Supplementary Material for Adversarial Robustness with Non-uniform Perturbations

Ecenaz Erdemir * Imperial College London e.erdemir17@imperial.ac.uk Jeffrey Bickford Amazon Web Services jbick@amazon.com Luca Melis Amazon Web Services lucmeli@amazon.com

Sergül Aydöre Amazon Web Services saydore@amazon.com

A.1 Toy Example for Non-uniform Perturbations

Adversarial training can be represented as a *min-max optimization*. Given a dataset $\{x_i, y_i\}_{i=1}^n$ with input $x_i \in \mathbb{R}^d$ and classes $y_i \in \mathcal{Y}$, the objective of adversarial training is denoted by

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \max_{\delta \in \Delta} \ell(f_{\theta}(x_i + \delta), y_i)$$
(A.1)

where $f_{\theta} : \mathbb{R}^d \to \mathcal{Y}$ is DNN function, $\ell(.)$ is the loss, e.g. cross-entropy, and Δ is the set of possible adversarial perturbations around the original samples. The adversary's objective is the inner maximization term in equation A.1, and the perturbed samples found as a solution to the norm-constrained inner maximization are called adversarial examples, or AEs.

Consider the 2D toy example of binary classification in Figure A.1 which is obtained by modifying [1]. Figure A.1 illustrates adversarially robust decision boundaries with red and blue regions, and l_2 norm perturbation limits around the data points with black circles. While Figure A.1a shows that adversarially trained model with input constraint $\|\delta\|_2 \leq 0.5$ gains complete robustness against input perturbations, in Figure A.1b there is loss of clean performance due to overlapping regions of increased allowed perturbations. Although the constraint $\|\delta\|_2 \leq 0.5$ might provide sufficient robustness in x-axis, there are still uncovered regions in y-axis in Figure A.1a. On the other hand, when we fit the allowable perturbations to yaxis by choosing a larger perturbation $\|\delta\|_2 \leq 0.8$, x-axis suffers from unnecessary overlaps. This can be solved by customizing the perturbation constraint such that the perturbation radius in x-axis fol-



Figure A.1: Classification boundaries from adversarial training with uniform perturbation limits for (a) $\|\delta\|_2 \le 0.5$, (b) $\|\delta\|_2 \le 0.8$ and non-uniform perturbation limits for (c) $|\delta_x| \le 0.5$ and $|\delta_y| \le 0.8$.

lows $|\delta_x| \leq 0.5$ and the radius in y-axis follows $|\delta_y| \leq 0.8$, which results in an ellipsoid perturbation

^{*}Work done at Amazon Web Services.

³⁵th Conference on Neural Information Processing Systems (NeurIPS 2021).

region in 2D as shown in Figure A.1c. This toy example highlights the advantage of a non-uniform constraint across both axes.

Uniformly perturbing all pixels in an image is often imperceptible to the human eye, but uniform perturbations are wholly inappropriate in many tabular datasets, where positive and negative correlations are strong, consistent, and meaningful. For example, in the German dataset used in Section 3.2, we find the largest positive correlation (0.62) between the amount of credit and the payment duration, while the largest negative correlation (-0.31) is between the checking account status and the credit risk score. Both relationships are intuitive, and both would be broken by applying uniform perturbations.

A.2 Ember Dataset Features

The EMBER dataset [2] consists of two types of features:

- 1. **Parsed features** are extracted after parsing the portable executable (PE) file. Parsed features include 5 different groups:
 - *General file information*: virtual size of the file; number of imported/exported functions and symbols; whether the file has a debug section, thread local storage, resources, relocations, or a signature.
 - *Header information*: timestamp in the header; target machine; list of image and DLL characteristics; target subsystem; file magic; image, system and subsystem versions; code, headers and commit sizes (hashing trick).
 - Imported functions: functions extracted from the import address table (hashing trick)
 - *Exported functions*: list of exported functions (hashing trick).
 - *Section information*: name, size, entropy, virtual size, and a list of strings representing section characteristics (hashing trick).
- 2. Format-agnostic features do not require parsing the PE file structure and include:
 - Byte histogram: counts of each byte value within the file (256 integer values).
 - Byte-entropy histogram: quantized and normalized of the joint distribution p(H, X) of entropy H and byte value X (256 bins).
 - *String information*: number of strings and their average length; a histogram of the printable characters within those strings; entropy of characters across all printable strings.

A.3 DNN Architecture and Pre-processing

In all applications, we use a fully-connected neural network model composed of 4 densely connected layers with the first three using *ReLU* activations followed by a *softmax* activation in the last layer. After each of the first three layers, we apply 20% *Dropout* rate for regularization during training. We use 5 random initialization for malware and 10 for both credit risk and spam detection use-cases to report average results.

For pre-processing, we use standardization as a normalization method, which is a common practice with many machine learning techniques. Min-max scaling transforms all features into the same scale while standardization, which is recommended in presence of outliers [3], only ensures zero mean and unit standard deviation. This approach does not guarantee same range (min and max) for all features. As a result, it is possible that the features have different scales even after normalization.

A.4 Theorem Proofs

Theorem 3.1. If the AEs are generated according to MD constraint, then their γ -consistency has a direct relation to ϵ such that

$$0 < \sqrt{2C - 2\log\gamma} \le \epsilon. \tag{A.2}$$

where $C = -\log(2\pi)^{d/2} |\Sigma_y|^{1/2}$, d is the dimension of x, and $\sqrt{\delta^T \Sigma_y^{-1} \delta} \leq \epsilon$.

Proof. For an AE x that is generated under the Mahalanobis distance constraint, i.e., $x \in \tilde{\Delta}_{\epsilon,2}$, we can write the following bound:

$$\min_{x \in \tilde{\Delta}_{\epsilon,2}} \log f(x \mid y) = C - \frac{1}{2} \delta^T \Sigma_y^{-1} \delta = \log \gamma$$
(A.3)

where the second equality is a result of γ -consistency assumption. Then, by using the upper limit of ℓ_2 Mahalanobis distance of δ for $M = \Sigma_y^{-1}$, we get

$$\sqrt{\delta^T \Sigma_y^{-1} \delta} = \sqrt{2C - 2\log\gamma} \le \epsilon.$$
 (A.4)

Theorem 2.1 implies that there is a direct relationship between limiting the Mahalonobis distance of δ and ensuring consistent samples when the data is Gaussian.

Theorem 4.1. The dual of the linear program 8 can be written as

$$\begin{aligned} \underset{\hat{\nu},\nu}{\text{maximize}} &\quad -\sum_{i=1}^{k-1} \nu_{i+1}^{T} b_{i} + \sum_{i=2}^{k-1} \sum_{j \in \mathcal{I}_{i}} l_{i,j} [\hat{\nu}_{i,j}]_{+} - \hat{\nu}_{1}^{T} x - \epsilon || \Omega^{-1} \hat{\nu}_{1} ||_{q} \\ \text{s.t.} &\quad \nu_{k} = -c, \ \hat{\nu}_{i} = (W_{i}^{T} \nu_{i+1}), \ \text{for } i = k - 1, \dots, 1 \\ &\quad \nu_{i,j} = \begin{cases} 0 & j \in \mathcal{I}_{i}^{-} \\ \hat{\nu}_{i,j} & j \in \mathcal{I}_{i}^{+} \\ \frac{u_{i,j}}{u_{i,j} - l_{i,j}} [\hat{\nu}_{i,j}]_{+} - \eta_{i,j} [\hat{\nu}_{i,j}]_{-} & j \in \mathcal{I}_{i} \end{cases} \end{aligned}$$
(A.5)

where \mathcal{I}_i^- , \mathcal{I}_i^+ and \mathcal{I}_i represent the activation sets in layer *i* for *l* and *u* are both negative, both positive and span zero, respectively.

Proof. The linear program with non-uniform input perturbation and relaxed ReLU constraints can be written as minimize $c^T \hat{z}_k$

$$\begin{array}{ll} \underset{\hat{z}_{k}}{\text{minimize}} & c^{r} z_{k} \\ \text{s.t.} & \hat{z}_{i+1} = W_{i} z_{i} + b_{i}, i = 1, \dots, k-1 \\ & ||\Omega(z_{1} - x)||_{p} \leq \epsilon \\ & z_{i,j} = 0, i = 2, \dots, k-1, j \in \mathcal{I}_{i}^{-} \\ & z_{i,j} = \hat{z}_{i,j}, i = 2, \dots, k-1, j \in \mathcal{I}_{i}^{+} \\ & z_{i,j} \geq 0, \ z_{i,j} \geq \hat{z}_{i,j}, \\ & ((u_{i,j} - l_{i,j})z_{i,j} - u_{i,j}\hat{z}_{i,j}) \leq -u_{i,j}l_{i,j} \end{array} \right\}_{\substack{i=2,\dots,k-1 \\ j \in \mathcal{I}_{i}}} (A.6)$$

We associate the following Lagrangian variables with each of the constraints except the ℓ_p norm constraint in Problem A.6,

$$\hat{z}_{i+1} = W_i z_i + b_i \Rightarrow \nu_{i+1}$$

$$\delta = z_1 - x \Rightarrow \psi$$

$$-z_{i,j} \leq 0 \Rightarrow \mu_{i,j}$$

$$\hat{z}_{i,j} - z_{i,j} \leq 0 \Rightarrow \tau_{i,j}$$

$$((u_{i,j} - l_{i,j})z_{i,j} - u_{i,j}\hat{z}_{i,j}) \leq -u_{i,j}l_{i,j} \Rightarrow \lambda_{i,j}.$$
(A.7)

We do not define explicit dual variables for $z_{i,j} = 0$ and $z_{i,j} = \hat{z}_{i,j}$ since they will be zero in the optimization. Then, we create the following Lagrangian by grouping up the terms with z_i , \hat{z}_i :

$$\begin{split} L(\mathbf{z}, \hat{\mathbf{z}}, \nu, \delta, \lambda, \tau, \mu, \psi) &= -\left(W_{1}^{T}\nu_{2} + \psi\right)^{T} z_{1} - \sum_{\substack{i=2\\j \in \mathcal{I}_{i}}}^{k-1} (\mu_{i,j} + \tau_{i,j} - \lambda_{i,j}(u_{i,j} - l_{i,j}) + (W_{i}^{T}\nu_{i+1})_{j}) z_{i,j} \\ &+ \sum_{\substack{i=2\\j \in \mathcal{I}_{i}}}^{k-1} (\tau_{i,j} - \lambda_{i,j}u_{i,j} + \nu_{i,j}) \hat{z}_{i,j} + (c + \nu_{k})^{T} \hat{z}_{k} - \sum_{i=1}^{k-1} \nu_{i+1}^{T} b_{i} \\ &+ \sum_{\substack{i=2\\j \in \mathcal{I}_{i}}}^{k-1} \lambda_{i,j}u_{i,j} l_{i,j} + \psi^{T} x + \psi^{T} \delta \\ \text{subject to} \quad ||\Omega\delta||_{p} \leq \epsilon \end{split}$$
(A.8)

Now, we take the minimum of L(.) w.r.t \mathbf{z} , $\hat{\mathbf{z}}$ and δ :

$$\inf_{\mathbf{z}, \hat{\mathbf{z}}, \delta} L(\mathbf{z}, \hat{\mathbf{z}}, \nu, \delta, \lambda, \tau, \mu, \psi) = -\inf_{\substack{z_{i,j} \\ j \in \mathcal{I}_i}} \sum_{\substack{i=2 \\ j \in \mathcal{I}_i}}^{k-1} \left(\mu_{i,j} + \tau_{i,j} - \lambda_{i,j} (u_{i,j} - l_{i,j}) + (W_i^T \nu_{i+1})_j \right) z_{i,j} \\
+ \inf_{\hat{\mathbf{z}}} \left(\sum_{\substack{i=2 \\ j \in \mathcal{I}_i}}^{k-1} (\tau_{i,j} - \lambda_{i,j} u_{i,j} + \nu_{i,j}) \hat{z}_{i,j} + (c + \nu_k)^T \hat{z}_k \right) - \sum_{i=1}^{k-1} \nu_{i+1}^T b_i \\
+ \sum_{\substack{i=2 \\ j \in \mathcal{I}_i}}^{k-1} \lambda_{i,j} u_{i,j} l_{i,j} + \psi^T x + \inf_{||\Omega\delta||_p \le \epsilon} \psi^T \delta - \inf_{z_1} (W_1^T \nu_2 + \psi)^T z_1.$$
(A.9)

We can represent the term $\inf_{||\Omega\delta||_p \le \epsilon} \psi^T \delta$ independent of δ using the following dual norm definition.

Cauchy-Schwarz inequality for dual norm:

We can write the Cauchy-Schwarz inequality as $\alpha^T \beta \leq ||\alpha||_p ||\beta||_q$, where $\frac{1}{p} + \frac{1}{q} = 1$ and q norm represents the dual of p norm. Let $\hat{u} = \frac{\alpha}{||\alpha||_p}$, the definition of dual norm is

$$||\beta||_q = \sup_{||\hat{u}||_p \le 1} \hat{u}^T \beta.$$
 (A.10)

We can write $\inf_{\substack{||\Omega\delta||_p \leq \epsilon}} \psi^T \delta = -\sup_{\substack{||\Omega\delta||_p \leq \epsilon}} (-\psi^T \delta) = -\sup_{\substack{||\Omega\delta||_p \leq \epsilon}} \psi^T \delta$. For $\alpha = \frac{\Omega\delta}{\epsilon}$ and $\beta = \epsilon \Omega^{-1} \psi$, we get $\delta^T \psi \leq ||\frac{\Omega\delta}{\epsilon}||_p ||\epsilon \Omega^{-1} \psi||_q$ which implies $-\sup_{\substack{||\Omega\delta||_p \leq \epsilon}} \psi^T \delta = -\epsilon ||\Omega^{-1} \psi||_q$.

Hence, the minimization of L(.) becomes,

$$\inf_{\mathbf{z}, \hat{\mathbf{z}}, \delta} L(.) = \begin{cases}
-\sum_{i=1}^{k-1} \nu_{i+1}^T b_i + \sum_{\substack{i=2\\j \in \mathcal{I}_i}}^{k-1} \lambda_{i,j} u_{i,j} l_{i,j} + \psi^T x - \epsilon ||\Omega^{-1} \psi||_q & \text{if cond.} \\ \\
-\infty & \text{o.w.,}
\end{cases}$$
(A.11)

where the conditions are

$$\nu_{k} = -c$$

$$W_{1}^{T}\nu_{2} = -\psi$$

$$\nu_{i,j} = 0, \ j \in \mathcal{I}_{i}^{-}$$

$$\nu_{i,j} = (W_{i}^{T}\nu_{i+1})_{j}, \ j \in \mathcal{I}_{i}^{+}$$

$$((u_{i,j} - l_{i,j})\lambda_{i,j} - \mu_{i,j} - \tau_{i,j}) = (W_{i}^{T}\nu_{i+1})_{j}$$

$$= u_{i,j}\lambda_{i,j} - \tau_{i,j} \begin{cases} i=2,...,k-1 \\ j \in \mathcal{I}_{i} \end{cases}$$
(A.12)

The dual problem can be rearranged and reduced to the standard form

Ţ

$$\max_{\nu,\psi,\lambda,\tau,\mu} \qquad -\sum_{i=1}^{k-1} \nu_{i+1}^T b_i + \psi^T x - \epsilon ||\Omega^{-1}\psi||_q + \sum_{i=2}^{k-1} \lambda_i^T(u_i l_i)$$
(A.13)

 ν,ψ,λ s.t.

$$\nu_k = c \tag{A.14}$$

$$V_1^{\scriptscriptstyle I} \nu_2 = -\psi \tag{A.15}$$

$$\nu_{i,j} = 0, \ j \in \mathcal{I}_i^- \tag{A.16}$$

$$\nu_{i,j} = (W_i^T \nu_{i+1})_j, \ j \in \mathcal{I}_i^+$$
(A.17)

$$\left((u_{i,j} - l_{i,j})\lambda_{i,j} - \mu_{i,j} - \tau_{i,j} \right) = (W_i^T \nu_{i+1})_j \begin{cases} i=2,\dots,k-1 \\ j \in \mathcal{I}_i \end{cases}$$
(A.18)

$$\lambda, \tau, \mu \ge 0. \tag{A.19}$$

The insight of the dual problem is that it can also be written in the form of a deep network. Consider the equality constraint A.18, the dual variable λ corresponds to the upper bounds in the convex ReLU relaxation, while μ and τ correspond to the lower bounds $z \ge 0$ and $z \ge \hat{z}$, respectively. By the complementary property, these variables will be zero of ReLU constraint is non-tight, and non-zero if the ReLU constraint is tight. since the upper and lower bounds cannot be tight simultaneously, either λ or $\mu + \tau$ must be zero. Hence, at the optimal solution to the dual problem,

$$(u_{i,j} - l_{i,j})\lambda_{i,j} = [(W_i^T \nu i + 1)_j]_+ \tau_{i,j} + \mu_{i,j} = [(W_i^T \nu i + 1)_j]_-.$$
(A.20)

Combining this with the constraint $\nu_{i,j} = u_{i,j}\lambda_{i,j} - \tau_{i,j}$ leads to

$$\nu_{i,j} = \frac{u_{i,j}}{u_{i,j} - l_{i,j}} [(W_i^T \nu i + 1)_j]_+ - \eta [(W_i^T \nu i + 1)_j]_-$$
(A.21)

for $j \in \mathcal{I}_i$ and $0 \le \eta \le 1$. This is a leaky ReLU operation with a slope of $\frac{u_{i,j}}{u_{i,j}-l_{i,j}}$ in the positive portion and and a negative slope η between 0 and 1. Also note that from A.15 $-\psi$ denotes the preactivation variable for the first layer. For the sake of simplicity, we use $\hat{\nu}_i$ to denote the pre-activation variable for layer *i*, then the objective of the dual problem becomes

$$S_{D_{\epsilon}}(x,\nu) = -\sum_{i=1}^{k-1} \nu_{i+1}^{T} b_{i} + \sum_{i=2}^{k-1} \sum_{j \in \mathcal{I}_{i}} \frac{u_{i,j} l_{i,j}}{u_{i,j} - l_{i,j}} [\hat{\nu}_{i,j}]_{+} - \hat{\nu}_{1}^{T} x - \epsilon ||\Omega^{-1} \hat{\nu}_{1}||_{q}$$

$$= -\sum_{i=1}^{k-1} \nu_{i+1}^{T} b_{i} + \sum_{i=2}^{k-1} \sum_{j \in \mathcal{I}_{i}} l_{i,j} [\hat{\nu}_{i,j}]_{+} - \hat{\nu}_{1}^{T} x - \epsilon ||\Omega^{-1} \hat{\nu}_{1}||_{q}$$
(A.22)

Hence, the final form of the dual problem can be rewritten as a network with objective $S_{D_{\epsilon}}(x,\nu)$, input -c and activations \mathcal{I} as follows:

$$\begin{array}{ll} \underset{\hat{\nu},\nu}{\text{maximize}} & -\sum_{i=1}^{k-1} \nu_{i+1}^{T} b_{i} + \sum_{i=2}^{k-1} \sum_{j \in \mathcal{I}_{i}} l_{i,j} [\hat{\nu}_{i,j}]_{+} - \hat{\nu}_{1}^{T} x - \epsilon || \Omega^{-1} \hat{\nu}_{1} ||_{q} \\ \text{s.t.} & \nu_{k} = -c \\ & \hat{\nu}_{i} = (W_{i}^{T} \nu_{i+1}), i = k - 1, \dots, 1 \\ & \nu_{i,j} = \begin{cases} 0 & j \in \mathcal{I}_{i}^{-} \\ \hat{\nu}_{i,j} & j \in \mathcal{I}_{i}^{+} \\ \frac{u_{i,j}}{u_{i,j} - l_{i,j}} [\hat{\nu}_{i,j}]_{+} - \eta [\hat{\nu}_{i,j}]_{-} & j \in \mathcal{I}_{i} \end{cases} \quad (A.23) \end{array}$$

Theorem 4.2. In binary classification problem, suppose $\underline{p}_a \in (\frac{1}{2}, 1]$ satisfies $\mathbb{P}(f(x+n) = a) \geq \underline{p}_a$. Then $g(x+\delta) = a$ for all $\sqrt{\delta^T \Sigma^{-1} \delta} \leq \Phi_{r,n}^{-1}(\underline{p}_a) - q_{50}$, where $r := \sqrt{\delta^T \Sigma^{-1} \delta}$, $\Phi_{r,n}^{-1}(\underline{p}_a)$ is the quantile function of the χ distribution of d degrees of freedom, and q_{50} is the 50^{th} quantile.

Proof. Let X and Y be random variables such that $X \sim \mathcal{N}(x, \Sigma)$ and $Y \sim \mathcal{N}(x + \delta, \Sigma)$. Next, we define the set $\mathcal{A} := \left\{ z \mid \delta^T \Sigma^{-1}(z - x) \leq \sqrt{\delta^T \Sigma^{-1} \delta} \Phi_{r,d}^{-1}(\underline{p}_a) \right\}$, where $r := \sqrt{\delta^T \Sigma^{-1} \delta}$ and $\Phi_{r,n}^{-1}(\underline{p}_a)$ is the quantile function of the χ distribution of d degree of freedom for the probability p_a , so that $\mathbb{P}(X \in \mathcal{A}) = \underline{p}_a$. Consequently, $\mathbb{P}(Y \in \mathcal{A}) = \Phi_{r,d} \left(\Phi_{r,d}^{-1}(\underline{p}_a) - \sqrt{\delta^T \Sigma^{-1} \delta} \right)$. To ensure that Y is classified as class A, we need

$$\Phi_{r,d}\left(\Phi_{r,d}^{-1}(\underline{p_a}) - \sqrt{\delta^T \Sigma^{-1} \delta}\right) \ge 1/2 \tag{A.24}$$

which can be satisfied if and only if $\sqrt{\delta^T \Sigma^{-1} \delta} \leq \Phi_{r,d}^{-1}(\underline{p_a}) - q_{50}$.

A.5 Algorithm for Section 5.1

Activation Bounds: The dual objective function provides a bound on any linear function $c^T \hat{z}_k$. Therefore, we can compute the dual objective for c = -I and c = I to obtain lower and upper bounds. For c = I, value of ν_i for all activations simultaneously is given by

$$\hat{\nu}_{i} = W_{i}^{T} D_{i+1} W_{i+1}^{T} \dots D_{n} W_{n}^{T} \text{ and } \nu_{i} = D_{i} \hat{\nu}_{i}, \text{ where } (D_{i})_{jj} = \begin{cases} 0 & j \in \mathcal{I}_{i}^{-} \\ 1 & j \in \mathcal{I}_{i}^{+} \\ \frac{u_{i,j}}{u_{i,j} - l_{i,j}} & j \in \mathcal{I}_{i} \end{cases}$$
(A.25)

Similar to [4], bounds for ν_i and $\hat{\nu}_i$ can be computed for each layer by cumulatively generating bounds for \hat{z}_2 , then \hat{z}_3 and so on. By initializing $\hat{\nu}_1 := W_1^T$, $\zeta_1 := b_1^T$, first bounds are $l_2 := x^T W_1^T + b_1^T - \epsilon ||\Omega^{-1} W_1^T||_q$ and $u_2 := x^T W_1^T + b_1^T + \epsilon ||\Omega^{-1} W_1^T||_q$, where the norms are taken over the columns. Calculation of the bounds for each layer is given below in Algorithm 1.

Algorithm 1 Activation Bound Calculation

Input: Network parameters $\{W_i, b_i\}$, input data x, input constraint matrix Ω and ball size ϵ , norm type q.

type q. Initialize $\hat{\nu}_1 := W_1^T$, $\zeta_1 := b_1^T$ $l_2 = x^T W_1^T + b_1^T - \epsilon ||\Omega^{-1} W_1^T||_q$ $u_2 = x^T W_1^T + b_1^T + \epsilon ||\Omega^{-1} W_1^T||_q$ $\nu_{2,\mathcal{I}_2} := (D_2)_{\mathcal{I}_2} W_2^T$ for i = 2 to k - 1 do $l_{i+1} = x^T \hat{\nu}_1 + \sum_{j=1}^i \zeta_j - \epsilon ||\Omega^{-1} \hat{\nu}_1||_q + \sum_{i=2,i' \in \mathcal{I}_i}^i l_{j,i'} [-\nu_{j,i'}]_+$ $u_{i+1} = x^T \hat{\nu}_1 + \sum_{j=1}^i \zeta_j + \epsilon ||\Omega^{-1} \hat{\nu}_1||_q - \sum_{i=2,i' \in \mathcal{I}_i}^i l_{j,i'} [\nu_{j,i'}]_+$ $\nu_{j,\mathcal{I}_j} = \nu_{j,\mathcal{I}_j} (D_i)_{\mathcal{I}_i} W_i^T$ $\zeta_j = \zeta_j D_i W_i^T$ $\hat{\nu}_1 = \hat{\nu}_1 (D_i)_{\mathcal{I}_i} W_i^T$ end for Output: $\{l_i, u_i\}_{i=2}^k$

A.6 Experiments for Section 3.1

In this section, we present a detailed explanation about the winner attacks [5] of malware competition [6], and show detailed evasion success of these attacks in Table A.1.

GREEDY ATTACK: Bytes in a range 256 are added iteratively to the malware binaries to make sure the prediction score for a known model lowers and none of the packing, functionality, or antitampering checks are affected. Byte addition is stopped when the prediction score gets lower than a threshold value or the file size exceeds 5MB. We generate 1000 adversarial examples from the malicious binaries of EMBER test set for each target model, such as standard trained neural network, adversarially trained model with ℓ_2 -PGD for $\epsilon = 5$ and LGBM model which were provided as benchmark together with EMBER dataset [2]; and we call these adversarial example sets GNN, GAdv and GLGBM, respectively.

CONSTANT PADDING ATTACK: A new section is created in the binary file and filled with a constant value of size 10000. This attack is applied to 2000 binaries from EMBER malicious test set for constants "169" and "0", and we call these adversarial example sets C1 Pad. and C2 Pad., respectively.

STRING PADDING ATTACK: Strings of size 10000 from a benign file, such as Microsoft's End User License Agreement (EULA), are added to a new section created in the malware binary. We generate 2000 adversarial examples, which we call set Str. Pad., by string padding EMBER malicious test set.

Table A.1: **Malware Use-case:** Average number of successful evasions on standard training, uniform and non-uniform ℓ_2 -PGD adversarial trainings by the adversarial example sets out of 1000 samples for approximately equal $\|\delta\|_2$. Defense success rates shown in Table A.2 and Figure 1a are calculated by averaging the success rate over these individual attacks results.

Model	$ \delta _2$	GNN	GLGBM	GAdv	C1 Pad.	C2 Pad.	Str. Pad.
Std. Training	-	832	217	337	168	35	123
Uniform- δ	0.1	472.6	105	249.6	66.3	37.6	114.9
NU-δ-Mask	0.1	408.5	89.2	241.7	46.2	35.2	74.5
NU- δ -SHAP	0.1	392.8	86.8	206.8	64.9	39	104.7
NU- δ -Pearson	0.1	417.6	92.8	221.4	45.1	38.2	74.5
NU-δ-MD	0.1	413	101	216	56	38.7	81.8
NU- δ -MDtarget	0.1	391.6	84.2	234.6	52.2	38.7	79
Uniform- δ	1	447.2	111.8	273.8	50.1	38.5	83.4
NU- δ -Mask	1	299.4	88.2	223.4	58.3	40	91
NU- δ -SHAP	1	359.7	82.2	244.5	53.8	33.6	81.7
NU- δ -Pearson	1	304	96.2	265	60.5	38.8	99.2
NU- δ -MD	1	373.2	89.5	244	54.7	37	81.8
NU- δ -MDtarget	1	360.8	103.4	246.6	45.1	36.7	72.4
Uniform- δ	6.7	231.5	129	333	37.7	38	58.7
NU-δ-Mask	6.7	104.4	68.4	153.4	43.4	47.3	70.8
NU- δ -SHAP	6.7	170	113	302.5	32.7	41.2	39.7
NU- δ -Pearson	6.7	213	78	304	38	38	48.6
NU- δ -MD	6.7	234	91	314	27.7	31	34.2
NU-δ-MDtarget	6.7	196	61	301	37.5	33.5	36.5
Uniform- δ	11	177	77.6	278	37.8	41.3	44.6
NU-δ-Mask	11	94.4	45.2	160.8	30.8	43.7	50.5
NU- δ -SHAP	11	178	62	296	32	40	35
NU- δ -Pearson	11	142	75.7	273	31.6	40.7	42.8
NU- δ -MD	11	195	46	247	40	32.5	43
NU- δ -MDtarget	11	122.7	44	251.7	34	41	48
Uniform- δ	18	152.2	57.3	234	42.7	51.6	52.3
NU- δ -Mask	18	44.5	20.2	116.5	27.1	48.2	47.2
NU- δ -SHAP	18	159.4	48.6	207.2	53.1	59.6	61.3
NU- δ -Pearson	18	154.2	49	220.4	42.6	61.7	47.2
NU- δ -MD	18	144.2	49.2	204.6	53	54	63.8
NU-δ-MDtarget	18	132.4	52.4	215	50.6	53.4	53.2
Uniform-δ	25	233.2	58	228	59.3	51	68.4
NU- δ -Mask	25	25	14.8	108	21.8	48.9	34.8
NU- δ -SHAP	25	193.8	53.4	226.2	44.7	56.9	58.7
NU-δ-Pearson	25	158.2	59.5	191.2	67.6	65.6	75.8
NU-δ-MD	25	199.7	54	248.5	58.6	59.5	59.7
NU- δ -MDtarget	25	210	55	225.6	57.7	56.4	60.5

Table A.1 shows the average number of adversarial examples out of 1000 which successfully evade the corresponding models. While $NU-\delta$ -Mask and $NU-\delta$ -MDtarget have better performance against Greedy attacks for most of the time, i.e., sets GNN, GLGBM and GAdv, $NU-\delta$ -Pearson, $NU-\delta$ -SHAP and $NU-\delta$ -MD have better accuracy against padding attacks, i.e., sets C1 Pad., C2 Pad. and Str. Pad.

Table A.2: **Malware Use-case:** Clean accuracy (Ac.) and defense success rate (S.R.) of standard training, uniform and non-uniform ℓ_2 -PGD adversarial trainings with EMBER dataset for approximately equal $\|\delta\|_2$. Non-uniform perturbation defense approaches outperform the uniform perturbation for all cases against adversarial attacks.

Model	$\ \delta\ _2$	Clean Ac., %	Defense S.R., $\%$
Std. Training	-	96.6	73
Uniform- δ	0.1	96.2	82.7 ± 0.88
NU-δ-Mask	0.1	96.2	85.3 ± 0.25
NU-δ-SHAP	0.1	96.2	85.2 ± 0.39
NU- δ -Pearson	0.1	96.1	85.3 ± 0.94
NU-δ-MD	0.1	96.3	85 ± 0.99
NU- δ -MDtarget	0.1	96.2	85.4 ± 0.80
Uniform- δ	1	96.1	83.3 ± 0.41
NU- δ -Mask	1	96.1	86.7 ± 0.68
NU- δ -SHAP	1	96.3	85.5 ± 0.61
NU- δ -Pearson	1	96.2	85.7 ± 0.45
NU- δ -MD	1	96.3	85.4 ± 0.67
NU- δ -MDtarget	1	96.3	85.9 ± 0.19
Uniform- δ	6.7	95.8	86.3 ± 0.15
NU-δ-Mask	6.7	95.7	92 ± 0.07
NU- δ -SHAP	6.7	95.8	88.3 ± 0.33
NU- δ -Pearson	6.7	95.9	88.2 ± 0.30
NU-δ-MD	6.7	96	87.7 ± 0.32
NU- δ -MDtarget	6.7	95.8	89 ± 0.18
Uniform- δ	11	95.6	89.3 ± 0.54
NU-∂-Mask	11	95.8	92.9 ± 0.57
NU- δ -SHAP	11	96	90.3 ± 0.36
NU- δ -Pearson	11	95.8	90 ± 0.36
NU-δ-MD	11	95.9	89.9 ± 0.25
NU- δ -MDtarget	11	95.7	90.9 ± 0.29
Uniform- δ	18	95.5	90.17 ± 0.71
NU-∂-Mask	18	95.8	94.8 ± 0.51
NU- δ -SHAP	18	95.3	90.45 ± 0.30
NU- δ -Pearson	18	95.3	90.46 ± 0.25
NU-δ-MD	18	95.4	90.54 ± 0.46
NU-δ-MDtarget	18	95.4	90.7 ± 0.51
Uniform-δ	25	95.6	88.4 ± 0.39
NU-δ-Mask	25	95.7	95.8 ± 0.21
NU- δ -SHAP	25	95.5	89.5 ± 0.27
NU- δ -Pearson	25	94.9	89.7 ± 0.40
NU-δ-MD	25	95.2	88.6 ± 0.26
NU- δ -MDtarget	25	95.2	89 ± 0.57

Table A.3: Credit Risk Use-case: Clean accuracy (Ac.) and defense success rate (S.R.) of standard training, uniform and non-uniform ℓ_2 -PGD adversarial trainings with German Credit dataset for approximately equal $\|\delta\|_2$. Non-uniform perturbation defense approaches outperform the uniform perturbation for all cases against adversarial attacks.

Table A.4: **Spam Detection Use-case:** Clean accuracy and defense success rate of standard training, uniform and non-uniform ℓ_2 -PGD adversarial trainings with Twitter Spam dataset for approximately equal $\|\delta\|_2$.

Model	$\ \delta\ _2$	Clean Ac., $\%$	Defense S.R., %	
Std. Training	-	69.7	60	
Uniform- δ	0.01	69	61.3 ± 0.40	
NU- δ -SHAP	0.01	68.3	61.3 ± 0.35	
NU-δ-Pearson	0.01	68.3	61.9 ± 0.37	
NU-δ-MD	0.01	69.6	61.6 ± 0.32	
$\textbf{NU-}\delta\textbf{-MDtarget}$	0.01	69.7	61.9 ± 0.30	
Uniform- δ	0.1	67.7	63.4 ± 0.31	
NU-δ-SHAP	0.1	67.1	64.5 ± 0.20	
NU-δ-Pearson	0.1	66.8	64.3 ± 0.56	
NU-δ-MD	0.1	66.7	64.2 ± 0.32	
NU-δ-MDtarget	0.1	66.7	64.5 ± 0.41	
Uniform- δ	0.3	66.7	66.4 ± 0.22	
NU- δ -SHAP	0.3	65.8	67.6 ± 0.30	
NU-δ-Pearson	0.3	66	68 ± 0.21	
NU-δ-MD	0.3	66.5	67.1 ± 0.64	
NU- δ -MDtarget	0.3	66.3	69 ± 0.32	
Uniform- δ	0.5	66.2	68 ± 0.32	
NU- δ -SHAP	0.5	66.5	69.7 ± 0.37	
NU-δ-Pearson	0.5	65.9	69.4 ± 0.27	
NU-δ-MD	0.5	66.3	69.2 ± 0.35	
NU- δ -MDtarget	0.5	66	69.8 ± 0.13	
Uniform- δ	0.7	66.1	69.6 ± 0.20	
NU-δ-SHAP	0.7	65.8	71.1 ± 0.57	
NU-δ-Pearson	0.7	65.6	71 ± 0.37	
NU-δ-MD	0.7	66.4	70.5 ± 0.30	
NU- δ -MDtarget	0.7	65.6	70.3 ± 0.30	
Uniform- δ	1	65.3	70.6 ± 0.44	
NU-δ-SHAP	1	64.5	71.3 ± 0.32	
NU-δ-Pearson	1	64.3	71.3 ± 0.32	
NU-δ-MD	1	64.9	71 ± 0.37	
NU-δ-MDtarget	1	65	71 ± 0.21	

Model	$\ \delta\ _2$	Clean Ac., $\%$	Defense S.R., $\%$
Std. Training	-	94.6	17.5
Uniform- δ	0.1	91.1	34.4 ± 0.16
NU- δ -SHAP	0.1	93.9	35.3 ± 0.32
NU- δ -Pearson	0.1	94	$36 \pm 0.50.$
NU- δ -MD	0.1	93.9	36.7 ± 0.48
NU- δ -MDtarget	0.1	93.9	38.3 ± 0.50
Uniform- δ	0.3	92.6	58.3 ± 0.66
NU- δ -SHAP	0.3	91.9	66.5 ± 0.86
NU- δ -Pearson	0.3	91.8	65 ± 0.21
NU-δ-MD	0.3	91.9	69.4 ± 0.25
NU-δ-MDtarget	0.3	92	67.9 ± 0.25
Uniform- δ	0.5	91.3	82.8 ± 0.46
NU- δ -SHAP	0.5	90.9	86.1 ± 0.14
NU-δ-Pearson	0.5	91.2	87.3 ± 0.20
NU-δ-MD	0.5	91.1	85.3 ± 0.30
NU-δ-MDtarget	0.5	91.2	86.8 ± 0.28
Uniform- δ	0.7	91.1	89.6 ± 0.48
NU- δ -SHAP	0.7	90.5	90.5 ± 0.19
NU-δ-Pearson	0.7	90.6	90.7 ± 0.11
NU-δ-MD	0.7	90.5	89.8 ± 0.35
NU- δ -MDtarget	0.7	90.5	89.1 ± 0.18
Uniform- δ	1	90.5	87.3 ± 0.62
NU- δ -SHAP	1	89.8	91.4 ± 0.62
NU- δ -Pearson	1	89.9	92 ± 0.53
NU-δ-MD	1	89.7	93.3 ± 0.30
NU- δ -MDtarget	1	89.8	92.5 ± 0.64

A.7 Experiments for Section 3.4

We further investigate the performance of our non-uniform approach against uniformly norm-bounded attacks for generalizability as in Section 3.4. We use the same setting as in spam detection use-case, and craft AEs using standard PGD attack, i.e., the attack in *Uniform*- δ , for $\epsilon = \{0.1, 0.3, 0.5, 0.7\}$. For a fair comparison between the uniform and non-uniform approaches, we set approximately equal $||\delta||_2$ for both models in the average sense. In this section, we also consider a non-uniform robust model which enforces the AT constraint first on $||\Omega\delta||_2$ and then $||\delta||_2$. That is, the non-uniform attack is always a valid uniform attack in the strict sense. We call this defense *Combo* due to using the combination of both projections in (3) and (5).

Table A.5 shows the defense success rates of *Uniform-* δ , *NU-* δ *-MDt* and *MDt-Combo*, which denotes the *Combo* approach for Ω selected as the Mahalanobis matrix for the benign samples, against PGD attacks for Spam Detection Use-case. We observe that our non-uniform approach outperforms the uniform approach for all cases, hence it is also effective against the uniformly norm-bounded attacks which makes it generalizable. Furthermore, Table A.5 shows that *MDt-Combo* performs in between *Uniform-* δ and *NU-* δ *-MDt*. This is due to the fact that the strict constraint on $||\delta||_2$ reduces the effect of non-uniform projection.

Table A.5: Defense success rates of *Uniform-* δ , *NU-* δ *-MDt* and *MDt-Combo* against PGD attacks for Spam Detection Use-case. Both non-uniform defenses outperform the uniform approach while *NU-* δ *-MDt* also outperforms *MDt-Combo* for all cases.

Defenses	$ \delta _2$	Attack ϵ =0.1	Attack ϵ =0.3	Attack ϵ =0.5	Attack ϵ =0.7
Uniform-δ NU-δ-MDt MDt-Combo	0.1	$\begin{array}{c} 90.6 \pm 0.18 \\ \textbf{92.8} \pm \textbf{0.21} \\ 91.6 \pm 0.24 \end{array}$	$\begin{array}{c} 83.9 \pm 0.34 \\ \mathbf{88.2 \pm 0.41} \\ 86.3 \pm 0.28 \end{array}$	$\begin{array}{c} 16.6 \pm 0.47 \\ \textbf{34.95} \pm \textbf{0.5} \\ 24.4 \pm 0.38 \end{array}$	$\begin{array}{c} 14.8 \pm 0.65 \\ \textbf{21.4} \pm \textbf{0.22} \\ 19.2 \pm 0.32 \end{array}$
Uniform-δ NU-δ-MDt MDt-Combo	0.3	$\begin{array}{c} 92.6 \pm 0.14 \\ \textbf{93.2} \pm \textbf{0.10} \\ 93 \pm 0.11 \end{array}$	$\begin{array}{c} 89.05 \pm 0.24 \\ \textbf{90.95} \pm \textbf{0.22} \\ 89.24 \pm 0.19 \end{array}$	$\begin{array}{c} 30.5 \pm 0.42 \\ \textbf{61.75} \pm \textbf{0.51} \\ 47.88 \pm 0.72 \end{array}$	$20.85 \pm 0.58 \\ 46.3 \pm 0.41 \\ 31.5 \pm 0.39$
Uniform-δ NU-δ-MDt MDt-Combo	0.5	$\begin{array}{c} 92.9 \pm 0.08 \\ \textbf{93.3} \pm \textbf{0.05} \\ 93.1 \pm 0.10 \end{array}$	$\begin{array}{c} 91.4 \pm 0.05 \\ \textbf{91.45} \pm \textbf{0.06} \\ 91.4 \pm 0.11 \end{array}$	$\begin{array}{c} 88 \pm 0.22 \\ \textbf{89.45} \pm \textbf{0.17} \\ 89.30 \pm 0.14 \end{array}$	$\begin{array}{c} 86.5 \pm 0.25 \\ 87.7 \pm 0.12 \\ 87.2 \pm 0.18 \end{array}$
Uniform-δ NU-δ-MDt MDt-Combo	1	$\begin{array}{c} 93.2 \pm 0.14 \\ \textbf{94.5} \pm \textbf{0.11} \\ 94.39 \pm 0.10 \end{array}$	$\begin{array}{c} 91.9 \pm 0.25 \\ \textbf{94.17} \pm \textbf{0.42} \\ 92.42 \pm 0.28 \end{array}$	$\begin{array}{c} 90.18 \pm 0.20 \\ \textbf{93.33} \pm \textbf{0.15} \\ 91.44 \pm 0.19 \end{array}$	$\begin{array}{c} 88.38 \pm 0.22 \\ \textbf{93.14} \pm \textbf{0.31} \\ 91.33 \pm 0.26 \end{array}$
Uniform-δ NU-δ-MDt MDt-Combo	1.5	$\begin{array}{c} 93.22 \pm 0.16 \\ \textbf{94.45} \pm \textbf{0.12} \\ 94.27 \pm 0.11 \end{array}$	$\begin{array}{c} 92.01 \pm 0.27 \\ \textbf{94.38} \pm \textbf{0.31} \\ 93.1 \pm 0.20 \end{array}$	$\begin{array}{c} 90.61 \pm 0.24 \\ \textbf{93.76} \pm \textbf{0.16} \\ 92.3 \pm 0.27 \end{array}$	$89.78 \pm 0.15 \\ \textbf{93.48} \pm \textbf{0.11} \\ 91.8 \pm 0.17 \\ \end{cases}$

References

- [1] Eric Wong and Zico Kolter. Provably robust neural networks. 2018. URL https://github.com/locuslab/convex_adversarial.
- [2] Hyrum S. Anderson and Phil Roth. EMBER: an open dataset for training static PE malware machine learning models. *arXiv preprint arXiv: 1804.04637*, 2018.
- [3] Jiawei Han, Micheline Kamber, and Jian Pei. Data transformation and data discretization. *Data Mining: Concepts and Techniques. Elsevier*, pages 111–118, 2011.
- [4] Eric Wong and Zico Kolter. Provable defenses against adversarial examples via the convex outer adversarial polytope. In *International Conference on Machine Learning*, pages 5286–5295. PMLR, 2018.
- [5] William Fleshman. Evading Machine Learning Malware Classifiers, 2019. URL https://towardsdatascience.com/ evading-machine-learning-malware-classifiers-ce52dabdb713.
- [6] DEFCON. Machine learning static evasion competition, 2019. URL https://www.elastic. co/blog/machine-learning-static-evasion-competition.