subsection, we will make the reasoning component R more concrete by instantiating
it as a Markov logic network (MLN). The output of a sensing-reasoning pipeline on the input data
example X is the expectation of the output of reasoning component R: $\mathbb{E}[R(\{p_i(X)\}_{i\in[n]})]$.

Example. A sensing-reasoning pipeline provides a generic, principled way of integrating domain
knowledge with the output of statistical predictive models such as neural networks. One such example
is [10] the task of ImageNet classification. Here each sensing model corresponds to the classifier
for one specific class in ImageNet, e.g., $S_{dog}(X)$ and $S_{animal}(X)$. The reasoning component then
encodes domain knowledge such that "*If an image is classified as a dog then it must also be classified
as an animal*" using a PGM. There is no prior work considering the certified robustness of such a
knowledge-enabled ML pipeline. Figure 2 illustrates a concrete sensing-reasoning pipeline, in which
the reasoning component is implemented as an MLN.

2.2 Reasoning Component as Markov Logic Networks

Given the generic definition of a sensing-reasoning pipeline, one can use different models to imple-
ment the reasoning components. In this paper, we focus on Markov logic networks (MLN), which is
a popular way to define a probabilistic graphical model using first-order logic [40]. Concretely, we
define the reasoning component implemented as an MLN, which contains a set of weighted first-order
logic rules, as illustrated in Figure 2(b). After grounding, an MLN defines a joint probabilistic
distribution among a collection of random variables, as illustrated in Figure 2(c). We adapt the
standard MLN semantics to a sensing-reasoning pipeline and use a slightly more general variant
compared with the original MLN [40]. Each MLN program corresponds to a factor graph — Due to
the space limitation, we will not discuss the grounding part and point the readers to [40]. We focus
on defining the result after grounding, i.e., the factor graph.

Specifically, a grounded MLN is a factor graph $\mathcal{G} = (\mathcal{V}, \mathcal{F})$, where $\mathcal{V}$ is a set of Boolean random
variables. Specific to a sensing-reasoning pipeline, there are two types of random variables $\mathcal{V} = \mathcal{X} \cup \mathcal{Y}$:

1. **Interface Variables** $\mathcal{X} = \{x_i\}_{i\in[n]}$: Each sensing model S_i corresponds to one interface
   variable x_i in the grounded factor graph;

2. **Interior variables** $\mathcal{Y} = \{y_i\}_{i\in[m]}$ are other variables introduced by the MLN model.

Each factor $F \in \mathcal{F}$ contains a weight w_F and a factor function f_F defined over a subset of variables
$\bar{\mathbf{v}}_F \subseteq \mathcal{V}$ that *returns* $\{0, 1\}$. There are two sets of factors $\mathcal{F} = \mathcal{G} \cup \mathcal{H}$:

1. **Interface Factors** $\mathcal{G}$: For each interface variable x_i, we create one interface factor G_i with
   weight $w_{G_i} = \log[p_i(X)/(1 - p_i(X))]$ and factor function $f_{G_i}(a) = \mathcal{I}[a = 1]$ defined
   over $\bar{\mathbf{v}}_{f_{G_i}} = \{x_i\}$.

2. **Interior Factors** $\mathcal{H}$ are other factors introduced by the MLN program.

Remarks: MLN-specific Structure. Our result applies to a more general family of factor graphs and
are not necessarily specific to those grounded by MLN. Moreover, MLN provides an intuitive way of

grounding such a factor graph with domain knowledge, and factor graphs grounded by MLN have certain properties that we will use later, e.g., all factors only return non-negative values, and there are no unusual weight sharing structures.

The above factor graph defines a joint probability distribution among all variables $\mathcal{V}$. We define a *possible world* as a function $\sigma : \mathcal{V} \mapsto \{0, 1\}$ that corresponds to one possible assignment of values to each random variable. Let Σ denote the set of all (exponentially many) possible worlds.

The *statistical inference* process of a reasoning component implemented using MLNs [40] computes the marginal probability of a given variable $v \in \mathcal{V}$:

$$\mathbb{E}[R_{MLN}(\{p_i(X)\}_{i\in[n]})] = \mathbf{Pr}\,[v = 1] = Z_1(\{p_i(X)\}_{i\in[n]})/Z_2(\{p_i(X)\}_{i\in[n]})$$

where the partition functions Z_1 and Z_2 are defined as

$$Z_1(\{p_i(X)\}_{i\in[n]}) = \sum_{\sigma\in\Sigma\wedge\sigma(v)=1} \exp\left\{\sum_{G_i\in\mathcal{G}} w_{G_i}\sigma(x_i) + \sum_{H\in\mathcal{H}} w_H f_H(\sigma(\bar{\mathbf{v}}_H))\right\}$$

$$Z_2(\{p_i(X)\}_{i\in[n]}) = \sum_{\sigma\in\Sigma} \exp\left\{\sum_{G_i\in\mathcal{G}} w_{G_i}\sigma(x_i) + \sum_{H\in\mathcal{H}} w_H f_H(\sigma(\bar{\mathbf{v}}_H))\right\}$$

Why $w_{G_i} = \log[p_i(X)/(1 - p_i(X))]$? When the MLN does not introduce any interior variables and interior factors, it is easy to see that setting $w_{G_i} = \log[p_i(X)/(1 - p_i(X))]$ ensures that the marginal probability of each interface variable equals to the output of the original sensing model $p_i(X)$. This means that if we do not have additional knowledge in the reasoning component, the pipeline outputs the *same* distribution as the original sensing component.

Learning Weights for Interior Factors? In this paper, we view all weights for interior factors as hyperparameters. These weights can be learned by maximizing the likelihood with weight learning algorithms for MLNs [28].

Beyond Marginal Probability for a Single Variable. We have assumed that the output of a sensing-reasoning pipeline is the marginal probability distribution of a given random variable in the grounded factor graph. However, our result can be more general — given a function over possible worlds and outputs $\{0, 1\}$, the output of a pipeline can be the marginal probability of such a function. This will not change the algorithm that we propose later.

3 Hardness of Certifying Reasoning Robustness

Given a reasoning component R, how hard is it to reason about its robustness? In this section, we aim at understanding this fundamental question. In order to provide the certified robustness of the reasoning component, which is defined as the lower bound of model prediction accuracy for inputs considering an adversarial perturbation with bounded magnitude [8], we need to analyze the hardness of this certification problem first. Specifically, we present the hardness results of determining the robustness of the reasoning component defined above, before we can provide our certification algorithm in Section 4.2. We start by defining the counting [48] and robustness problems on general distribution. We prove that counting can be reduced to checking for reasoning robustness, and hence the latter is at least as hard; We then prove the complexities of reasoning with MLN.

3.1 Harness of Certifying General Reasoning Model

Let $X = \{x_1, x_2, \ldots, x_n\}$ be a set of variables. Let π_α be a distribution over $D^{[n]}$ defined by a set of parameters $\alpha \in P^{[m]}$, where D is the domain of variables, either discrete or continuous, and P is the domain of parameters. We call π *accessible* if for any $\sigma \in D^{[n]}$, $\pi_\alpha(\sigma) \propto w(\sigma; \alpha)$, where $w : D^{[n]} \times P^{[m]} \to \mathbb{R}_{\geq 0}$ is a polynomial-time computable function. We will restrict our attention to accessible distributions only. We use $Q : D^{[n]} \to \{0, 1\}$ to denote a Boolean query, which is a polynomial-time computable function. We define the following two oracles:

Definition 1 (COUNTING)**.** Given input polynomial-time computable weight function $w(\cdot)$ and query function $Q(\cdot)$, parameters α, a real number $\epsilon > 0$, a COUNTING oracle outputs a real number Z that

$$1 - \epsilon \leq \frac{Z}{\mathbb{E}[\sigma \sim \pi_\alpha]Q(\sigma)} \leq 1 + \epsilon.$$

Definition 2 (ROBUSTNESS). Given input polynomial-time computable weight function $w(\cdot)$ and query function $Q(\cdot)$, parameters α, two real numbers $\epsilon > 0$ and $\delta > 0$, a ROBUSTNESS oracle decides, for any $\alpha' \in P^{[m]}$ such that $\|\alpha - \alpha'\|_\infty \leq \epsilon$, whether the following is true:

$$|\mathbb{E}[\sigma \sim \pi_\alpha]Q(\sigma) - \mathbb{E}[\sigma \sim \pi_{\alpha'}]Q(\sigma)| < \delta.$$

We can prove that ROBUSTNESS is at least as hard as COUNTING by a reduction argument.

Theorem 1 (COUNTING $\leq_t$ ROBUSTNESS). *Given polynomial-time computable weight function $w(\cdot)$ and query function $Q(\cdot)$, parameters α and real number $\epsilon > 0$, the instance of* COUNTING, (w, Q, α, ϵ) *can be determined by up to $O(1/\varepsilon_c^2)$ queries of the* ROBUSTNESS *oracle with input perturbation $\epsilon = O(\varepsilon_c)$.*

Proof-sketch. We define the partition function $Z_i := \sum_{\sigma:Q(\sigma)=i} w(\sigma; \alpha)$ and $\mathbb{E}[\sigma \sim \pi_\alpha]Q(\sigma) = Z_1/(Z_0 + Z_1)$. We then construct a new weight function $t(\sigma; \alpha) := w(\sigma; \alpha)\exp(\beta Q(\sigma))$ by introducing an additional parameter β, such that $\tau_\beta(\sigma) \propto t(\sigma; \beta)$, and $\mathbb{E}[\sigma \sim \tau_\beta]Q(\sigma) = \frac{e^\beta Z_1}{Z_0 + e^\beta Z_1}$. Then we consider the perturbation $\beta' = \beta \pm \epsilon$, with $\epsilon = O(\varepsilon_c)$ and query the ROBUSTNESS oracle with input $(t, Q, \beta, \epsilon, \delta)$ multiple times to perform a binary search in δ to estimate $|\mathbb{E}[\sigma \sim \pi_\beta]Q(\sigma) - \mathbb{E}[\sigma \sim \pi_{\beta'}]Q(\sigma)|$. Perform a further "outer" binary search to find the β which maximizes the perturbation. This yields a good estimator for $\log \frac{Z_0}{Z_1}$ which in turn gives $\mathbb{E}[\sigma \sim \pi_\alpha]Q(\sigma)$ with ε_c multiplicative error. We leave detailed proof to Appendix A.

3.2 Hardness of Certifying Markov Logic Networks

Given Theorem 1, we can now state the following result specifically for MLNs:

Theorem 2 (MLN Hardness). *Given an MLN whose grounded factor graph is $\mathcal{G} = (\mathcal{V}, \mathcal{F})$ in which the weights for interface factors are $w_{G_i} = \log p_i(X)/(1 - p_i(X))$ and constant thresholds $\delta, \{C_i\}_{i \in [n]}$, deciding whether*

$$\forall\{\epsilon_i\}_{i \in [n]} \quad (\forall i. |\epsilon_i| < C_i) \implies |\mathbb{E}R_{MLN}(\{p_i(X)\}_{i \in [n]}) - \mathbb{E}R_{MLN}(\{p_i(X) + \epsilon_i\}_{i \in [n]})| < \delta$$

is as hard as estimating $\mathbb{E}R_{MLN}(\{p_i(X)\}_{i \in [n]})$ up to ε_c multiplicative error, with $\epsilon_i = O(\varepsilon_c)$.

Proof. Let $\alpha = [p_i(X)]$, query function $Q(.) = R_{MLN}(.)$ and π_α defined by the marginal distribution over interior variables of MLN. Theorem 1 directly implies that $O(1/\varepsilon_c^2)$ queries of a ROBUSTNESS oracle can be used to efficiently estimate $\mathbb{E}R_{MLN}(\{p_i(X)\}_{i \in [n]})$. $\square$

In general, statistical inference in MLNs is #P-complete, and checking robustness for general MLNs is also #P-hard.

4 Certifying the Robustness of Sensing-Reasoning Pipeline

Given a sensing-reasoning pipeline with n sensors $\{S_i\}_{i \in [n]}$ and a reasoning component R, we will first formally define its end-to-end certified robustness and then its connection to the robustness of each component. Finally, based on the above hardness result for *certifying reasoning robustness* in Section 3, we will provide an effective certification method for the reasoning component by making oracle assumption for the inference of reasoning component, which will lead to the final certification of the sensing-reasoning pipeline combined with sensing certification.

Definition 3 $((C_I, C_E, p)$-robustness). A sensing-reasoning pipeline with n sensors $\{S_i\}_{i \in [n]}$ and a reasoning component R is (C_I, C_E, p)-robust on the input X, if for input perturbation $\eta, \|\eta\|_p \leq C_I$

$$\left|\mathbb{E}[R(\{p_i(X)\}_{i \in [n]})] - \mathbb{E}[R(\{p_i(X + \eta)\}_{i \in [n]})]\right| \leq C_E.$$

I.e., a perturbation $\|\eta\|_p < C_I$ on the input only changes the final pipeline output by at most C_E.

Sensing Robustness and Reasoning Robustness. We decompose the end-to-end certified robustness of the pipeline into two components. The first component, which we call the *sensing robustness*, has been studied by the research community recently [20, 44, 8] — given a perturbation $\|\eta\|_p < C_I$ on the input X, we say each sensor S_i is $(C_I, C_S^{(i)}, p)$-robust if

$$\forall\eta, \|\eta\|_p \leq C_I \implies |p_i(X) - p_i(X + \eta)| \leq C_S^{(i)}$$

The robustness of the *reasoning component* R is defined as: Given a perturbation $|\epsilon_i| < C_S^{(i)}$ on the output of each sensor $S_i(X)$, we say the reasoning component R is $\left(\{C_S^{(i)}\}_{i \in [n]}, C_E\right)$-robust if

$$\forall\epsilon_1, ..., \epsilon_n, (\forall i. |\epsilon_i| \leq C_S^{(i)}) \implies \left|\mathbb{E}[R(\{p_i(X)\}_{i \in [n]})] - \mathbb{E}[R(\{p_i(X) + \epsilon_i\}_{i \in [n]})]\right| \leq C_E.$$

It is easy to see that when the sensing component is $\left(C_I, \{C_S^{(i)}\}_{i\in[n]}, p\right)$-robust and the reasoning component is $\left(\{C_S^{(i)}\}_{i\in[n]}, C_E\right)$-robust on X, the sensing-reasoning pipeline is (C_I, C_E, p)-robust. Since the sensing robustness has been intensively studied by previous work, in this paper, we mainly focus on the reasoning robustness and therefore analyze the robustness of the pipeline.

4.1 Certifying Sensing Robustness

There are several existing ways to certify the robustness of sensing models, such as Interval Bound Propagation (IBP) [16], Randomized Smoothing [8], and others [58, 50]. Here we will leverage randomized smoothing to provide an example for certifying the robustness of sensing components.

Corollary 1. *Given a sensing model S_i, we construct a smoothed sensing model $g_i(X; \hat{\sigma}) = \mathbb{E}_{\xi\sim\mathcal{N}(0,\hat{\sigma}^2)}p_i(X + \xi)$. With input perturbation $||\eta||_2 \leq C_I$, the smoothed sensing model satisfies*

$$\Phi(\Phi^{-1}(g_i(X;\hat{\sigma})) - C_I/\hat{\sigma}) \leq g_i(X + \eta; \hat{\sigma}) \leq \Phi(\Phi^{-1}(g_i(X;\hat{\sigma})) + C_I/\hat{\sigma})$$

where Φ is the Gaussian CDF and Φ^{-1} as its inverse.

Thus, the output probability of smoothed sensing model can be bounded given input perturbations. Note that the specific ways of certifying sensing robustness is orthogonal to certifying reasoning robustness, and one can plug in different sensing certification strategies.

4.2 Certifying Reasoning Robustness

Given the hardness results for certifying reasoning robustness in Section 3.2, in this paper, we assume that we have access to an oracle for statistical inference, and provide a novel algorithm to certify the reasoning robustness. I.e., we assume that we are able to calculate the two partition functions $Z_1(\{p_i(X)\}_{i\in[n]})$ and $Z_2(\{p_i(X)\}_{i\in[n]})$.

Lemma 4.1 (MLN Robustness). *Given access to partition functions $Z_1(\{p_i(X)\}_{i\in[n]})$ and $Z_2(\{p_i(X)\}_{i\in[n]})$, and maximum perturbations $\{C_i\}_{i\in[n]}$, $\forall \epsilon_1, ..., \epsilon_n$, if $\forall i. |\epsilon_i| < C_i$, we have that $\forall \lambda_1, ..., \lambda_n \in \mathbb{R}$,*

Algorithm 1 Algorithms for MLN robustness upper bound (algorithm of lower bound is similar)

input : Oracles calculating $\widetilde{Z_1}$ and $\widetilde{Z_2}$; maximal perturbations $\{C_i\}_{i\in[n]}$.
output : An upper bound for input $R_{MLN}(\{p_i(X) + \epsilon_i\})$

1: $\overline{R}_{min} \leftarrow 1$
2: initialize λ
3: **for** $b \in$ search budgets **do**
4: $\quad \lambda \rightarrow$ update$(\{\lambda\}; \lambda_i \in (-\infty, -1] \cup [0, +\infty))$
5: $\quad$ **for** $i = 1$ **to** n **do**
6: $\quad\quad$ **if** $\lambda_i \geq 0$ **then**
7: $\quad\quad\quad \epsilon_i = C_i, \epsilon_i' = -C_i$
8: $\quad\quad$ **else if** $\lambda_i \leq -1$ **then**
9: $\quad\quad\quad \epsilon_i = -C_i, \epsilon_i' = C_i$
10: $\quad\quad$ **end if**
11: $\quad\quad \overline{R} \leftarrow \widetilde{Z_1}(\{\epsilon_i\}_{i\in[n]}) - \widetilde{Z_2}(\{\epsilon_i'\}_{i\in[n]})$
12: $\quad\quad \overline{R}_{min} \leftarrow \min(\overline{R}_{min}, \overline{R})$
13: $\quad$ **end for**
14: **end for**
15: **return** $\overline{R}_{min}$

$$\max_{\{|\epsilon_i|<C_i\}} \ln \mathbb{E}[R_{MLN}(\{p_i(X) + \epsilon_i\}_{i\in[n]})] \leq \max_{\{|\epsilon_i|<C_i\}} \widetilde{Z_1}(\{\epsilon_i\}_{i\in[n]}) - \min_{\{|\epsilon_i'|<C_i\}} \widetilde{Z_2}(\{\epsilon_i'\}_{i\in[n]})$$

$$\min_{\{|\epsilon_i|<C_i\}} \ln \mathbb{E}[R_{MLN}(\{p_i(X) + \epsilon_i\}_{i\in[n]})] \geq \min_{\{|\epsilon_i|<C_i\}} \widetilde{Z_1}(\{\epsilon_i\}_{i\in[n]}) - \max_{\{|\epsilon_i'|<C_i\}} \widetilde{Z_2}(\{\epsilon_i'\}_{i\in[n]})$$

where

$$\widetilde{Z_r}(\{\epsilon_i\}_{i\in[n]}) = \ln Z_r(\{p_i(X) + \epsilon_i\}_{i\in[n]}) + \sum_i \lambda_i \epsilon_i.$$

We leave the proof to the Appendix B. The high-level proof idea is to decouple Z_1/Z_2 into two sub-problems via a collection of Lagrangian multipliers, i.e., $\{\lambda_i\}$. For any assignment of $\{\lambda_i\}$, we obtain a valid upper/lower bound, which reduces the certification process to the process of *searching* for an assignment of these multipliers that minimize the upper bound (maximize the lower bound).

To efficiently search for the optimal assignment of $\{\lambda_i\}$, it is crucial to consider the interactions between these $\{\lambda_i\}$ and the corresponding solution of $\widetilde{Z_r}$, which hinges on the structure of MLN. In particular, we can prove the following (Detailed proofs and discussions in Appendix C):

Proposition 1 (Monotonicity). *When $\lambda_i \geq 0$, $\widetilde{Z_r}(\{\epsilon_i\}_{i\in[n]})$ monotonically increases w.r.t. ϵ_i; When $\lambda_i \leq -1$, $\widetilde{Z_r}(\{\epsilon_i\}_{i\in[n]})$ monotonically decreases w.r.t. ϵ_i.*

Proposition 2 (Convexity). *$\widetilde{Z_r}(\{\tilde{\epsilon}_i\}_{i\in[n]})$ is a convex function in $\tilde{\epsilon}_i$, $\forall i$ with*

$$\tilde{\epsilon}_i = \log\left[\frac{(1 - p_i(X))(p_i(X) + \epsilon_i)}{p_i(X)(1 - p_i(X) - \epsilon_i)}\right].$$

274 *Implication.* Given the monotonicity region, the maximal and minimal of $\widetilde{Z_r}$ are achieved at
275 either $\epsilon_i = -C_i$ or $\epsilon_i = C_i$ respectively. Given the convexity region, the maximal is achieved
276 at $\epsilon_i \in \{-C_i, C_i\}$, and the minimal is achieved at $\epsilon_i \in \{-C_i, C_i\}$ or at the zero gradient of
277 $\widetilde{Z_r}(\{\tilde{\epsilon}_i\}_{i \in [n]})$. As a result, our analysis leads to the following certification algorithm.

Algorithm of Certifying Reasoning Robustness. Algorithm 1 illustrates the detailed algorithm
279 based on the above result to upper bound the robustness of MLN. The main step is to explore different
280 regimes of the $\{\lambda_i\}$. In this paper, we only explore regimes where $\lambda \in (-\infty, -1] \cup [0, +\infty)$ as
281 this already provides reasonable solutions in our experiments. The function $\texttt{update}(\{\lambda_i\})$ defines
282 the exploration strategy — Depending on the scale of the problem, one can explore $\{\lambda_i\}$ using grid
283 search, random sampling, or even gradient-based methods. For experiments in this paper, we use
284 either grid search or random sampling. It is an exciting future direction to understand other efficient
285 exploration and search strategies. We leave the detailed explanation of the algorithm to Appendix C.

5 Experiments

287 We conduct intensive experiments on five datasets to evaluate the certified robustness of the sensing-
288 reasoning pipeline. We focus on two tasks with different modalities: *image classification* task on
289 Road Sign dataset created based on GTSRB dataset [43] following the standard setting as [17];
290 and *information extraction* task with stocks news on text data. We also report additional results on
291 two other image classification tasks (Word50 [6] and PrimateNet, which is a subset of ImageNet
292 ILSVRC2012 [9]) with natural knowledge rules in Appendix G and Appendix F. We also report
293 results on standard image benchmarks (MNIST and CIFAR10) with manually constructed knowl-
294 edge rules in Appendix H. The code is provided at $\texttt{https://github.com/Sensing-Reasoning/}$
295 $\texttt{Sensing-Reasoning-Pipeline}$.

5.1 Experimental Setup

Datasets and Tasks. For the *road sign classification* task, we follow [17] and use the same dataset
298 GTSRB [43], which contains 12 types of German road signs {"Stop", "Priority Road", "Yield",
299 "Construction Area", "Keep Right", "Turn Left", "Do not Enter", "No Vihicles", "Speed Limit 20",
300 "Speed Limit 50", "Speed Limit 120", "End of Previous Limitation"}. It consists of 14880 training
301 samples, 972 validation samples, and 3888 testing samples. We also include 13 additional detectors
302 for knowledge integration, detecting attributes such as whether the border has an octagon shape (See
303 Appendix D for a full list).

304 For the *information extraction* task, we use the HighTech dataset which consists of both daily closing
305 asset price and financial news from *2006* to *2013* [12]. We choose 9 companies with the most news,
306 resulting in 4810 articles related to 9 stocks filtered by company name. We split the dataset into
307 training and testing days chronologically. We define three information extraction tasks as our
308 sensing models: $\texttt{StockPrice(Day, Company, Price)}$, $\texttt{StockPriceChange(Day, Company,}$
309 $\texttt{Percent)}$, $\texttt{StockPriceGain(Day, Company)}$. The domain knowledge that we integrate depicts
310 the relationships between these relations (See Appendix E for more details).

Knowledge Rules. We integrate different types of knowledge rules for these two applications. We
312 provide the full list of knowledge rules in the Appendix D.

313 For *road sign classification*, we follow [17], which includes two different types of knowledge rules —
314 *Indication rules* (road sign class u indicates attribute v) and *Exclusion rules* (attribute classes u and v
315 with the same general type such as "Shape", "Color", "Digit" or "Content" are naturally exclusive).

316 For *information extraction*, we integrate knowledge about the relationships between the sensing mod-
317 els (e.g., $\texttt{StockPrice}$, $\texttt{StockPriceChange}$, $\texttt{StockPriceGain}$). For example, the stock prices
318 of two consecutive days, $\texttt{StockPrice}(d_1, Company, p_1)$ and $\texttt{StockPrice}(d_2, Company, p_2)$,
319 should be consistent with $\texttt{StockPriceChange}(d_2, Company, p)$, i.e., $p = (p_2 - p_1)/p_1$.

Implementation Details. Throughout the road sign classification experiment, we implement all
321 sensing models using the GTSRB-CNN [13] architecture. During training, we train all sensors with
322 Isotropic Gaussian $\epsilon \sim \mathcal{N}(0, \hat{\sigma}^2 I_d)$ augmented data with 50000 training iterations until converge and
323 tune the training parameters on the validation set, following [8]. We use the SGD-momentum with
324 the initial learning rate as 0.01 and the weight decay parameter as 10^{-4} to train all the sensors for
325 50000 iterations with 200 as the batch size, following [17]. During certification, we adopt the same
326 smoothing parameter for training to construct the smoothed model based on Monte-Carlo sampling.

327 For information extraction, we use BERT as our model architecture. During training, we use the
328 final hidden state of the first token [CLS] from BERT as the representation of the whole input and

Table 1: (**Road sign classification**) *Certified accuracy* under different input perturbation magnitudes (C_I). Models are smoothed with different Gaussian noises $\epsilon \sim \mathcal{N}(0, \hat{\sigma}^2 I_d), \hat{\sigma} \in \{0.12, 0.25, 0.50\}$. Rows with $*$ denote the best certified accuracy among all the smoothing parameters for each method. The bold numbers show the higher certified accuracy under the same $(C_I, \hat{\sigma})$ setting and the numbers with underline show the highest certified accuracy for each C_I among different smoothing parameters. (All certificates hold with 99.9% confidence)

Methods	$\hat{\sigma}$	$C_I = 0.12$	$C_I = 0.25$	$C_I = 0.50$	$C_I = 1.00$
Vanilla Smoothing (w/o knowledge)	0.12	90.8	87.1	0.0	0.0
	0.25	89.6	88.4	71.6	0.0
	0.50	84.0	80.2	73.2	61.7
	$*$	90.8	88.4	73.2	61.7
Sensing-Reasoning Pipeline (w/ knowledge)	0.12	**96.0**	**89.0**	**73.2**	**24.2**
	0.25	**93.4**	**91.0**	**74.0**	**49.2**
	0.50	**89.3**	**85.4**	**75.5**	**62.5**
	$*$	**96.0**	**91.0**	**75.5**	**62.5**

apply dropout with probability $p = 0.5$ on this final hidden state. Additionally, there is a fully connected layer added on top of BERT for classification. To fine-tune the BERT classifiers for three information tasks, we use the Adam optimizer with the initial learning rate as 10^{-5} and the weight decay parameter as 10^{-4}. We train all the sensors for 30 epochs, and the batch size 32.

Evaluation Metrics. We adopt the standard *certified accuracy* as our evaluation metric, defined by the percentage of instances that can be certified under certain ℓ_p-norm bounded perturbations. Specifically, given the input x with ground-truth label y, once we can certify the bound of the model's output confidence on predicting label y under the norm-bounded perturbation as $[\mathcal{L}, \mathcal{U}]$, the certified accuracy can be defined by: $\frac{1}{N} \sum_{i=1}^{N} \mathbb{I}([\mathcal{L}_i > 0.5])$ where $\mathbb{I}(\cdot)$ denotes the indicator function. Since each sensing component's certification is performed by randomized smoothing, which yields the failure probability characterized by ζ_0, we will control the failure probability ζ for the whole sensing-reasoning pipeline pipeline with n sensing models as $\zeta_0 = 1 - (1 - \zeta)^{1/n}$ by applying the union bound. Throughout all the experiments, ζ is kept to 0.001 so our end-to-end certification is guaranteed to be correct with at least 99.9% confidence.

5.2 Results of *Road Sign Classification*

In this section, we evaluate the certified robustness of our sensing-reasoning pipeline under the ℓ_2-norm bounded perturbation. We first report the ℓ_2 certified accuracy of our sensing-reasoning pipeline and compare it to a strong baseline as a vanilla randomized smoothing trained model (without knowledge). Note that it is flexible to replace the sensing component with other robust training algorithms. We conduct our evaluation under different smoothing parameters $\hat{\sigma} = \{0.12, 0.25, 0.50\}$ and various ℓ_2 perturbation magnitudes on the input image $C_I = \{0.12, 0.25, 0.50, 1.00\}$ (Table 1). During certification, we evaluate our certification time per sample with 25 sensors as 5.39s, which shows that the overall certification time is generally acceptable.

As shown in Table 1, we can see that with knowledge integration, sensing-reasoning pipeline achieves consistently higher certified accuracy compared to the baseline smoothed ML model without knowledge under all the perturbation magnitudes C_I and smoothing parameter $\hat{\sigma}$ settings. Under the small perturbation magnitude cases, our improvement is very significant (around 5%). More interestingly, given large C_I but small smoothing parameter $\hat{\sigma}$, vanilla randomized smoothing-based certification directly fails (0% certified accuracy) due to the looseness of the hypothesis testing bound, while the sensing-reasoning pipeline could still achieve reasonable certified robustness (over 71% on $C_I = 0.50$, 49% on $C_I = 1.00$) under the same $(C_I, \hat{\sigma})$ settings. This indicates a very realistic case: we always **under-estimate** the attacker's ability easily under the real-world setting – in this case, the sensing-reasoning pipeline could remain robust even provide reasonable certified accuracy with a conservative smoothing parameter.

5.3 Results of *Information Extraction*

In this section, we conduct the certified robustness evaluation on the information extraction task on text data. Since there is no good certification method on discrete NLP data for sensing models, we directly assume the maximal perturbation on the output of sensors (C_S). Table 2 shows the certified accuracy on the final outputs of the reasoning component. We see that the sensing-reasoning pipeline provides significantly higher certified robustness, and even under a high perturbation magnitude on all sensing models' output confidence ($C_S = 0.5$), which means the sensing-reasoning pipeline can still leverage the knowledge to help enhance the robustness given strong attacker. To further

Table 2: **(Information extraction)** *Certified accuracy* under different perturbation magnitudes (C_S) based on the sensing models' output uncertainty. (All certificates hold with 99.9% confidence)

Methods	$C_S = 0.1$	$C_S = 0.5$	$C_S = 0.9$
Vanilla Smoothing (w/o knowledge)	99.7	94.7	38.4
Sensing-Reasoning Pipeline (w/ knowledge)	**100.0**	**100.0**	**58.8**

Figure 3: **(Information extraction)** Histogram of the **robustness margin** (the difference between the probability of the correct class (lower bound) and the top wrong class (upper bound)) under perturbations. If such a difference is positive, it means that the classifier makes the right prediction under perturbations.

illustrate intuitively why such knowledge-based reasoning helps, Figure 3 shows the "margin" — the probability of the ground truth class minus the probability of the wrong class — with or without knowledge integration. We see that, with knowledge integration, we can significantly increase the number of examples with a large "margin" under adversarial perturbations. This explains the improvement of certified robustness, which highly relies on such prediction confident margin.

We also conduct experiments on PrimateNet, Word50, MNIST, CIFAR10 datasets for the image classification tasks in Appendix F, Appendix G, Appendix H. We observe similar results that the sensing-reasoning pipeline with knowledge integration will significantly boost the certified robustness.

6 Related Work

Robustness for Single ML model and Ensemble Lots of efforts have been made to improve the robustness of single ML or ensemble models. Adversarial training [15], and its variations [46, 30, 51] have generally been more successful in practice, but usually come at the cost of accuracy and increased training time [47, 51]. To further provide certifiable robustness guarantees for ML models, various certifiable defenses and robustness verification approaches have been proposed [20, 44, 8]. Among these strategies, randomized smoothing [8] has achieved scalable performance. With improvements in training, including pretraining and adversarial training, the certified robustness bound can be further improved [4, 41]. In addition to the single ML model, some work proposed to promote the diversity of classifiers and therefore develop a robust ensemble [33, 56, 55]. Although promising, these defense approaches, either empirical or theoretical, can only improve the robustness of a single ML model. Certifying or improving the robustness of such single or pure ensemble models is very challenging, given that there is no additional information that can be utilized. In practice, the ML learning process usually favors a pipeline that is able to incorporate different sensing components as well as domain knowledge. Thus, certifying the robustness of such pipelines is of great importance.

Robustness of End-to-end Systems There have been intensive studies on joint inference between multiple models and predictions within an end-to-end pipeline can help to improve their accuracy [53, 10, 37, 32, 7, 5] and have been applied to a range of real-world applications [2, 36, 31]. Often, these approaches use different statistical inference models such as factor graphs [49], Markov logic networks [40], Bayesian networks [34] as a way to integrate knowledge. In this paper, we take a different perspective on this problem — instead of treating joint inference as a way to improve the *application accuracy*, we explore the possibility of using it as a way to improve the end-to-end *certified robustness*. A recent work [17] explores the empirical robustness improvement via knowledge integration, while there is no guarantee provided. As we show in this paper, by integrating domain knowledge, we can improve the *certified robustness* of the ML pipeline significantly.

7 Conclusions

We provide the first certified robustness analysis for the sensing-reasoning pipeline with knowledge-based logical reasoning. Our theoretical results provide the certified robustness of such ML pipelines together with its complexity analysis. Our empirical results demonstrate the robustness of sensing-reasoning pipeline, and we believe our work would shed light on future research towards improving and certifying robustness for general ML frameworks as well as different ways to integrate logical reasoning with statistical learning.

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