CERTIFIED ROBUSTNESS TO DATA POISONING IN GRADIENT-BASED TRAINING

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ABSTRACT

Modern machine learning pipelines leverage large amounts of public data, making it infeasible to guarantee data quality and leaving models open to poisoning and backdoor attacks. Provably bounding model behavior under such attacks remains an open problem. In this work, we address this challenge by developing the first framework providing provable guarantees on the behavior of models trained with potentially manipulated data without modifying the model or learning algorithm. In particular, our framework certifies robustness against untargeted and targeted poisoning, as well as backdoor attacks, for bounded and unbounded manipulations of the training inputs and labels. Our method leverages convex relaxations to over-approximate the set of all possible parameter updates for a given poisoning threat model, allowing us to bound the set of all reachable parameters for any gradient-based learning algorithm. Given this set of parameters, we provide bounds on worst-case behavior, including model performance and backdoor success rate. We demonstrate our approach on multiple real-world datasets from applications including energy consumption, medical imaging, and autonomous driving.

1 INTRODUCTION

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To achieve state-of-the-art performance, modern machine learning pipelines involve pre-training on
 massive, uncurated datasets; subsequently, models are fine-tuned with task-specific data to maximize
 downstream performance (Han et al., 2021). Unfortunately, the datasets used in both steps are
 potentially untrustworthy and of such scale that rigorous quality checks become impractical.

Data Poisoning. Yet, adversarial manipulation, i.e., *poisoning attacks*, affecting even a small proportion of data used for either pre-training or fine-tuning can lead to catastrophic model failures (Carlini et al., 2023). For instance, Yang et al. (2017) show how popular recommender systems on sites such as YouTube, Ebay, and Yelp can be easily manipulated by poisoning. Likewise, Zhu et al. (2019) show that poisoning even 1% of training data can lead models to misclassify targeted examples, and Han et al. (2022) use poisoning to selectively trigger backdoor vulnerabilities in lane detection systems to force critical errors.

040 **Poisoning Defenses.** Despite the gravity of the failure modes induced by poisoning attacks, counter-041 measures are generally attack-specific and only defend against known attack methods (Tian et al., 042 2022). The result of attack-specific defenses is an effective "arms race" between attackers trying 043 to circumvent the latest defenses and counter-measures being developed for the new attacks. In 044 effect, even best practices, i.e., using the latest defenses, provide no guarantees of protection against poisoning attacks. To date, relatively few approaches have sought provable guarantees against poisoning attacks. These methods are often limited in scope, e.g., applying only to linear models 046 (Rosenfeld et al., 2020; Steinhardt et al., 2017) or only providing approximate guarantees for a limited 047 set of poisoning settings (Rosenfeld et al., 2020; Xie et al., 2022). Other approaches partition datasets 048 into hundreds or thousands of disjoint shards and then aggregate predictions such that the effects of poisoning is provably limited (Levine & Feizi, 2020; Wang et al., 2022). In contrast, our goal in this work is not to produce a robust learning algorithm, but to efficiently analyze the sensitivity of 051 (un-modified) algorithms. Further discussion of related works is provided in Appendix A. 052

This Work: General Certificates of Poisoning Robustness. We present an approach for computing sound and general certificates of robustness to poisoning attacks for any model trained with first-order

optimization methods, e.g., stochastic gradient descent or Adam (Kingma & Ba, 2014). The proposed 055 strategy begins by treating various poisoning attacks as constraints over an adversary's perturbation 056 'budget' in input and label spaces. Following the comprehensive taxonomy by Tian et al. (2022), we view the objective of each poisoning attack as an optimization problem. We consider three 058 objectives: (i) untargeted attacks: reducing model test performance to cause denial-of-service, (ii) targeted attacks: compromising model performance on certain types of inputs, and (iii) backdoor attacks: leaving the model performance stable, but introducing a trigger pattern that causes errors 060 at deployment time. Our approach then leverages convex relaxations of both the training problem 061 and the constraint sets defining the threat model to compute a sound (but incomplete) certificate that 062 bounds the impact of the poisoning attack. 063

Paper Outline. The paper is organized as follows. We first provide a general framework for poisoning attacks, describing how our formulation captures the settings studied in prior works (related works are reviewed in Appendix A). We then present *abstract gradient training* (AGT), our technique for over-approximating the effect of a given poisoning attack and discuss implementation details, including a novel, explicit formulation of CROWN-like bounds (Zhang et al., 2018) on the weight gradients. We conclude with extensive ablation experiments on datasets from household energy consumption, medical image classification, and autonomous vehicle driving. In summary, this paper makes the following key contributions:

- A framework, including a novel bound propagation strategy, for computing sound bounds on the influence of a poisoning adversary on any model trained with gradient-based methods.
- Based on the above, a series of formal proofs that allow us to bound the effect of poisoning attacks that seek to corrupt the system with targeted, untargeted, or backdoor attacks.
- An extensive empirical evaluation demonstrating the effectiveness of our approach.
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2 PRELIMINARIES: POISONING ATTACKS

We denote a machine learning model as a parametric function f with parameters θ , feature space $x \in \mathbb{R}^{n_{\text{in}}}$, and label space $y \in \mathcal{Y}$. The label space \mathcal{Y} may be discrete (e.g. classification) or continuous (e.g. regression). We operate in the supervised learning setting with a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$ where we index the dataset such that $\mathcal{D}_x^{(i)}$ is the i^{th} feature vector and $\mathcal{D}_y^{(i)}$ is the i^{th} label. We denote the parameter initialization θ' and a training algorithm M as $\theta = M(f, \theta', \mathcal{D})$, i.e., given a model, initialization, and data, the training function M returns a "trained" parameterization θ . Finally, we assume the loss function is computed element-wise from the dataset, denoted as $\mathcal{L}(f(x^{(i)}), y^{(i)})$.

Given this abstraction of model training, we now turn to developing an abstraction of the data poisoning attacks, defining their capabilities to adversarially manipulate the training input. To complete the threat model, we formulate adversary goals, i.e., what the adversaries seek to accomplish with their manipulation as optimization problems. Typical threat models additionally specify the adversary's system knowledge; however, as we aim to upper bound a worst-case adversary, we assume unrestricted access to all training information including model architecture and initialization, data, data ordering, hyper-parameters, etc.

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096 2.1 POISONING ATTACK CAPABILITIES

This section defines the capabilities of the poisoning attack adversaries that we seek to certify against. We consider two distinct threat models: (1) ℓ_p -norm bounded adversaries, which are commonly assumed in backdoor attack models (Saha et al., 2020; Weber et al., 2023); (2) unbounded adversaries, which are more general and have the capability to inject arbitrary data into the training set. In both cases, we consider adversaries able to modify both features and labels simultaneously.

Bounded Attacks. Under a bounded attack setting, we allow an adversary to perturb a subset of the training data in both the feature and label space, where the magnitude of the perturbation is bounded in a given norm. In feature space, we allow for an adversary to modify at most n datapoints by a distance of up to ϵ in the ℓ_p -norm. Similarly, we define the label-space poisoning capability as modifying at most m labels by magnitude at most ν in an ℓ_q -norm. Note that label-space poisoning encompasses both classification and (multivariate) regression settings. Common label-flipping attacks

108 can be considered under this attack model by setting q = 0. Formally, given a dataset \mathcal{D} and an 109 adversary $\langle n, \epsilon, p, m, \nu, q \rangle$, the set of potentially poisoned datasets is defined as 110

$$\mathcal{T}_{m,\nu,q}^{n,\epsilon,p}(\mathcal{D}) := \left\{ \widetilde{\mathcal{D}} \middle| \begin{array}{c} \|\mathcal{D}_x^{(i)} - \widetilde{\mathcal{D}}_x^{(i)}\|_p \le \epsilon \; \forall i \in I, \quad \mathcal{D}_x^{(i')} = \widetilde{\mathcal{D}}_x^{(i')} \; \forall i' \notin I, \quad \forall I \in \mathcal{S}_n \\ \|\mathcal{D}_y^{(j)} - \widetilde{\mathcal{D}}_y^{(j)}\|_q \le \nu \; \forall j \in J, \quad \mathcal{D}_y^{(j')} = \widetilde{\mathcal{D}}_y^{(j')} \; \forall j' \notin J, \quad \forall J \in \mathcal{S}_m \end{array} \right\}$$
(1)

113 where S_n is the set of all subsets of integers less than N with cardinality at most n. The index sets I 114 and J refer to the data-points that have been poisoned in the feature and label spaces, respectively. 115 Note that in a paired modification setting, adversaries must choose a set of inputs and modify both 116 their features and labels, which corresponds to setting I = J in the above. Our more general setting 117 allows for adversaries to modify features and labels of different inputs. 118

Unbounded Attacks. It may not always be realistic to assume that the effect of a poisoning adversary 119 is bounded. A more powerful adversary may be able to inject arbitrary data points into the training 120 data set, for example by exploiting the collection of user data. In this unbounded attack setting, we 121 consider only a 'paired' modification setting, where an adversary can substitute both the features and 122 labels of any n data-points. Specifically, for a dataset \mathcal{D} , the set of potentially poisoned datasets is 123

$$\mathcal{T}^{n}(\mathcal{D}) := \left\{ \widetilde{\mathcal{D}} = (\mathcal{D} \setminus \mathcal{D}^{r}) \cup \mathcal{D}^{a} \mid |\mathcal{D}^{a}| \le n, |\mathcal{D}^{r}| \le n, \mathcal{D}^{a} \subset \mathcal{D} \right\}$$
(2)

where $|\cdot|$ is the cardinality operator, \mathcal{D}^a is a set of arbitrary added data-points, and \mathcal{D}^r is the set of corresponding data-points removed from the original dataset. To simplify the exposition below, we interchangeably refer to \mathcal{T}^n as either the poisoning adversary or the set of poisoned datasets. We use \mathcal{T} to refer to cases where either the bounded or unbounded adversaries may be applied.

2.2 POISONING ATTACK GOALS

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132 Here, we cover the different goals poisoning adversaries may pursue and briefly outline what it means to certify that a training algorithm is robust against such an adversary. 133

Untargeted Poisoning. Untargeted attacks aim to prevent training convergence, leading to an unusable model and denial of service (Tian et al., 2022). Given the training dataset $\{(x^{(i)}, y^{(i)})\}_{i=1}^{k}$ the adversary's objective is thus:

$$\max_{\mathcal{D}'\in\mathcal{T}} \frac{1}{k} \sum_{i=1}^{k} \mathcal{L}\left(f^{M(f,\theta',\mathcal{D}')}(x^{(i)}), y^{(i)}\right)$$
(3)

We can certify robustness to this kind of attack using a sound upper bound on the solution of (3).

142 **Targeted Poisoning.** Targeted poisoning is more task-specific and is typically evaluated over the test dataset. Rather than simply attempting to increase the loss, the adversary seeks to make model 143 predictions fall outside a 'safe' set of outputs $S(x^{(i)}, y^{(i)})$ (e.g., the set of predictions matching the 144 ground truth). The safe set can be more specific however, i.e., mistaking a lane marking for a person 145 is safe, but not vice versa. The adversary's objective is given by: 146

$$\max_{\mathcal{D}' \in \mathcal{T}} \frac{1}{k} \sum_{i=1}^{k} \mathbb{1}\left(f^{M(f,\theta',\mathcal{D}')}(x^{(i)}) \notin S(x^{(i)}, y^{(i)}) \right)$$
(4)

150 As before, a sound upper bound on (4) bounds the success rate of any targeted poisoning attacker. Note that with k = 1 we recover the pointwise certificate setting studied by Rosenfeld et al. (2020). 151 This setting also covers 'unlearnable examples', such as the attacks considered by Huang et al. (2021). 152

153 Backdoor Poisoning. Backdoor attacks deviate from the above attacks by assuming that test-time 154 data can be altered, via a so-called trigger manipulation. However, backdoor attacks typically aim to 155 leave the model performance on 'clean' data unchanged. By assuming that the trigger manipulation(s) are bounded to a set V(x) (e.g., an ℓ_{∞} ball around the input), one can formulate the backdoor attack's 156 157 goal as producing predictions outside a safe set $S(x^{(i)}, y^{(i)})$ (defined as before) for manipulated inputs: 158

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$$\max_{\mathcal{D}'\in\mathcal{T}} \frac{1}{k} \sum_{i=1}^{k} \mathbb{1}\left(\exists x^{\star} \in V(x^{(i)}) \ s.t. \ f^{M(f,\theta',\mathcal{D}')}(x^{\star}) \notin S(x^{(i)}, y^{(i)})\right)$$
(5)

Any sound upper bound to the above is a sound bound on the success rate of any backdoor attacker.

162 3 METHODOLOGY 163

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164 This section develops a novel approach for certifying robustness to poisoning attacks starting by 165 assuming we have access to the set of all reachable trained models in the form of intervals over model 166 parameters. We first show how these intervals can be used to certify robustness to the above attacks. 167 We then formulate a general algorithm for bounding the effect of adversaries on model parameters, 168 producing an interval containing all reachable training parameters. We then instantiate it using a novel formulation of CROWN-style bounds which can soundly compute the quantities required within. 169

3.1 PARAMETER-SPACE CERTIFICATES OF POISONING ROBUSTNESS

The key concept behind our framework is to bound the parameters obtained via the training function $M(f, \theta', \mathcal{D})$ given $\mathcal{T}(\mathcal{D})$. Before detailing the method, we first formalize our definition of parameterspace bounds and how they can be translated into formal, provable guarantees on poisoning robustness.

Definition 1. (Valid parameter-space bounds) An interval over parameters $[\theta^L, \theta^U]$ such that $\forall i, \theta_i^L \leq \theta_i^U$ is a valid parameter-space bound on a poisoning adversary, $\mathcal{T}(\mathcal{D})$, if $\forall i$:

$$\theta_i^L \le \min_{\mathcal{D}' \in \mathcal{T}(\mathcal{D})} M(f, \theta', \mathcal{D}')_i \le M(f, \theta', \mathcal{D})_i \le \max_{\mathcal{D}' \in \mathcal{T}(\mathcal{D})} M(f, \theta', \mathcal{D}')_i \le \theta_i^U$$
(6)

Intuitively, Definition 1 allows us to measure the poisoning adversary's influence in parameter space. 182 From such bounds, we can then derive guarantees on the poisoning robustness against any of the aforementioned attack vectors.

184 **Theorem 3.1.** Given valid parameter bounds $[\theta^L, \theta^U]$ for an adversary $\mathcal{T}(\mathcal{D})$, one can compute a 185 sound upper bound (i.e., certificate) on any poisoning objective by optimization over the parameter space, rather than dataset space: 187

$$\max_{\mathcal{D}' \in \mathcal{T}} J\big(f^{M(f,\theta',\mathcal{D}')}(x)\big) \le \max_{\theta^{\star} \in [\theta^{L},\theta^{U}]} J\big(f^{\theta^{\star}}(x)\big)$$

where J is one of the objective functions from (3)–(5). Full expressions are provided in Appendix I.1.

The advantage of Theorem 3.1 is that each of these upper-bounds can be computed directly using 192 bounds from works studying certification of adversarial robustness of probabilistic models (Adams 193 et al., 2023; Wicker et al., 2020; 2023). 194

3.2 ABSTRACT GRADIENT TRAINING FOR VALID PARAMETER SPACE BOUNDS

197 In this section, we provide an intuition and high-level framework for computing parameter bounds 198 that respect Definition 1. We call this framework *abstract gradient training* (AGT). Our framework 199 is applicable to any training function M based on first-order optimization, e.g., stochastic gradient 200 descent or Adam. To keep our exposition intuitive, we choose to focus on SGD, written as: 201

$$\theta \leftarrow \theta - \alpha \frac{1}{|\mathcal{B}|} \sum_{(x,y) \in \mathcal{B}} \nabla_{\theta} \mathcal{L} \left(f^{\theta}(x), y \right)$$
(7)

204 where $\mathcal{B} \subseteq \mathcal{D}$ is the sampled batch at the current iteration. The function $M(f, \theta', \mathcal{D})$, in the simplest 205 case, iteratively applies the update (7) for a fixed, finite number of iterations starting from $\theta^{(0)} = \theta'$. 206 Therefore, to bound the effect of a poisoning attack, we can iteratively apply bounds on update 207 (7). In Algorithm 1, we present a general framework for computing parameter-space bounds on the 208 output of SGD given a poisoning adversary \mathcal{T} . In particular, we highlight that Algorithm 1 first 209 computes the standard stochastic gradient descent update (lines 4-5), and then computes a bound on 210 the set of all possible descent directions that could be taken at this iteration. Note that the gradient 211 clipping operation, highlighted in purple, is optional for a bounded adversary, and is only required 212 for the unbounded adversary to limit the maximum contribution of any added data-points. This bound on the descent direction is then soundly combined with the existing parameter space bound to 213 obtain an updated reachable parameter interval $[\theta^L, \theta^U]$. Since the reachable parameter interval is 214 maintained over every iteration of the algorithm, we have the following theorem (which we prove in 215 Appendix I.2):

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17	Algo	rithm 1: Abstract Gradient Training for Poisoning Certification	
18 19	ir o	iput : f - ML model, θ' - param. initialisation, \mathcal{D} - nominal dataset, E - epochs, α - learning rate allowable dataset perturbations (poisoning adversary), κ - optional clipping parameter. utput: θ - nominal SGD parameter, $[\theta^L, \theta^U]$ - reachable parameter interval.	e, Τ
20 21 22	$\begin{array}{c c} 1 & \theta \\ 2 & \mathbf{f} \\ 3 \end{array}$	$ \leftarrow \theta'; [\theta^L, \theta^U] \leftarrow [\theta', \theta'] $ or <i>E-many epochs</i> do for <i>each batch</i> $\mathcal{B} \subset \mathcal{D}$ do	
23		/* Compute the (optionally clipped) SGD update.	*/
24 25	4	$\Delta \theta \leftarrow \frac{1}{ \mathcal{B} } \sum_{(x,y) \in \mathcal{B}} \operatorname{Clip}_{\kappa} \left[\nabla_{\theta} \mathcal{L} \left(f^{\theta}(x), y \right) \right]$	
26	5	$\theta \leftarrow \theta - \alpha \Delta \theta$	
27 28 29 30	6	$ \left \begin{array}{l} /* \text{ Define the set of descent directions possible under } \mathcal{T} \text{.} \\ \Delta \Theta \leftarrow \left\{ \frac{1}{ \widetilde{\mathcal{B}} } \sum_{(\tilde{x}, \tilde{y}) \in \widetilde{\mathcal{B}}} \operatorname{Clip}_{\kappa} \left[\nabla_{\theta'} \mathcal{L} \left(f^{\theta'}(\tilde{x}), \tilde{y} \right) \right] \mid \widetilde{\mathcal{B}} \in \mathcal{T} \left(\mathcal{B} \right), \theta' \in \left[\theta^L, \theta^U \right] \right\} \end{aligned} \right\} $	*/
31		/* Bound the set of descent directions possible under $\mathcal{T}.$	*/
32	7	Compute $\Delta \theta^L$, $\Delta \theta^U$ s.t. $\Delta \theta^L \preceq \Delta \theta \preceq \Delta \theta^U$ for all $\Delta \theta \in \Delta \Theta$	
3		/* Update the reachable parameter interval under ${\cal T}.$	*/
4	8	$\left[\left[\theta^L, \theta^U \right] \leftarrow \left[\theta^L - \alpha \Delta \theta^U, \theta^U - \alpha \Delta \theta^L \right] \right]$	
5	9 re	eturn $ heta, [heta^L, heta^U]$	

Theorem 3.2. Algorithm 1 returns valid parameter-space bounds on a $T_{n,\epsilon,p}^{m,\nu,q}(\mathcal{D})$ poisoning adversary for a stochastic gradient descent training procedure $M(f, \theta', \mathcal{D})$.

240 **Bounding the Descent Direction.** The main complexity in Algorithm 1 is in bounding the set $\Delta \Theta$, 241 which is the set of all possible descent directions at the given iteration under \mathcal{T} . In particular, $\mathcal{B} \in$ 242 $\mathcal{T}(\mathcal{B})$ represents the effect of the adversary's perturbations on the *current* batch, while the reachable 243 parameter interval $\theta' \in [\theta^L, \theta^U]$ represents the worst-case effect of adversarial manipulations to 244 all *previously seen* batches. Exactly computing the set $\Delta \Theta$ is not computationally tractable, so we 245 instead seek over-approximate element-wise bounds that can be computed efficiently within the 246 training loop. We present a procedure for computing bounds for the bounded poisoning adversary 247 in the following theorem. The analogous theorem for the unbounded adversary can be found in 248 Appendix B. 249

Theorem 3.3 (Bounding the descent direction for a bounded adversary). Given a nominal batch $\mathcal{B} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{b}$ of size b, a parameter set $[\theta^{L}, \theta^{U}]$, and a bounded adversary $\langle n, \epsilon, p, m, \nu, q \rangle$, the SGD parameter update $\Delta \theta = \frac{1}{b} \sum_{\widetilde{B}} \nabla_{\theta} \mathcal{L} (f^{\theta} (\tilde{x}^{(i)}), \tilde{y}^{(i)})$ is bounded element-wise by 253

$$\Delta \theta^{L} = \frac{1}{b} \left(\operatorname{SEMin}_{m+n} \left\{ \tilde{\delta}_{L}^{(i)} - \delta_{L}^{(i)} \right\}_{i=1}^{b} + \sum_{i=1}^{b} \delta_{L}^{(i)} \right), \quad \Delta \theta^{U} = \frac{1}{b} \left(\operatorname{SEMax}_{m+n} \left\{ \tilde{\delta}_{U}^{(i)} - \delta_{U}^{(i)} \right\}_{i=1}^{b} + \sum_{i=1}^{b} \delta_{U}^{(i)} \right)$$

for any $\widetilde{\mathcal{B}} \in T_{m,\nu,q}^{n,\epsilon,p}(\mathcal{B})$ and $\theta \in [\theta^L, \theta^U]$. The terms $\delta_L^{(i)}, \delta_U^{(i)}$ are sound bounds that account for the effect of previous adversarial manipulations. Likewise, the terms $\widetilde{\delta}_L^{(i)}, \widetilde{\delta}_U^{(i)}$ are bounds on the worst-case adversarial manipulations of the *i*-th data-point in the current batch, *i.e.*

$$\delta_L^{(i)} \preceq \delta \preceq \delta_U^{(i)} \quad \forall \delta \in \left\{ \nabla_{\theta'} \mathcal{L} \left(f^{\theta'}(x^{(i)}), y^{(i)} \right) \mid \theta' \in [\theta^L, \theta^U] \right\},\tag{8}$$

$$\tilde{\delta}_{L}^{(i)} \preceq \tilde{\delta} \preceq \tilde{\delta}_{U}^{(i)} \quad \forall \tilde{\delta} \in \left\{ \nabla_{\theta'} \mathcal{L}\left(f^{\theta'}\left(\tilde{x}\right), \tilde{y}\right) \mid \theta' \in [\theta^{L}, \theta^{U}], \|x^{(i)} - \tilde{x}\|_{p} \le \epsilon, \|y^{(i)} - \tilde{y}\|_{q} \le \nu \right\}.$$
(9)

The operations SEMax_a and SEMin_a correspond to taking the sum of the element-wise top/bottom-*a* elements over each index of the input vectors. The update rule in Theorem 3.3 accounts for the effect of poisoning in previous batches by taking the lower and upper bounds on the gradient $(\delta_L^{(i)}, \delta_U^{(i)})$ for all θ reachable at the current iteration. Then, we bound the effect of adversarial manipulation in the current batch by taking the n + m points that have the worst-case gradient bounds $\tilde{\delta}_L^{(i)}, \tilde{\delta}_U^{(i)}$ under poisoning. We assume that $m + n \leq b$. If m + n > b, we take SEMin/Max with respect to

270 $\min(b, m+n)$ instead. Since we wish to soundly over-approximate this operation for all parameters, 271 we perform this bounding operation independently over each index of the parameter vector. This 272 is certainly a loose approximation, as the n + m points that maximize the gradient at a particular 273 index will likely not maximize the gradient of other indices. However, this relaxation allows us 274 to efficiently compute and propagate interval enclosures between successive iterations of AGT. A further relaxation is taken when computing gradient bounds $\delta_L^{(i)}, \delta_U^{(i)}$, since they are computed independently for each sample *i* and the min/max for different samples may be attained for different 275 276 $\theta' \in [\theta^L, \theta^U]$. Performing this computation independently for each *i*, however, allows for efficient 277 278 bound-propagation that we describe in more detail in subsequent sections.

For the bounded adversary, gradient clipping is not a requirement and we can directly bound the un-modified SGD training procedure. However, it can still be desirable to add gradient clipping even in the bounded adversary case, as it can improve the tightness of our descent direction bounds and subsequently improve the guarantees afforded by AGT with little cost to training performance.

3.3 COMPUTATION OF SOUND GRADIENT BOUNDS

This section presents a novel algorithm for computing bounds on the following optimization problem

$$\min_{x^*, y^*, \theta^*} \left\{ \nabla_{\theta'} \mathcal{L}\left(f^{\theta'}\left(\tilde{x}\right), \tilde{y} \right) \mid \theta' \in [\theta^L, \theta^U], \|x^{(i)} - \tilde{x}\|_p \le \epsilon, \|y^{(i)} - \tilde{y}\|_q \le \nu \right\}.$$
(10)

Computing the exact solution to this problem is, in general, a non-convex and NP-hard optimization problem. However, we require only over-approximate solutions; while these can introduce (significant) over-approximation of the reachable parameter set, they will always maintain soundness. Future work could investigate exact solutions, e.g., via mixed-integer programming (Huchette et al., 2023; Tsay et al., 2021). Owing to their tractability, our discussion focuses on the novel linear bound propagation techniques we develop for abstract gradient training. Noting that problems of the form (8) can be recovered by setting $\nu = \epsilon = 0$, we focus solely on this more general case in this section.

Neural networks. While the algorithm presented in Section 3.2 is general to any machine learning model trained via stochastic gradient descent, we focus our discussion on neural network models for the remained of the paper. We first define a neural network model $f^{\theta} : \mathbb{R}^{n_{\text{in}}} \to \mathbb{R}^{n_{\text{out}}}$ with K layers and parameters $\theta = \{(W^{(i)}, b^{(i)})\}_{i=1}^{K}$ as:

 $\hat{z}^{(k)} = W^{(k)} z^{(k-1)} + b^{(k)}, \quad z^{(k)} = \sigma\left(\hat{z}^{(k)}\right)$

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where $z^{(0)} = x$, $f^{\theta}(x) = \hat{z}^{(K)}$, and σ is the activation function, which we take to be ReLU.

Solving problems of the form $\min \{ \cdot | ||x - x^*||_p \le \epsilon \}$ for neural networks has been well-studied in the context of adversarial robustness certification. However, optimizing over inputs, labels and parameters, e.g., $\min \{ \cdot | \theta^* \in [\theta^L, \theta^U], ||x - x^*||_p \le \epsilon, ||y - y^*||_q \le \nu \}$ is much less well-studied, and to-date similar problems have appeared primarily in the certification of probabilistic neural networks (Wicker et al., 2020).

Interval Arithmetic. For ease of exposition, we will represent interval matrices with bold symbols i.e., $A := [A_L, A_U] \subset \mathbb{R}^{n_1 \times n_2}$ and interval matrix multiplication as \otimes , meaning $AB \in A \otimes B$ for all $A \in A$ and $B \in B$. Additionally, we define \odot and \oplus as element-wise interval matrix multiplication and addition, respectively. This implies $A \circ B \in A \odot B$ (where \circ is the element-wise product) and $A + B \in A \oplus B$ for all $A \in A$ and $B \in B$, which can be computed using standard interval arithmetic techniques. We denote interval vectors as $a := [a_L, a_U]$ with analogous operations. More details of interval arithmetic operations over matrices and vectors can be found in Appendix C.

316 Forward Pass Bounds Mirroring developments in robustness certification of neural networks, we 317 provide a novel, explicit extension of the CROWN algorithm (Zhang et al., 2018) to account for 318 interval-bounded weights. The standard CROWN algorithm bounds the outputs of the *m*-th layer of a 319 neural network by back-propagating linear bounds over each intermediate activation function to the 320 input layer. We extend this framework to interval parameters, where the weights and biases involved 321 in these linear relaxations are themselves intervals. We note that linear bound propagation with interval parameters has been studied previously in the context of floating-point sound certification 322 (Singh et al., 2019). In the interest of space, we present only the upper bound of our extended 323 CROWN algorithm here, with the full version presented in Appendix D.



Figure 1: Bounds on a classification threshold trained on the halfmoons dataset for a bounded adversary that can perturb up to n data-points by up to ϵ in the $p = \infty$ norm; in label space, the adversary may flip up to m labels (corresponding to $\gamma = 1, q = 0$). The white line shows the decision boundary of the nominal classification model. The coloured regions show the areas for which we *cannot* certify robustness for the given adversary strength.

Proposition 1 (Explicit upper bounds of neural network f with interval parameters). Given an m-layer neural network function $f : \mathbb{R}^{n_{in}} \to \mathbb{R}^{n_{out}}$ whose unknown parameters lie in the intervals $b^{(k)} \in \mathbf{b}^{(k)}$ and $W^{(k)} \in \mathbf{W}^{(k)}$ for k = 1, ..., m, there exist an explicit function

$$f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) = \Lambda_{j,:}^{(0)} x + \sum_{k=1}^m \Lambda_{j,:}^{(k)} \left(b^{(k)} + \Delta_{:,j}^{(k)}\right)$$
(11)

such that $\forall x \in \boldsymbol{x}$

$$f_j(x) \le \max\left\{f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) \mid \Lambda^{(k)} \in \mathbf{\Lambda}^{(k)}, b^k \in \mathbf{b}^{(k)}\right\}$$
(12)

where x is a closed input domain and $\Lambda^{(0:m)}$, $\Delta^{(1:m)}$ are the equivalent weights and biases of the linear upper bounds, respectively. The bias term $\Delta^{(1:m)}$ is explicitly computed based on the linear bounds on the activation functions. The weight $\Lambda^{(0:m)}$ lies in an interval $\Lambda^{(0:m)}$ which is computed in an analogous way to standard, non-interval CROWN (see Appendix D for further details).

Given the upper bound function $f_j^U(\cdot)$ defined above and intervals over all the relevant variables, we can compute the following closed-form global upper bound:

$$\gamma_j^U = \max\left\{ oldsymbol{\Lambda}_{j,:}^{(0)} \otimes oldsymbol{x} \oplus \sum_{k=1}^m oldsymbol{\Lambda}_{j,:}^{(k)} \otimes \left[oldsymbol{b}^{(k)} \oplus \Delta_{:,j}^{(k)}
ight]
ight\}$$

where max is performed element-wise and returns the upper bound of the interval enclosure. Then, we have $f_j(x) \le \gamma_j^U$ for all $x \in \boldsymbol{x}, b^{(k)} \in \boldsymbol{b}^{(k)}$ and $W^{(k)} \in \boldsymbol{W}^{(k)}$. The equivalent procedure for computing the global lower bound $f_j(x) \ge \gamma_j^L$ can be found in Appendix D.

Backward Pass Bounds. Given bounds on the forward pass of the neural network, we can bound the backward pass (the gradients) of the model. We do this by extending the interval arithmetic based approach of Wicker et al. (2022) (which bounds derivatives of the form $\partial \mathcal{L}/\partial z^{(k)}$) to additionally bound the derivatives w.r.t. the parameters. Details of this computation can be found in Appendix F.

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3.4 Algorithm Analysis and Discussion

368 Figure 1 visualizes the resulting worst-case decision boundaries for a simple binary classifier con-369 sisting of a neural network with a hidden layer of 128 neurons. In this classification setting, label 370 poisoning results in looser bounds than feature space poisoning, with m = 5 producing bounds of 371 approximately the same width as n = 50. This is due to the relatively large interval introduced by a 372 label flipping attack $y^{(i)} \in \{0, 1\}$, compared to an interval of width ϵ introduced in a feature-space 373 attack. We also emphasise that Algorithm 1 assumes at most m, n poisoned points *per batch*, rather 374 than per dataset. In regression settings, label poisoning is relatively weaker than feature poisoning 375 for a given strength $\epsilon = \nu$, since the feature-space interval propagates through both the forward and backward training passes, while the label only participates in the backward pass. This effect is partic-376 ularly pronounced in deep networks, since interval/CROWN bounds tend to weaken exponentially 377 with depth (Mao et al., 2023; Sosnin & Tsay, 2024).

Comparison to Interval Bound Propagation. The CROWN algorithm in § 3.3 is not strictly tighter
 than interval bound propagation (IBP). Specifically, the non-associativity of double-interval matrix
 multiplication leads to significantly different interval sizes depending on the order in which the
 multiplications are performed: IBP performs interval matrix multiplications in a 'forwards' ordering,
 while CROWN uses a 'backwards' ordering. Empirically, we observe that CROWN tends to be tighter
 for deeper networks, while IBP may outperform CROWN for smaller networks. In our numerical
 experiments, we compute both CROWN and IBP bounds and take the element-wise tightest bound.

Combined Forward and Backward Pass Bounds. The CROWN algorithm can be applied to any composition of functions that can be upper- and lower-bounded by linear equations. Therefore, it is possible to consider both the forwards and backwards passes in a single combined CROWN pass for many loss functions. However, linear bounds on the gradient of the loss function tend to be relatively loose, e.g., linear bounds on the softmax function may be orders-of-magnitude looser than constant [0, 1] bounds (Wei et al., 2023). As a result, we found that the tightest bounds were obtained using IBP/CROWN on the forward pass and IBP on the backward pass.

392 **Computational Complexity.** The computational complexity of Algorithm 1 depends on the method 393 used to bound on the gradients. In the simplest case, IBP can be used to compute bounds on the 394 gradients in $4 \times$ the cost of a standard forward and backward pass (see Appendix C). Likewise, our 395 CROWN bounds admit a cost of at most 4 times the cost of the original CROWN algorithm. For an m layer network with n neurons per layer and n outputs, the time complexity of the original CROWN 396 algorithm is $\mathcal{O}(m^2n^3)$ (Zhang et al., 2018). We further note that the SEMin / SEMax operations 397 required by Theorems B.1 and 3.3 can be computed in $\mathcal{O}(b)$ for each index and in practice can be 398 efficiently parallelized using GPU-based implementations. In summary, Abstract Gradient Training 399 using IBP has time complexity equivalent to standard neural network training ($\mathcal{O}(bmn^2)$) for each 400 batch of size b), but with our tighter, CROWN-based, bounds the complexity is $\mathcal{O}(bm^2n^3)$ per batch. 401

Limitations. While Algorithm 1 is able to obtain valid-parameter space bounds for any gradient-based 402 training algorithm, the tightness of these bounds depends on the exact architecture, hyperparameters 403 and training procedure used. In particular, bound-propagation between successive iterations of the 404 algorithm assumes the worst-case poisoning at *each parameter index*, which may not be achievable 405 by realistic poisoning attacks. Therefore, obtaining non-vacuous guarantees with our algorithm 406 often requires training with larger batch-sizes and/or for fewer epochs than is typical. Additionally, 407 certain loss functions, such as multi-class cross entropy, have particularly loose interval relaxations. 408 Therefore, AGT obtains relatively weaker guarantees for multi-class problems when compared to 409 regression or binary classification settings. We hope that tighter bound-propagation approaches, such 410 as those based on more expressive abstract domains, may overcome this limitation in future works.

411 Computing Certificates of Poisoning Robustness. Algorithm 1 returns valid parameter-space 412 bounds $[\theta_L, \theta_U]$ for a given poisoning adversary. To provide certificates of poisoning robustness for 413 a specific query at a point x, we first bound the model output $f^{\theta}(x) \forall \theta \in [\theta_L, \theta_U]$ using the bound-414 propagation procedure described above. In classification settings, the robustness of the prediction can 415 then be certified by checking if the lower bound on the output logit for the target class is greater than 416 the upper bounds of all other classes (i.e. $[f_i^{\theta}(x)]_L \ge [f_i^{\theta}(x)]_U \forall i \ne j$). If this condition is satisfied, 417 then the model always predicts class i at the point x for all parameters within our parameter-space bounds, and thus this prediction is certifiably robust to poisoning. Details on computing bounds on 418 other poisoning adversary objectives (3), (4), and (5) can be found in Appendix G. 419

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4 EXPERIMENTS

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Computational experiments were performed using a Python implementation of Algorithm 1. Bounds
 on accuracy/error are computed by bounding the respective optimization problem from Theorem 4.1
 using IBP/CROWN. To investigate the tightness of AGT, we also compare our bounds with heuristic
 poisoning attacks in Appendix H. The experimental set-up and datasets are described in Appendix J.

UCI Regression (Household Power Consumption). We first consider a relatively simple regression model for the household electric power consumption ('houseelectric') dataset from the UCI repository (Hebrail & Berard, 2012) with fully connected neural networks and MSE as loss function. Figure 2 (top) shows the progression of the nominal and worst/best-case MSE (computed for the test set) for a 1×50 neural network and various parameterizations of poisoning attacks. As expected, we observe

Feature poisoning ($\varepsilon = 0.01$) Feature poisoning (n = 1000)Label poisoning ($\nu = 0.05$) Label poisoning (m = 1000)Bounds $\nu = 0.75$ n = 10000 $\epsilon = 0.15$ m = 100000.4 n = 5000 $\varepsilon = 0.1$ m = 5000 $\nu = 0.5$ n = 1000 ε=0.05 m = 1000 $\nu = 0.25$ + 0.2 MSE 0.0 0 50 100 0 50 100 0 50 100 0 50 100 Depth (b)Width (w) Batch Size (b) Learning Rate (α) Bounds d=3w = 400b = 100 $\alpha = 0.1$ 0.4 d=2w = 300b = 1000 $\alpha = 0.05$ d=1w = 100b = 10000 $\alpha = 0.02$ MSE + 0.2 0.0 0 50 100 50 0 50 100 0 100 0 50 100 Training Iteration

that increasing each of n, m, ϵ , and ν results in looser performance bounds. We note that the settings of m = 10000 and n = 10000 correspond 100% of the data (batchsize b = 10000) being poisoned.

Figure 2: Mean squared error bounds on the UCI-houseelectric dataset. Top: Effect of adversary strength. Bottom: Effect of model/training hyperparameters (with $n = 100, \epsilon = 0.01, p = \infty$). Where not stated, d = 1, w = 50, b = 10000, and $\alpha = 0.02$.

Figure 2 (bottom) shows the progression of bounds on the MSE (computed for the test set) over the training procedure for a fixed poisoning attack ($n = 100, \epsilon = 0.01$) and various hyperparameters of the regression model. In general, we observe that increasing model size (width or depth) results in looser performance guarantees. As expected, increasing the batch size improves our bounds, as the number of potentially poisoned samples n remains fixed and their worst-case effect is 'diluted'. Increasing the learning rate accelerates both the model training and the deterioration of the bounds.

459 **MNIST Digit Recognition.** We consider a label-flipping attack 460 $(q = 0, \nu = 1)$ on the MNIST dataset. In label-only poisoning settings, it is common to use unsupervised learning approaches on 461 the (assumed clean) features prior to training a classification model 462 (e.g. SS-DPA (Levine & Feizi, 2020)). Therefore, we first project 463 the data into a 32-dimensional feature space using PCA and then 464 train a linear classifier using AGT to obtain a certified classification 465 model. Figure 3 illustrates the certifiable accuracy using this method-466 ology. Compared to regression or binary classification settings, AGT 467 provides limited guarantees for multi-class problems; we hope that 468 tighter bound propagation techniques will overcome this limitation 469 in the future. Stronger guarantees can be obtained by increasing the 470 gradient clipping parameter κ , at the cost of decreased model utility.



Figure 3: Certified accuracy on the MNIST dataset under a label-flipping attack.

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 472 a classifier trained on the retinal OCT dataset (OCTMNIST) (Yang

473 et al., 2021), which contains four classes—one normal and three abnormal. The dataset is unbalanced, 474 and we consider the simpler normal vs abnormal binary classification setting. We consider the 'small' 475 architecture from Gowal et al. (2018), comprising two convolutional layers of width 16 and 32 and 476 a dense layer of 100 nodes, and the following fine-tuning scenario: the model is first pre-trained 477 without the rarest class (Drusen) using the robust training procedure from Wicker et al. (2022), so that the resulting model is robust to feature perturbations during fine-tuning. We then assume Drusen 478 samples may be poisoned and add them as a new abnormal class to fine-tune the dense layer, with a 479 mix of 50% Drusen samples (b = 6000 with 3000 Drusen) per batch. 480

In general, this fine-tuning step improves accuracy on the new class (Drusen) from approximately 0.5 to over 0.8. Nevertheless, Figure 4 shows how increasing the amount of potential poisoning worsens the bound on prediction accuracy. With feature-only poisoning, a poisoning attack greater than $\epsilon = 0.02$ over $n \approx 500$ samples produces bounds worse than the prediction accuracy of the original pre-trained model. With an unbounded label and feature poisoning adversary, the bounds are weaker, as expected. Higher certified accuracy can be obtained by increasing the clipping parameter κ , at the



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Figure 4: Certified accuracy (left) and backdoor accuracy (right) for a binary classifier fine-tuned on the Drusen class of OCTMNIST for an attack size up to 10% poisoned data per batch ($b = 6000, p = \infty, q = 0, \nu = 1$). Dashed lines show the nominal accuracy of each fine-tuned model.



Figure 5: Left: Fine-tuning PilotNet on unseen data with a bounded label poisoning attack ($q = \infty$). Right: Steering angle prediction bounds after fine-tuning ($m = 300, q = \infty, \nu = 0.01$).

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512cost of nominal model accuracy (Figure 4, center right). With label-only poisoning, the certificates513are relatively stronger, as the training procedure requires approximately $m \ge 600$ poisoned samples514for the prediction accuracy bound to reach the original pre-trained model's accuracy. The setting of515m = 600 corresponds to 20% of the Drusen data per batch being mis-labeled as healthy.

Finally, we consider a backdoor attack setting where the ϵ used at training and inference times is the same. The model is highly susceptible to adversarial perturbations at inference time even without data poisoning, requiring only $\epsilon = 0.009$ to reduce the certified backdoor accuracy to < 50%. As the strength of the (bounded) adversary increases, the accuracy that we are able to certify decreases. We note that tighter verification algorithms can be applied at inference time to obtain stronger guarantees.

Fine-Tuning PilotNet. Finally, we fine-tune a model that predicts steering angles for autonomous driving given an input image (Bojarski et al., 2016). The model contains convolutional layers of 24, 36, 48, and 64 filters, followed by fully connected layers of 100, 50, and 10 nodes. The fine-tuning setting is similar to above: first, we pre-train the model on videos 2–6 of the Udacity self-driving car dataset (github.com/udacity/self-driving-car/tree/master). We then fine-tune the dense layers on video 1 (challenging lighting conditions) assuming potential label poisoning.

Figure 5 shows the bounds on mean squared error for the video 1 data and visualizes how the bounds translate to the predicted steering angle. We again see that fine-tuning improves accuracy on the new data, but also that the MSE bounds deteriorate as the number of potentially poisoned samples increases (Figure 5, left). The rate of deterioration depends strongly on poisoning strength ν .

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5 CONCLUSIONS

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We proposed a mathematical framework for computing sound parameter-space bounds on the influence of a poisoning attack for gradient-based training. Our framework defines generic constraint sets
to represent general poisoning attacks and propagates them through the forward and backward passes
of model training. Based on the resulting parameter-space bounds, we provided rigorous bounds
on the effects of various poisoning attacks. Finally, we demonstrated our proposed approach to be effective on tasks including autonomous driving and the classification of medical images.

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A RELATED WORKS

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Data Poisoning. Poisoning attacks have existed for nearly two decades and are a serious security concern (Biggio & Roli, 2018; Biggio et al., 2014; Newsome et al., 2006). In Muñoz-González et al. (2017) the authors formulate a general gradient-based attack that generates poisoned samples that corrupt model performance when introduced into the dataset (now termed, untargeted attack). Backdoor attacks manipulate a small proportion of the data such that, when a specific pattern is seen at test-time, the model returns a specific, erroneous prediction Chen et al. (2017); Gu et al. (2017); Han et al. (2022); Zhu et al. (2019). Popular defenses are attack specific, e.g., generating datasets using known attack strategies to classify and reject potentially poisoned inputs (Li et al., 2020). Alternative strategies apply noise or clipping to mitigate certain attacks (Hong et al., 2020).

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Poisoning Defenses. General defenses to poisoning attacks seek to provide upper-bounds on the effectiveness of *any* attack strategy. In this area, Steinhardt et al. (2017) provide such upper-bounds for linear models trained with gradient descent. Rosenfeld et al. (2020) present a statistical upper-bound on the effectiveness of ℓ_2 perturbations on training labels for linear models using randomized smoothing. Xie et al. (2022) observe that differential privacy, which usually covers addition or removal of data points, can also provide statistical guarantees in some limited poisoning settings.

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Certified Poisoning Robustness Relative to inference-time adversarial robustness (also referred to 722 as evasion attacks), less attention has been devoted to provable guarantees against data poisoning 723 adversaries. Existing methods for deterministic certification of robustness to poisoning adversaries 724 involve design of a learning process with careful partitioning and ensembling such that the resulting 725 model has poisoning robustness guarantees (Levine & Feizi, 2020; Wang et al., 2022; Rezaei et al., 726 2023). We refer to these methods as "aggregation" methods. In contrast, our approach is a method 727 for analysis and certification of standard, unmodified machine learning algorithms. Aggregation 728 approaches have been shown to offer strong guarantees against poisoning adversaries albeit at a 729 substantial computational cost including: storing and training thousands of models on (potentially 730 disjoint) subsets of the dataset and the requirement to evaluate each of the potentially thousands of 731 models for each prediction; additionally, these methods require that one have potentially thousands of times more data than is necessary for training a single classifier. By designing algorithms to be 732 robust to poisoning adversaries aggregation based approaches are able to scale to larger models than 733 are considered in this work (Levine & Feizi, 2020; Wang et al., 2022; Rezaei et al., 2023). Yet, 734 the computational cost of our approach, in the simplest case, is only four times that of standard 735 training and inference and we do not require that one has access to enough data to train multiple 736 well-performing models. Furthermore, our approach enables reasoning about backdoor attacks, where 737 these partitioning approaches cannot. We finally highlight that the method presented in this paper 738 is orthogonal/complementary to the partitioning approach, and thus future works may be able to 739 combine the two effectively.

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Certified Adversarial Robustness. Sound algorithms (i.e., no false positives) for upper-bounding 742 the effectiveness of inference-time adversaries are well-studied for trained models (Gehr et al., 2018) 743 and training models for robustness (Gowal et al., 2018; Müller et al., 2022). These approaches 744 typically utilize ideas from formal methods (Katz et al., 2017; Wicker et al., 2018) or optimization 745 (Botoeva et al., 2020; Bunel et al., 2018; Huchette et al., 2023). Most related to this work are strategies 746 that consider intervals over both model inputs and parameters (Wicker et al., 2020), as well as some 747 preliminary work on robust explanations that bound the input gradients of a model Wicker et al. 748 (2022). Despite these methodological relationships, none of these methods directly apply to the 749 general training setting studied here.

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- B BOUNDING THE DESCENT DIRECTION FOR AN UNBOUNDED ADVERSARY
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- **Theorem B.1** (Bounding the descent direction for an unbounded adversary). Given a nominal batch $\mathcal{B} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{b}$ with batchsize b, a parameter set $[\theta^L, \theta^U]$, and a clipping level κ , the clipped

SGD parameter update
$$\Delta \theta = \frac{1}{b} \sum_{\widetilde{B}} \operatorname{Clip}_{\kappa} \left[\nabla_{\theta} \mathcal{L} \left(f^{\theta} \left(\tilde{x}^{(i)} \right), \tilde{y}^{(i)} \right) \right]$$
 is bounded element-wise by

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$$\Delta \theta^{L} = \frac{1}{b} \left(\operatorname{SEMin}_{b-n} \left\{ \delta_{L}^{(i)} \right\}_{i=1}^{b} - n\kappa \mathbf{1}_{d} \right), \quad \Delta \theta^{U} = \frac{1}{b} \left(\operatorname{SEMax}_{b-n} \left\{ \delta_{U}^{(i)} \right\}_{i=1}^{b} + n\kappa \mathbf{1}_{d} \right)$$
(13)

for any poisoned batch $\widetilde{\mathcal{B}}$ derived from \mathcal{B} by substituting up to n data-points with poisoned data and any $\theta \in [\theta^L, \theta^U]$. The terms $\delta_L^{(i)}, \delta_U^{(i)}$ are sound bounds that account for the worst-case effect of additions/removals in any previous iterations. That is, they bound the gradient given any parameter $\theta^* \in [\theta^L, \theta^U]$ in the reachable set, i.e. for all i = 1, ..., b, we have $\delta_L^{(i)} \preceq \delta_U^{(i)}$ for any

$$\delta^{(i)} \in \left\{ \operatorname{Clip}_{\kappa} \left[\nabla_{\theta'} \mathcal{L} \left(f^{\theta'}(x^{(i)}), y^{(i)} \right) \right] \mid \theta' \in \left[\theta^L, \theta^U \right] \right\}.$$
(14)

768 The operations $SEMax_a$ and $SEMin_a$ correspond to taking the sum of the element-wise top/bottom-a 769 elements over each index of the input vectors. Therefore, the update step in (13) corresponds to 770 substituting the n elements with the *largest / smallest* gradients (by taking the sum of only the min / 771 max b - n gradients) with the *minimum / maximum* possible gradient updates ($-\kappa, \kappa$, respectively, due to the clipping operation). Since we wish to soundly over-approximate this operation for all 772 parameters, we perform this bounding operation independently over each index of the parameter 773 vector. This is certainly a loose approximation, as the n points that maximize the gradient at a 774 particular index will likely not maximize the gradient of other indices. Note that without clipping, the 775 min / max effect of adding arbitrary data points into the training data is unbounded and we cannot 776 compute any guarantees. 777

C INTERVAL MATRIX ARITHMETIC

781 In this appendix, we provide a basic introduction to interval matrix arithmetic, which forms the basic 782 building block of our CROWN-style bounds. We denote intervals over matrices as $\mathbf{A} := [A_L, A_U] \subseteq$ 783 $\mathbb{R}^{n \times m}$ such that for all $A \in \mathbf{A}, A_L \leq A \leq A_U$.

Definition 2 (Interval Matrix Arithmetic). Let $\mathbf{A} = [A_L, A_U]$ and $\mathbf{B} = [B_L, B_U]$ be intervals over matrices. Let \oplus , \otimes , \odot represent interval matrix addition, matrix multiplication and elementwise multiplication, such that

$A + B \in [\boldsymbol{A} \oplus \boldsymbol{B}]$	$\forall A \in \boldsymbol{A}, B \in \boldsymbol{B},$
$A \times B \in [\boldsymbol{A} \otimes \boldsymbol{B}]$	$\forall A \in \boldsymbol{A}, B \in \boldsymbol{B},$
$A \circ B \in [\boldsymbol{A} \odot \boldsymbol{B}]$	$\forall A \in \boldsymbol{A}, B \in \boldsymbol{B}.$

These operations can be computed using standard interval arithmetic techniques in at most $4 \times$ the cost of a standard matrix operation. For example, interval matrix multiplication can be computed using the following procedure.

Definition 3 (Interval Matrix Multiplication). *Given element-wise intervals over matrices* $[A_L, A_U]$ where $A_L, A_U \in \mathbb{R}^{n \times m}$ and $[B_L, B_U]$ where $B_L, B_U \in \mathbb{R}^{m \times k}$, define the matrices $A_\mu = (A_U + A_L)/2$ and $A_r = (A_U - A_L)/2$. Allow B_μ and B_r to be defined analogously, then computing using Rump's algorithm (Rump, 1999),

$$C_L = A_{\mu}B_{\mu} - |A_{\mu}|B_r - A_r|B_{\mu}| - A_rB_r$$

$$C_U = A_{\mu}B_{\mu} + |A_{\mu}|B_r + A_r|B_{\mu}| + A_rB_r,$$

801 we have that $C_{Li,j} \leq [A'B']_{i,j} \leq C_{Ui,j} \forall A' \in [A_L, A_U], B' \in [B_L, B_U]$. Nguyen (2012) showed 802 that the above bounds have a worst-case overestimation factor of 1.5.

Interval arithmetic is commonly applied as a basic verification or adversarial training technique by propagating intervals through the intermediate layers of a neural network (Gowal et al., 2018).

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D CROWN WITH INTERVAL PARAMETERS

In this section, we present our full extension of the CROWN algorithm (Zhang et al., 2018) for neural networks with interval parameters. The standard CROWN algorithm bounds the outputs of the

m-th layer of a neural network by back-propagating linear bounds over each intermediate activation
 function to the input layer. We extend this framework to interval parameters, where the weights
 and biases involved in these linear relaxations are themselves intervals. We note that linear bound
 propagation with interval parameters has been studied previously in the context of floating-point
 sound certification (Singh et al., 2019). Here, we present an explicit instantiation of the CROWN
 algorithm for interval parameters, which we recall from Section 3.3.

Proposition 1 (Explicit output bounds of neural network f with interval parameters). Given an m-layer neural network function $f : \mathbb{R}^{n_{in}} \to \mathbb{R}^{n_{out}}$ whose unknown parameters lie in the intervals $b^{(k)} \in \mathbf{b}^{(k)}$ and $W^{(k)} \in \mathbf{W}^{(k)}$ for k = 1, ..., m, there exist two explicit functions

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$$f_j^L\left(x,\Omega^{(0:m)},\Theta^{(1:m)},b^{(1:m)}\right) = \Omega_{j,:}^{(0)}x + \sum_{k=1}^m \Omega_{j,:}^{(k)}\left(b^{(k)} + \Theta_{:,j}^{(k)}\right)$$
(15)

$$f_j^U\left(x,\Lambda^{(0:m)},\Delta^{(1:m)},b^{(1:m)}\right) = \Lambda_{j,:}^{(0)}x + \sum_{k=1}^m \Lambda_{j,:}^{(k)}\left(b^{(k)} + \Delta_{:,j}^{(k)}\right)$$
(16)

such that $\forall x \in \boldsymbol{x}$

$$f_{j}(x) \geq \min \left\{ f_{j}^{L} \left(x, \Omega^{(0:m)}, \Theta^{(1:m)}, b^{(1:m)} \right) \mid \Omega^{(k)} \in \mathbf{\Omega}^{(k)}, b^{k} \in \mathbf{b}^{(k)} \right\}$$
$$f_{j}(x) \leq \max \left\{ f_{j}^{U} \left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)} \right) \mid \Lambda^{(k)} \in \mathbf{\Lambda}^{(k)}, b^{k} \in \mathbf{b}^{(k)} \right\}$$

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where \boldsymbol{x} is a closed input domain and $\Lambda^{(0:m)}, \Delta^{(1:m)}, \Omega^{(0:m)}, \Theta^{(1:m)}$ are the equivalent weights and biases of the upper and lower linear bounds, respectively. The bias terms $\Delta^{(1:m)}, \Theta^{(1:m)}$ are explicitly computed based on the linear bounds on the activation functions. The weights $\Lambda^{(0:m)}, \Omega^{(0:m)}$ lie in intervals $\Lambda^{(0:m)}, \Omega^{(0:m)}$ which are computed in an analogous way to standard (non-interval) *CROWN*.

Computing Equivalent Weights and Biases. Our instantiation of the CROWN algorithm in Proposition 1 relies on the computation of the equivalent bias terms $\Delta^{(1:m)}$, $\Theta^{(1:m)}$ and interval enclosures over the equivalent weights $\Omega^{(0:m)}$, $\Lambda^{(0:m)}$. This proceeds similarly to the standard CROWN algorithm but now accounting for intervals over the parameters $b^{(1:m)}$, $W^{(1:m)}$ of the network. All interval operations are as described in Appendix C.

The standard CROWN algorithm bounds the outputs of the *m*-th layer of a neural network by backpropagating linear bounds over each intermediate activation function to the input layer. In the case of interval parameters, the sign of a particular weight may be ambiguous (when the interval spans zero), making it impossible to determine which linear bound to back-propagate. In such cases, we propagate a concrete bound for that neuron instead of its linear bounds.

When bounding the *m*-th layer of a neural network, we assume that we have pre-activation bounds $\hat{z}^{(k)} \in [l^{(k)}, u^{(k)}]$ on all previous layers on the network. Given such bounds, it is possible to form linear bounds on any non-linear activation function in the network. For the *r*-th neuron in *k*-th layer with activation function $\sigma(z)$, we define two linear functions

 $h_{L,r}^{(k)}(z) = \alpha_{L,r}^{(k)}\left(z + \beta_{L,r}^{(k)}\right), \quad h_{U,r}^{(k)}(z) = \alpha_{U,r}^{(k)}\left(z + \beta_{U,r}^{(k)}\right)$

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such that $h_{L,r}^{(k)}(z) \le \sigma(z) \le h_{U,r}^{(k)}(z) \ \forall z \in \left[l_r^{(k)}, u_r^{(k)}\right]$. The coefficients $\alpha_{U,r}^{(k)}, \alpha_{L,r}^{(k)}, \beta_{U,r}^{(k)}, \beta_{L,r}^{(k)} \in \mathbb{R}$ are readily computed for many common activation functions (Zhang et al., 2018).

Given the pre-activation and activation function bounds, the interval enclosures over the weights $\Omega^{(0:m)}, \Lambda^{(0:m)}$ are computed via a back-propagation procedure. The back-propagation is initialised

with $\mathbf{\Omega}^{(m)} = \mathbf{\Lambda}^{(m)} = [I^{n_m}, I^{n_m}]$ and proceeds as follows:

$$\mathbf{\Lambda}^{(k-1)} = \left(\mathbf{\Lambda}^{(k)} \otimes \mathbf{W}^{(k)}\right) \odot \lambda^{(k-1)}, \quad \lambda_{j,i}^{(k)} = \begin{cases} \alpha_{U,i}^{(k)} & \text{if } k \neq 0, \ 0 \leq \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \\ \alpha_{L,i}^{(k)} & \text{if } k \neq 0, \ 0 \geq \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \\ 0 & \text{if } k \neq 0, \ 0 \in \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \end{cases}$$

$$\begin{array}{c} \mathbf{870} \\ \mathbf{871} \\ \mathbf{872} \\ \mathbf{873} \\ \mathbf{873} \\ \mathbf{874} \\ \mathbf{875} \\ \mathbf{876} \\ \mathbf{877} \end{array} \qquad \mathbf{\Omega}^{(k-1)} = \left(\mathbf{\Omega}^{(k)} \otimes \mathbf{W}^{(k)}\right) \odot \omega^{(k-1)}, \quad \omega_{j,i}^{(k)} = \begin{cases} \alpha_{L,i}^{(k)} & \text{if } k \neq 0, \ 0 \leq \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \\ \alpha_{U,i}^{(k)} & \text{if } k \neq 0, \ 0 \geq \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \\ 0 & \text{if } k \neq 0, \ 0 \in \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)}\right]_{j,i} \\ 1 & \text{if } k = 0. \end{cases}$$

where we use $0 \leq [\cdot]$ and $0 \geq [\cdot]$ to denote that an interval is strictly positive or negative, respectively. Finally, the bias terms $\Delta^{(k)}, \Theta^{(k)}$ for all k < m can be computed as

$$\Delta_{i,j}^{(k)} = \begin{cases} \beta_{U,i}^{(k)} & \text{if } 0 \le \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \\ \beta_{L,i}^{(k)} & \text{if } 0 \ge \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \\ u^{(k)} & \text{if } 0 \in \left[\mathbf{\Lambda}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \\ \end{cases}_{j,i}^{(k)}, \Theta_{i,j}^{(k)} = \begin{cases} \beta_{L,i}^{(k)} & \text{if } 0 \le \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \\ \beta_{U,i}^{(k)} & \text{if } 0 \ge \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \\ l^{(k)} & \text{if } 0 \in \left[\mathbf{\Omega}^{(k+1)} \otimes \mathbf{W}^{(k+1)} \right]_{j,i} \end{cases}$$

with the *m*-th bias terms given by $\Theta_{i,j}^{(m)} = \Delta_{i,j}^{(m)} = 0$.

Closed-Form Global Bounds. Given the two functions $f_i^L(\cdot), f_i^U(\cdot)$ as defined above and intervals over all the relevant variables, we can compute the following closed-form global bounds:

$$\gamma_{j}^{L} = \min\left\{\boldsymbol{\Omega}_{j,:}^{(0)} \otimes \boldsymbol{x} \oplus \sum_{k=1}^{m} \boldsymbol{\Omega}_{j,:}^{(k)} \otimes \left[\boldsymbol{b}^{(k)} \oplus \Theta_{:,j}^{(k)}\right]\right\}$$
$$\gamma_{j}^{U} = \max\left\{\boldsymbol{\Lambda}_{j,:}^{(0)} \otimes \boldsymbol{x} \oplus \sum_{k=1}^{m} \boldsymbol{\Lambda}_{j,:}^{(k)} \otimes \left[\boldsymbol{b}^{(k)} \oplus \Delta_{:,j}^{(k)}\right]\right\}$$

where \min / \max are performed element-wise and return the lower / upper bounds of each interval enclosure. Then, we have $\gamma_j^L \leq f_j(x) \leq \gamma_j^U$ for all $x \in \mathbf{x}$, $b^{(k)} \in \mathbf{b}^{(k)}$ and $W^{(k)} \in \mathbf{W}^{(k)}$, which suffices to bound the output of the neural network as required to further bound the gradient of the network.

Е **BOUNDS ON LOSS FUNCTION GRADIENTS**

In this section we present the computation of bounds on the first partial derivative of the loss function required for Algorithm 1. In particular, we consider bounding the following optimization problem via interval arithmetic:

$$\min \& \max \left\{ \partial \mathcal{L} \left(y^{\star}, y' \right) / \partial y^{\star} \mid y^{\star} \in \left[y^{L}, y^{U} \right], \| y' - y^{t} \|_{q} \leq \nu \right\}$$

for some loss function \mathcal{L} where $[y^L, y^U]$ are bounds on the logits of the model (obtained via the bound-propagation procedure), y^t is the true label and y' is the poisoned label.

Mean Squared Error Loss Taking $\mathcal{L}(y^*, y') = \|y^* - y'\|_2^2$ to be the squared error and considering the $q = \infty$ norm, the required bounds are given by:

$$egin{aligned} \partial l^L &= 2\left(y^L - y^t -
u
ight) \ \partial l^U &= 2\left(y^U - y^t +
u
ight) \end{aligned}$$

The loss itself can be upper-bounded by $l^U = \max\{(y^L - y^t)^2, (y^U - y^t)^2\}$ and lower bounded by

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$$l^{L} = \begin{cases} 0 & \text{if } y^{t} \in [y^{L}, y^{U}] \\ \min\{(y^{L} - y^{t})^{2}, (y^{U} - y^{t})^{2}\} & \text{otherwise} \end{cases}$$
(17)

Cross Entropy Loss To bound the gradient of the cross entropy loss, we first bound the output probabilities $p_i = [\sum_j \exp(y_j^* - y_i^*)]^{-1}$ obtained by passing the logits through the softmax function:

$$p_i^L = \left[\sum_j \exp\left(y_j^U - y_i^L\right)\right]^{-1}, \quad p_i^U = \left[\sum_j \exp\left(y_j^L - y_i^U\right)\right]^{-1}$$

The categorical cross entropy loss and its first partial derivative are given by

$$\mathcal{L}(y^{\star}, y') = -\sum_{i} y_{i}^{t} \log p_{i}, \quad \frac{\partial \mathcal{L}(y^{\star}, y')}{\partial y^{\star}} = p - y^{t}$$

where y^t is a one-hot encoding of the true label. Considering label flipping attacks ($q = 0, \nu = 1$), we can bound the partial derivative by

$$\left[\partial l^L\right]_i = p^L_i - 1, \quad \left[\partial l^U\right]_i = p^U_i - 0$$

In the case of targeted label flipping attacks (e.g. only applying label flipping attacks to / from specific classes), stronger bounds can be obtained by considering the 0-1 bounds only on the indices y_i^t affected by the attack. The cross entropy loss itself is bounded by $l^L = -\sum_i y_i^t \log p_i^U$, $l^U = -\sum_i y_i^t \log p_i^L$.

F BACKWARDS PASS BOUNDS

Given bounds on the forward pass of the neural network, we now turn to bounding the objective of our original problem (10), replacing the forward pass constraints with their bounds computed using our CROWN algorithm,

$$\min \& \max\left\{\frac{\partial}{\partial \theta^{\star}} \left(\mathcal{L}\left(\hat{z}^{(K)}, y^{\star}\right) \right) \mid \theta^{\star} \in \left[\theta^{L}, \theta^{U}\right], \hat{z}^{(k)} \in \left[\hat{z}_{L}^{(k)}, \hat{z}_{U}^{(k)}\right], \|y - y^{\star}\|_{q} \le \nu \right\}.$$
(18)

We extend the interval arithmetic based approach of Wicker et al. (2022), which bounds derivatives of the form $\partial \mathcal{L}/\partial z^{(k)}$, to additionally compute bounds on the derivatives w.r.t. the parameters. First, we back-propagate intervals over y^* (the label) and $\hat{z}^{(K)}$ (the logits) to compute an interval over $\partial \mathcal{L}/\partial \hat{z}^{(K)}$, the gradient of the loss w.r.t. the logits of the network. The procedure for computing this interval is described in Appendix E for a selection of loss functions. We then use interval bound propagation to back-propagate this interval through the network to compute intervals over all gradients:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^{(k-1)}} = \left(\boldsymbol{W}^{(k)}\right)^{\top} \otimes \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{z}}^{(k)}}, \quad \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{z}}^{(k)}} = \left[H\left(\hat{z}_{L}^{(k)}\right), H\left(\hat{z}_{U}^{(k)}\right)\right] \odot \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^{(k)}} \\ \frac{\partial \mathcal{L}}{\partial \boldsymbol{W}^{(k)}} = \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{z}}^{(k)}} \otimes \left[\left(z_{L}^{(k-1)}\right)^{\top}, \left(z_{U}^{(k-1)}\right)^{\top}\right], \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}^{(k)}} = \frac{\partial \mathcal{L}}{\partial \hat{\boldsymbol{z}}^{(k)}}$$

where $H(\cdot)$ is the Heaviside function, and \circ is the element-wise product. The resulting intervals are valid bounds the objective of our original problem (10) and its relaxation (18). That is, the gradients of the network lie within these intervals for all $W^{(k)} \in \mathbf{W}^{(k)}$, $b^{(k)} \in \mathbf{b}^{(k)}$, $||x - x^*||_p \leq \epsilon$, and $||y - y^*||_q \leq \nu$.

G COMPUTING BOUNDS ON POISONING OBJECTIVES

In this section, we describe a procedure for computing bounds on each of the poisoning adversary's objectives. Given any objective J and a test set $\{(x^{(i)}, y^{(i)})\}_{i=1}^k$, the poisoning adversary's objective can be relaxed by taking each test sample independently, i.e.

$$\max_{\theta^{\star} \in [\theta^{L}, \theta^{U}]} \frac{1}{k} \sum_{i=1}^{k} J(\theta^{\star}, x^{(i)}, y^{(i)}) \le \frac{1}{k} \sum_{i=1}^{k} \max_{\theta^{\star} \in [\theta^{L}, \theta^{U}]} J(\theta^{\star}, x^{(i)}, y^{(i)}).$$
(19)

971 Thus to bound the original poisoning objectives (3), (4), and (5), it suffices to compute bounds on the required quantity for each test sample independently.

972 **Denial of Service.** Computing bounds on the optimization problem

$$\max_{\star \in [\theta^L, \theta^U]} \mathcal{L}\left(f^{\theta^\star}(x^{(i)}), y^{(i)}\right) \tag{20}$$

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for the cross-entropy and mean-squared-error losses is described in Section E.

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Certified Prediction and Backdoor Robustness. Computing an bounds on

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$$\max_{\mathfrak{t}^{\star} \in [\theta^{L}, \theta^{U}]} \mathbb{1}\left(f^{\theta^{\star}}(x^{(i)}) \notin S\right)$$
(21)

corresponds to checking if $f^{\theta^{\star}}(x^{(i)})$ lies within the safe set S for all $\theta^{\star} \in [\theta^L, \theta^U]$. As before, we first compute bounds f^L, f^U on $f^{\theta^{\star}}(x^{(i)})$ using our CROWN-based bounds. Given these bounds and assuming a multi-class classification setting, the predictions *not* reachable by any model within $[\theta^L, \theta^U]$ are those whose logit upper bounds lie below the logit lower bound of any other class. That is, the set of possible predictions S' is given by

$$S' = \left\{ i \text{ s.t. } \nexists j : f_i^U \le f_j^L \right\}.$$

$$(22)$$

988 If $S' \subseteq S$, then $\max_{\theta^*} \mathbb{1}(f^{\theta^*}(x^{(i)}) \notin S) = 0$.

Backdoor attack robustness is computed in an analogous way, with the only difference being the logit bounds f^L , f^U being computed over all $x \in V(x)$ and $\theta^* \in [\theta^L, \theta^U]$. This case is also computed via our CROWN-based bound propagation.

H COMPARISON WITH EMPIRICAL ATTACKS

In this section, we compare the tightness of our bounds with simple heuristic poisoning attacks for both the UCI-houseelectric and OCT-MNIST datasets.

H.1 VISUALISING ATTACKS IN PARAMETER SPACE (UCI-HOUSEELECTRIC)



Figure 6: Training trajectory for selected parameters under parameter-targeted feature poisoning with an adversary of $\epsilon = 0.02, n = 2000, p = \infty$. The coloured boxes show the bounds $[\theta_L, \theta_U]$ obtained at each training iteration using AGT.

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First, we investigate the tightness of our bounds in parameter space via a feature poisoning attack. The attack's objective is to maximize a given scalar function of the parameters, which we label $f^{\text{targ}}(\theta)$. We then take the following poisoning procedure at each training iteration:

- 1. Randomly sample a subset of n samples from the current training batch.
- 2. For each selected sample $x^{(i)}$, compute a poison $v^{(i)}$ such that $x^{(i)} + v^{(i)}$ maximizes the gradient $\partial f^{\text{targ}}/\partial x$ subject to $\|v^{(i)}\|_p \leq \epsilon$.
- 3. Add the noise to each of the *n* sampled points to produce the poisoned dataset.

1022 The noise in step 2 is obtained via projected gradient descent (PGD). To visualise the effect of our 1023 attack in parameter space, we plot the trajectory taken by two randomly selected parameters θ_i, θ_j 1024 from the network. We then run our poisoning attack on a collection of poisoning objectives f^{targ} , 1025 such as $\theta_i + \theta_j, \theta_i, -\theta_j$, etc. The effect of our poisoning attack is to perturb the training trajectory in the direction to maximize the given objective. Figure 6 shows the result of this poisoning procedure for a random selection of parameter training trajectories. We can see that the poisoned trajectories (in black) lie close the clean poisoned trajectory, while our bounds represent an over-approximation of all the possible training trajectories.

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H.2 FEATURE-SPACE COLLISION ATTACK (UCI-HOUSEELECTRIC)



Figure 7: Mean squared error on the target point $(x^{\text{target}}, y^{\text{target}})$ in the UCI-house electric dataset. Black lines show loss trajectories under the randomized feature-collision poisoning attack.

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We now consider an unbounded attack setting where the adversary's goal is to prevent the model from learning a particular training example $(x^{\text{target}}, y^{\text{target}})$. We again consider a simple randomized attack setting, where the adversary first selects a subset of n samples from each training batch. The adversary then replaces the features of each of the n samples with x^{target} , and assigns each one a randomly generated label. In this way, the adversary aims to obscure the true target label and prevent the model from learning the pair $(x^{\text{target}}, y^{\text{target}})$.

Figure 7 shows the loss of the model on the target point at each training iteration. To investigate the tightness of our loss lower bound, we also consider the case where the adversary replaces all of the n sampled instances from the batch with the true $(x^{\text{target}}, y^{\text{target}})$, thus over-representing the sample within the batch and causing the model to fit the target point faster. The bounds (in red) are obtained from AGT with an unbounded adversary ($\kappa = 0.05$). We can see that although our bounds are not tight to any of the attacks considered, they remain sound for all the poisoned training trajectories.

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1064 H.3 RANDOMIZED LABEL FLIPPING ATTACK (OCT-MNIST)

Here, we present the results of a label-flipping attack conducted on the OCT-MNIST dataset. Following the approach 1067 described in Section 4, we begin by pre-training a binary 1068 classification model to distinguish between two diseased 1069 classes and a healthy class. Next, we fine-tune the model's 1070 final dense layers on the 'Drusen' class, which we assume 1071 to be potentially compromised, using a training set com-1072 posed of 50% clean data and 50% Drusen data, with 3000 1073 samples from each category in each batch. Given that the 1074 Drusen class is a minority, we simulate a scenario where a 1075 random subset of the Drusen data is incorrectly labeled as 1076 the 'healthy' class. Figure 8 displays the model's accuracy when trained on the poisoned dataset. We can see that train-1077 ing on the mis-labelled data results in a significant decrease 1078 in model accuracy, though the poisoned accuracy remains 1079 within the bounds of certified by AGT.



Figure 8: Accuracy on the OCT-MNIST dataset under a random label flipping attack on the Drusen class.

1080 I PROOFS

PROOF OF THEOREM 3.1 (BOUNDING ADVERSARY GOALS VIA PARAMETER SPACE I.1 BOUNDS) 1084

We begin the proof by writing out the form of the function we wish to optimize, J, for each attack setting considered. Below the right hand side of the inequality is taken to be the function J, and each 1086 inequality is the statement we would like to prove. 1087

1088 For denial of service our bound becomes:

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$$\max_{\mathcal{D}' \in \mathcal{T}} \frac{1}{k} \sum_{i=1}^{k} \mathcal{L} \left(f^{M(f,\theta',\mathcal{D}')}(x^{(i)}), y^{(i)} \right) \le \max_{\theta^{\star} \in [\theta^{L},\theta^{U}]} \frac{1}{k} \sum_{i=1}^{k} \mathcal{L} \left(f^{\theta^{\star}}(x^{(i)}), y^{(i)} \right)$$

For certified prediction poisoning robustness our bound becomes: 1093

$$\max_{\mathcal{D}'\in\mathcal{T}}\frac{1}{k}\sum_{i=1}^{k}\mathbb{1}\left(f^{M(f,\theta',\mathcal{D}')}(x^{(i)})\notin S\right)\leq \max_{\theta^{\star}\in[\theta^{L},\theta^{U}]}\frac{1}{k}\sum_{i=1}^{k}\mathbb{1}\left(f^{\theta^{\star}}(x^{(i)})\notin S\right)$$

And for backdoor attacks our bound becomes:

$$\max_{\mathcal{D}'\in\mathcal{T}} \frac{1}{k} \sum_{i=1}^{k} \mathbb{1}\left(\exists x^{\star} \in V(x^{(i)}) \ s.t. \ f^{M(f,\theta',\mathcal{D}')}(x^{\star}) \notin S\right)$$

$$\leq \max_{\theta^{\star} \in [\theta^{L}, \theta^{U}]} \frac{1}{k} \sum_{i=1}^{k} \mathbb{1} \left(\exists x^{\star} \in V(x^{(i)}) \ s.t. \ f^{\theta^{\star}}(x^{\star}) \notin S \right)$$

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1105 **Proof:** Without loss of generality, take the function we wish to optimize to be denoted simply by J. By definition, there exists a parameter, $\theta^{\circ} = M(f, \theta', \mathcal{D}')$ resulting from a particular dataset 1106 $\mathcal{D}' \in \mathcal{T}(\mathcal{D})$ such that θ° provides a (potentially non-unique) optimal solution to the optimization 1107 problem we wish to bound, i.e., the left hand side of the inequalities above. Given a valid parameter 1108 space bound $[\theta^L, \theta^U]$ satisfying Equation 6, we have that necessarily, $\theta^\circ \in [\theta^L, \theta^U]$. Therefore, the 1109 result of optimizing over $[\theta^L, \theta^U]$ can provide at a minimum the bound realized by θ° ; however, due 1110 to approximation, this bound might not be tight, so optimizing over $[\theta^L, \theta^U]$ provides an upper-bound, 1111 thus proving the inequalities above. 1112

1113 I.2 PROOF OF THEOREM 3.2 (ALGORITHM CORRECTNESS) 1114

1115 Here we provide a proof of correctness for our algorithm (i.e., proof of Theorem 3.2) as well as a 1116 detailed discussion of the operations therein.

1117 First, we recall the definition of valid parameter space bounds (Equation 6 in the main text): 1118

$$\theta_i^L \le \min_{\mathcal{D}' \in \mathcal{T}(\mathcal{D})} M(f, \theta', \mathcal{D}')_i \le M(f, \theta', \mathcal{D})_i \le \max_{\mathcal{D}' \in \mathcal{T}(\mathcal{D})} M(f, \theta', \mathcal{D}')_i \le \theta_i^U$$

1121 As well as the iterative equations for stochastic gradient descent:

$$\theta \leftarrow \theta - \alpha \Delta \theta, \qquad \Delta \theta \leftarrow \frac{1}{|\mathcal{B}|} \sum_{(x,y) \in \mathcal{B}} \nabla_{\theta} \mathcal{L}\left(f^{\theta}(x), y\right)$$

1125 For ease of notation, we assume a fixed data ordering (one may always take the element-wise 1126 maximums/minimums over the entire dataset rather than each batch to relax this assumption). 1127

Now, we proceed to prove by induction that Algorithm 1 maintains valid parameter space bounds 1128 on each step of gradient descent. We start with the base case of $\theta^L = \theta^{\hat{U}} = \theta'$ according to line 1129 1, which are valid parameter-space bounds. Our inductive hypothesis is that, given valid parameter 1130 space bounds satisfying Definition 1, each iteration of Algorithm 1 (lines 4–8) produces a new θ^L 1131 and θ^U that satisfy also Definition 1. 1132

First, we observe that lines 4–5 simply compute the normal forward pass. Second, we note that lines 1133 6–7 compute valid bounds on the descent direction for all possible poisoning attacks within $\mathcal{T}(\mathcal{D})$. In 1134 other words, the inequality $\Delta \theta^L \leq \Delta \theta \leq \Delta \theta^U$ holds element-wise for any possible batch $\tilde{\mathcal{B}} \in \mathcal{T}(\mathcal{D})$. Combining this largest and smallest possible update with the smallest and largest previous parameters yields the following bounds:

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1147 1148 $\theta^L - \alpha \Delta \theta^U \leq \theta - \alpha \Delta \theta \leq \theta^U - \alpha \Delta \theta^L$

which, by definition, constitute valid parameter-space bounds and, given that these bounds are exactly those in Algorithm 1, we have that Algorithm 1 provides valid parameter space bounds as desired. \Box

1142I.3PROOF OF THEOREM B.1 (DESCENT DIRECTION BOUND FOR UNBOUNDED1143ADVERSARIES)

The nominal clipped descent direction for a parameter θ is the averaged, clipped gradient over a training batch \mathcal{B} , defined as

$$\Delta \theta = \frac{1}{b} \sum_{i=1}^{b} \operatorname{Clip}_{\kappa} \left[\delta^{(i)} \right]$$

where each gradient term is given by $\delta^{(i)} = \nabla_{\theta} \mathcal{L} \left(f^{\theta} \left(x^{(i)} \right), y^{(i)} \right)$. Our goal is to bound this descent direction for the case when (up to) *n* points are removed or added to the training data, for any $\theta \in [\theta_L, \theta_U]$. We begin by bounding the descent direction for a fixed, scalar θ , then generalize to all $\theta \in [\theta_L, \theta_U]$ and to the multi-dimensional case (i.e., multiple parameters). We present only the upper bounds here; analogous results apply for lower bounds.

Bounding the descent direction for a fixed, scalar θ . Consider the effect of removing up to n data points from batch \mathcal{B} . Without loss of generality, assume the gradient terms are sorted in descending order, i.e., $\delta^{(1)} \ge \delta^{(2)} \ge \cdots \ge \delta^{(b)}$. Then, the average clipped gradient over all points can be bounded above by the average over the largest b - n terms:

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1178 1179 1180 $\Delta \theta = \frac{1}{b} \sum_{i=1}^{b} \operatorname{Clip}_{\kappa} \left[\delta^{(i)} \right] \leq \frac{1}{b-n} \sum_{i=1}^{b-n} \operatorname{Clip}_{\kappa} \left[\delta^{(i)} \right]$ This bound corresponds to removing the *n* points with the smallest gradients.

1163 Next, consider adding n arbitrary points to the training batch. Since each added point contributes at 1164 most κ due to clipping, the descent direction with up to n removals and n additions is bounded by 1165

$$\frac{1}{b}\sum_{i=1}^{b}\operatorname{Clip}_{\kappa}\left[\delta^{(i)}\right] \leq \frac{1}{b-n}\sum_{i=1}^{b-n}\operatorname{Clip}_{\kappa}\left[\delta^{(i)}\right] \leq \frac{1}{b}\left(n\kappa + \sum_{i=1}^{b}\operatorname{Clip}_{\kappa}\left[\delta^{(i)}\right]\right)$$

where the bound now accounts for replacing the n smallest gradient terms with the maximum possible value of κ from the added samples.

Bounding the effect of a variable parameter interval. We extend this bound to any $\theta \in [\theta_L, \theta_U]$. Assume the existence of upper bounds $\delta_U^{(i)}$ on the clipped gradients for each data point over the interval, such that

$$\delta_{U}^{(i)} \ge \operatorname{Clip}_{\kappa} \left[\nabla_{\theta'} \mathcal{L} \left(f^{\theta'}(x^{(i)}), y^{(i)} \right) \right] \quad \forall \, \theta' \in [\theta_L, \theta_U]$$

1176 Then, using these upper bounds, we further bound $\Delta \theta$ as

$$\Delta \theta \leq \frac{1}{b} \left(n\kappa + \sum_{i=1}^{b} \operatorname{Clip}_{\kappa} \left[\delta_{U}^{(i)} \right] \right)$$

1181 where, as before, we assume $\delta_U^{(i)}$ are indexed in descending order. 1182

Extending to the multi-dimensional case. To generalize to the multi-dimensional case, we apply the above bound component-wise. Since gradients are not necessarily ordered for each parameter component, we introduce the $SEMax_n$ operator, which selects and sums the largest *n* terms at each index. This yields the following bound on the descent direction:

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$$\Delta \theta \leq \frac{1}{b} \left(\operatorname{SEMax}_{b-n} \left\{ \delta_U^{(i)} \right\}_{i=1}^b + n\kappa \mathbf{1}_d \right)$$

1188 which holds for any $\theta \in [\theta_L, \theta_U]$ and up to *n* removed and replaced points. 1189

We have established the upper bound on the descent direction. The corresponding lower bound can 1190 be derived by reversing the inequalities and substituting SEMax with the analogous minimization 1191 operator, SEMin. 1192

1193 L.4 PROOF OF THEOREM 3.3 (DESCENT DIRECTION BOUND FOR BOUNDED ADVERSARIES) 1194

1195 The nominal descent direction for a parameter θ is the averaged gradient over a training batch \mathcal{B} , 1196 defined as $\Delta \theta = \frac{1}{b} \sum_{i=1}^{b} \delta^{(i)}$

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where each gradient term is given by $\delta^{(i)} = \nabla_{\theta} \mathcal{L}\left(f^{\theta}\left(x^{(i)}\right), y^{(i)}\right)$. Our goal is to upper bound 1201 this descent direction when up to n points are poisoned in the feature space and up to m points are 1202 poisoned in the label space. The bound is additionally computed with respect to any $\theta \in [\theta_L, \theta_U]$. 1203 We again begin by bounding the descent direction for a fixed θ , then generalize to all $\theta \in [\theta_L, \theta_U]$. We present only the upper bounds here, though corresponding results for the lower bound can be 1204 shown by reversing the inequalities and replacing SEMax with SEMin. 1205

1206 **Bounding the descent direction for a fixed** θ **.** Consider the effect of poisoning either the features or 1207 the labels of a data point. For a given data point, an adversary may choose to poison its features, its 1208 labels, or both. In total, at most n + m points may be influenced by the poisoning adversary, which 1209 corresponds to choosing a disjoint sets for label and feature poisoning. We assume that $m + n \le b$, 1210 otherwise take at most min(m + n, b) points to be poisoned.

1211 Assume that we have access to sound gradient upper bounds 1212

$$\delta^{(i)} \leq \tilde{\delta}_U^{(i)} \quad \forall \delta^{(i)} \in \left\{ \nabla_{\theta'} \mathcal{L}\left(f^{\theta'}\left(\tilde{x}\right), \tilde{y}\right) \mid \|x^{(i)} - \tilde{x}\|_p \leq \epsilon, \|y^{(i)} - \tilde{y}\|_q \leq \nu \right\}.$$

1215 where the inequalities are interpreted element-wise. Here, $\tilde{\delta}_{U}^{(i)}$ corresponds to an upper bound on the 1216 maximum possible gradient achievable at the data-point $(x^{(i)}, y^{(i)})$ through poisoning. 1217

The adversary's maximum possible impact on the descent direction at any point i is given by $\delta_{II}^{(i)} - \delta^{(i)}$. 1218 1219 To maximise an upper bound on $\Delta \theta$, we consider the n+m points with the largest possible adversarial contributions. Therefore, we obtain 1220

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where the SEMax operation corresponds to taking the sum of the largest n + m elements of its 1225 argument at each element. This bound captures the maximum increase in $\Delta \theta$ that an adversary can 1226 induce by poisoning up to m + n data points. 1227

 $\Delta \theta = \frac{1}{b} \sum_{i=1}^{b} \delta^{(i)} \le \frac{1}{b} \left(\operatorname{SEMax}_{m+n} \left\{ \tilde{\delta}_{U}^{(i)} - \delta^{(i)} \right\}_{i=1}^{b} + \sum_{i=1}^{b} \delta^{(i)} \right),$

Bounding the effect of a variable parameter interval. Now, we wish to compute a bound on $\Delta \theta$ 1228 for any $\theta \in [\theta_L, \theta_U]$. To achieve this, we extend our previous gradient bounds to account for the interval over our parameters. Specifically, we define upper bounds on the nominal and adversarially 1230 perturbed gradients that hold across the entire parameter interval: 1231

$$\begin{split} \delta &\leq \delta_U^{(i)} \quad \forall \delta \in \left\{ \nabla_{\theta'} \mathcal{L} \left(f^{\theta'}(x^{(i)}), y^{(i)} \right) \mid \theta' \in [\theta^L, \theta^U] \right\}, \\ \tilde{\delta} &\leq \tilde{\delta}_U^{(i)} \quad \forall \tilde{\delta} \in \left\{ \nabla_{\theta'} \mathcal{L} \left(f^{\theta'}\left(\tilde{x} \right), \tilde{y} \right) \mid \theta' \in [\theta^L, \theta^U], \|x^{(i)} - \tilde{x}\|_p \leq \epsilon, \|y^{(i)} - \tilde{y}\|_q \leq \nu \right\}. \end{split}$$

1236 Thus, the descent direction is upper bounded by

$$\Delta \theta \le \Delta \theta^U = \frac{1}{b} \left(\operatorname{SEMax}_{m+n} \left\{ \tilde{\delta}_U^{(i)} - \delta_U^{(i)} \right\}_{i=1}^b + \sum_{i=1}^b \delta_U^{(i)} \right)$$

for all $\theta \in [\theta_L, \theta_U]$, where the appropriate bounds with respect to the parameter interval have been 1241 substituted in.

1242 PROOF OF PROPOSITION 1 (CROWN BOUNDS) I.5 1243

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1244 To prove Proposition 1, we rely on the following result which we reproduce from Zhang et al. (2018): 1245 **Theorem I.1** (Explicit output bounds of a neural network f (Zhang et al., 2018)). Given an m-layer neural network function $\hat{f}: \mathbb{R}^{n_0} \to \mathbb{R}^{n_m}$, there exists two explicit functions $f_i^L: \mathbb{R}^{n_0} \to \mathbb{R}$ and 1246 $f_j^U : \mathbb{R}^{n_0} \to \mathbb{R}$ such that $\forall j \in [n_m], \forall x \in \mathbb{B}_p(x_0, \epsilon)$, the inequality $f_j^L(x) \le f_j^U(x)$ holds 1247 1248 true, where

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$$f_{j}^{U}(x) = \Lambda_{j,:}^{(0)} x + \sum_{k=1}^{m} \Lambda_{j,:}^{(k)} \left(b^{(k)} + \Delta_{:,j}^{(k)} \right), \quad \Lambda_{j,:}^{(k-1)} = \begin{cases} e_{j}^{\top} & \text{if } k = m+1; \\ \left(\Lambda_{j,:}^{(k)} W^{(k)} \right) \circ \lambda_{j,:}^{(k-1)} & \text{if } k \in [m]. \end{cases}$$
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$$f_{j}^{L}(x) = \Omega_{j,:}^{(0)}x + \sum_{k=1}^{m} \Omega_{j,:}^{(k)} \left(b^{(k)} + \Theta_{:,j}^{(k)} \right), \quad \Omega_{j,:}^{(k-1)} = \begin{cases} e_{j}^{\top} & \text{if } k = m+1; \\ \left(\Omega_{j,:}^{(k)} W^{(k)} \right) \circ \omega_{j,:}^{(k-1)} & \text{if } k \in [m] \end{cases}$$
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and $\forall i \in [n_k]$, we define four matrices $\lambda^{(k)}, \omega^{(k)}, \Delta^{(k)}, \Theta^{(k)} \in \mathbb{R}^{n_m \times n_k}$: 1255

$$\begin{array}{ll} \textbf{1256} \\ \textbf{1257} \\ \textbf{1258} \\ \textbf{1258} \\ \textbf{1259} \\ \textbf{1259} \\ \textbf{1260} \\ \textbf{1260}$$

$$\begin{array}{l} \mathbf{1261} \\ \mathbf{1262} \\ \mathbf{1263} \end{array} \quad \Delta_{i,j}^{(k)} = \begin{cases} \beta_{U,i}^{(k)} & \text{if } k \neq m, \Lambda_{j,i}^{(k+1)} W_{:,i}^{(k+1)} \geq 0; \\ \beta_{L,i}^{(k)} & \text{if } k \neq m, \Lambda_{j,i}^{(k+1)} W_{:,i}^{(k+1)} < 0; \\ 0 & \text{if } k = m. \end{cases} \quad \Theta_{i,j}^{(k)} = \begin{cases} \beta_{L,i}^{(k)} & \text{if } k \neq m, \Lambda_{j,i}^{(k+1)} W_{i,i}^{(k+1)} \geq 0; \\ \beta_{U,i}^{(k)} & \text{if } k \neq m, \Omega_{j,i}^{(k+1)} W_{i,i}^{(k+1)} < 0; \\ 0 & \text{if } k = m. \end{cases} \end{cases}$$

and \circ is the Hadamard product and $e_j \in \mathbb{R}^{n_m}$ is a standard unit vector at j th coordinate. 1264

1265 The terms $\alpha_{L,i}^{(k)}, \alpha_{U,i}^{(k)}, \beta_{L,i}^{(k)}$, and $\beta_{U,i}^{(k)}$ represent the coefficients of linear bounds on the activation 1266 functions, that is for the r-th neuron in k-th layer with activation function $\sigma(x)$, there exist two linear 1267 functions 1268

$$h_{L,r}^{(k)}(x) = \alpha_{L,r}^{(k)} \left(x + \beta_{L,r}^{(k)} \right), \quad h_{U,r}^{(k)}(x) = \alpha_{U,r}^{(k)} \left(x + \beta_{U,r}^{(k)} \right)$$

1270 such that $h_{L,r}^{(k)}(x) \leq \sigma(x) \leq h_{U,r}^{(k)}(x) \ \forall x \in \left[l_r^{(k)}, u_r^{(k)}\right]$. The terms $\left[l_r^{(k)}, u_r^{(k)}\right]$ are assumed to be sound bounds on all previous neurons in the network. We first note that, for any neuron r in the k-th 1271 1272 layer, the linear bounds may be replaced with concrete bounds by substituting $\alpha_{L,r}^{(k)} = \alpha_{U,r}^{(k)} = 0$ and 1273 $\beta_{L,r}^{(k)} = l_r^{(k)}, \beta_{U,r}^{(k)} = u_r^{(k)}$. Let S^L, S^U be index sets of tuples (i, k) indicating whether the lower and 1274 1275 upper bounds (respectively) of the *i*-th neuron in the *k*-th layer should be concretized in this way. 1276 Then, the equivalent weights and biases take the following form:

$$\begin{aligned} & 1277 \\ & 1278 \\ & 1279 \\ & 1279 \\ & 1280 \\ & 1280 \\ & 1281 \\ & 1281 \\ & 1282 \\ & 1281 \\ & 1282 \\ & 1282 \\ & 1282 \\ & 1282 \\ & 1282 \\ & 1282 \\ & 1283 \\ & 1284 \\ & 1285 \\ & 1284 \\ & 1285 \\ & 1285 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1286 \\ & 1287 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1288 \\ & 1289 \\ & 1290 \\ & 1290 \\ & 1291 \\ & 1290 \\ & 1291 \\ & 1291 \\ & 1292 \\ & 1292 \\ & 1292 \\ & 1292 \\ & 1292 \\ & 1293 \\ & \Theta_{...}^{(k)} = \begin{cases} & \alpha_{L,i}^{(k)} & \text{if } (i,k) \notin S^{U}, k \neq 0, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \alpha_{U,i}^{(k)} & \text{if } (i,k) \notin S^{U}, k \neq m, \Lambda_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \beta_{L,i}^{(k)} & \text{if } (i,k) \notin S^{U}, k \neq m, \Lambda_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & 0 & \text{if } (i,k) \notin S^{U}, k = m; \\ & u^{(k)} & \text{if } (i,k) \notin S^{U}, k = m; \\ & u^{(k)} & \text{if } (i,k) \notin S^{U}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} \geq 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,:}^{(k+1)}W_{:,i}^{(k+1)} < 0; \\ & \beta_{U,i}^{(k)} & \text{if } (i,k) \notin S^{L}, k \neq m, \Omega_{j,i}^{(k)} & W_{i,i}^{(k)} < 0; \\ & \beta_{U,i}^{(k)} & W_{i,i}^{(k)} & W_{i,i}^{(k)} & W_{i,i}^{(k$$

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$$0 \quad \text{if } (i,k) \notin S^L, k = m;$$

 $l^{(k)} \quad \text{if } (i,k) \in S^L.$

This is exactly the form described in Appendix D, where S^L and S^U are chosen to be the sets of neurons whose equivalent coefficient interval spans zero. Without this modification, the equivalent weights and biases of such neurons in the original formulation would be undefined. We now have bounds on the output of the neural network for which all operations are well-defined in interval arithmetic.

1301 1302 1303 1304 Replacing all operations in the computation of the equivalent weight terms by their interval arithmetic counterparts, we can compute sound, though over-approximated, intervals over $\Lambda^{(0:m)}$ and $\Omega^{(0:m)}$ which satisfy

$$\Lambda^{(k)} \in \boldsymbol{\Lambda}^{(k)} \quad \forall W^{(1:m)} \in \boldsymbol{W}^{(1:m)}, b^{(1:m)} \in \boldsymbol{b}^{(1:m)},$$
$$\Omega^{(k)} \in \boldsymbol{\Omega}^{(k)} \quad \forall W^{(1:m)} \in \boldsymbol{W}^{(1:m)}, b^{(1:m)} \in \boldsymbol{b}^{(1:m)}.$$

This is trivially true by the definitions of the interval arithmetic operations as given in Appendix C.

1309 Turning to the upper bound (though analagous arguments hold for the lower bound), we have

$$f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) = \Lambda_{j,:}^{(0)} x + \sum_{k=1}^m \Lambda_{j,:}^{(k)} \left(b^{(k)} + \Delta_{:,j}^{(k)}\right)$$

where $\Lambda^{(0:m)}$ are functions of the weights and biases of the network and $\Delta^{(1:m)}$ are constants that depend on the bounds on the intermediate layers of the network. Thus, given parameter intervals $\boldsymbol{b}^{(k)}, \boldsymbol{W}^{(k)}$, the following result holds

$$\begin{aligned} & f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) \leq \max\left\{ f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) \mid \begin{array}{l} W^{(1:m)} \in \boldsymbol{W}^{(1:m)} \\ b^{(1:m)} \in \boldsymbol{b}^{(1:m)} \end{array} \right\} \\ & \leq \max\left\{ f_j^U\left(x, \Lambda^{(0:m)}, \Delta^{(1:m)}, b^{(1:m)}\right) \mid \begin{array}{l} \Lambda^{(0:m)} \in \boldsymbol{\Lambda}^{(0:m)} \\ b^{(1:m)} \in \boldsymbol{b}^{(1:m)} \end{array} \right\} \end{aligned}$$

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for any set of intervals $\Lambda^{(0:m)}$ that satisfy $\{\Lambda^{(k)} | W^{(1:m)} \in W^{(1:m)}\} \subseteq \Lambda^{(k)}$. Since our intervals $\Lambda^{(0:m)}$ computed via interval arithmetic satisfy this property, we have that any valid bound on this maximization problem constitutes a bound on the output of the neural network $f_j(x)$ for any $W^{(1:m)} \in W^{(1:m)}$ and $b^{(1:m)} \in b^{(1:m)}$.

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J EXPERIMENTAL SET-UP AND ADDITIONAL RESULTS

This section details the datasets and hyper-parameters used for the experiments detailed in Section 4.
 All experiments were run on a server equipped with 2x AMD EPYC 9334 CPUs and 2x NVIDIA
 L40 GPUs using an implementation of Algorithm 1 written in Python using Pytorch.

Table 1 shows a run-time comparison of our implementation of Algorithm 1 with (un-certified)
training in Pytorch. We observe that training using Abstract Gradient Training typically incurs a
modest additional cost per iteration when compared to standard training.

	Time per iteration (seconds)				
Dataset	Abstract gradient training	Un-certified training			
UCI House-electric	0.25	0.12			
MNIST (inc. PCA projection)	1.6	1.1			
OCT-MNIST	0.96	0.10			
Udacity Self-Driving	53	42			

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Table 1: Comparison of the run-time of AGT and standard model training in Pytorch.

Table 2 details the datasets along with the number of epochs, learning rate (α) , decay rate (η) and batch size (b) used for each. We note that a standard learning rate decay of the form $(\alpha_n = \alpha/(1+\eta n))$ was applied during training. In the case of fine-tuning both OCT-MNIST and PilotNet, each batch consisted of a mix 70% 'clean' data previously seen during pre-training and 30% new, potentially poisoned, fine-tuning data.

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	Dataset	#Samples	#Features	#Epochs	α	η	b
1351	UCI House-electric	2049280	11	1	0.02	0.2	10000
1352	MNIST	60000	784	3	5.0	1.0	60000
1353	OCT-MNIST	97477	784	2	0.05	5.0	6000
1354	Udacity Self-Driving	31573	39600	$\frac{1}{2}$	0.25	10.0	10000
1355							

Table 2: Datasets and Hyperparameter Settings

COMPARISON WITH DEEP PARTITION AGGREGATION J.1

As discussed in Appendix A, existing approaches seeking certifiable robustness to data poisoning rely on partitioning the dataset and training large ensemble models. Figure 9 compares the guarantees provided by Abstract Gradient Training to those of a popular ensemble method, (Self-Supervised)-Deep Partition Aggregation (SS-DPA) (Levine & Feizi, 2020).

SS-DPA demonstrates both higher nominal and certified accuracies than AGT on the MNIST dataset. However, the ensemble approach is specifically designed to be robust to data poisoning attacks. On the other hand, AGT focuses on certifying an *existing* training algorithm by analyzing the sensitivity of standard training pipelines to data poisoning.

Additionally, our experiments show that AGT incurs a run-time cost of approximately 2-4 times standard training. In contrast, SS-DPA requires training an ensemble of thousands of classifiers, demanding significant data and computational costs. Finally, we highlight once again that AGT is complementary to ensemble approaches, and future works may seek to combine the two.



Figure 9: Comparison of Certified Accuracy on the MNIST dataset under a label flipping attack. Left: Certified Accuracy using AGT for a variety of clipping levels κ . Right: Certified Accuracy using SS-DPA for ensembles of size k = 3000 and k = 1200. Figure reproduced from Levine & Feizi (2020).