A Novel Plug-and-Play Approach for Adversarially Robust Generalization

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Abstract

In this work, we propose a robust framework that employs adversarially robust training to safeguard the machine learning models against perturbed testing data. We achieve this by incorporating the worst-case additive adversarial error within a fixed budget for each sample during model estimation. Our main focus is to provide a plug-and-play solution that can be incorporated in the existing machine learning algorithms with minimal changes. To that end, we derive the ready-to-use solution for several widely used loss functions with a variety of norm constraints on adversarial perturbation for various supervised and unsupervised ML problems, including regression, classification, two-layer neural networks, graphical models, and matrix completion. The solutions are either in closed-form, 1-D optimization, semidefinite programming, difference of convex programming or a sorting-based algorithm. Finally, we validate our approach by showing significant performance improvement on real-world datasets for supervised problems such as regression and classification, as well as for unsupervised problems such as matrix completion and learning graphical models, with very little computational overhead.

1 Introduction

Machine learning models are used in a wide variety of applications such as image classification, speech recognition and self-driving vehicles. The models employed in these applications can achieve a very high training time accuracy by training on a large number of samples. However, they can fail spectacularly to make trustworthy predictions on data coming from the test distribution with some unknown shifts from the training distribution \[4, 16\]. As the learning model never sees data from the target domain during training time due to the unknown shift, this leads to overfitting on training data and subsequently poor performance and generalization on test data. Thus, it becomes important for existing machine learning models to possess the ability of out-of-distribution generalization under distribution shift \[49, 24\].

The problem of out-of-distribution generalization can also be seen through an adversarial lens. It is now a well-known phenomena \[50, 14\] in the machine learning community that an adversary

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can easily force machine learning models to make bad predictions with high confidence by simply adding some perturbation to the input data. Robustness to such adversarial attacks remains a serious challenge for researchers. Recently, the field of adversarial training \cite{17, 44, 32}, i.e., preparing models for adversarial attack during the training time, has started making initial inroads to tackle this challenge.

The key idea of adversarial training is to train with perturbed input by adding adversarial error to improve the predictions during, possibly out-of-distribution, testing. In this scheme, the adversary tries to maximize the underlying loss function, while the learner tries to minimize it by estimating optimal model parameters. One of the earliest methods to solve this maximization problem was the Fast Gradient Signed Method \cite{14}. Several other variants of this approach also exist (See \cite{25, 32, 52} for further details). Some other works consider relaxation or approximation of the original optimization problem by maximizing over a convex polytope \cite{55}, using random projections \cite{56}, or constructing a semi-definite program (SDP) \cite{37, 38}. As all these approaches solve relaxed or approximate optimization problems, they run the risk of providing sub-optimal solutions which may not work well for out-of-distribution generalization. In this work, we focus on deriving the exact optimal solution within the bounds of norm constraints. Moreover, unlike other domain specific works such as \cite{18, 29, 6, 40} in natural language processing and \cite{15, 2} in computer vision, we aim to provide an adversarially robust training model which covers a large class of machine learning problems.

There are also few theoretical works which provide generalization bounds for worst-case adversarially robust training \cite{63, 59}. However, note that analyzing such bounds is not the focus of this work. Rather, here we consider the problem of out-of-distribution generalization in a more practical point of view. Often, practitioners do not have the luxury to incorporate complex models in their existing machine learning algorithms due to their potential impact on computational time. Thus, it becomes important to propose a simple plug-and-play framework which only requires little change in the existing models without imposing a large computational overhead. In particular, we provide ready-to-use results for a wide variety of loss functions and various norm constraints (See Table 1).

The closed-form solution may not exist for problems with a complex objective function. For example, the optimal solution in graphical models with euclidean norm constraint can be derived by constructing the dual problem, which has a convex objective function in one variable (refer Theorem 7, Table 1). Similarly, it may not be possible to derive the optimal solution for a complex objective function, such as in neural networks. We tackle this issue using well-established algorithms with theoretical guarantees for global convergence. We pose the non-convex objective function as a difference of two convex functions and utilize the well-established difference of convex programming \cite{51, 28} to arrive at the globally optimal solution for two-layer neural networks.

Intuitively, with no prior information on the shift of the testing distribution, it makes sense to be prepared for absolutely worst case scenarios. We incorporate this insight formally in our proposed adversarially robust training model. At each iteration of the training algorithm, we generate worst case adversarial samples using the current model parameters and “clean” training data within bounds of a maximum norm. The model parameters are updated using these worst case adversarial samples and next iteration is performed. Figure 1 provides a geometric interpretation of our training process.

Our Contributions. Broadly, we make the following contributions through this work:

- **Adversarially robust formulation**: We use the adversarially robust training framework of \cite{59} to handle out-of-distribution generalization using worst case adversarial attacks. Under this framework, we analyze several supervised and unsupervised ML problems, including
Table 1: A summary of our results for various loss functions and norm constraints which are used in a wide variety of applications.

| Problem                | Loss function | Norm Constraint | Prior results | Our solution               |
|------------------------|---------------|-----------------|---------------|----------------------------|
| Regression             | Squared loss  | Any norm        | Euclidean norm | Closed form, Theorem 9      |
| Classification         | Logistic loss | Any norm        | Euclidean norm | Closed form, Theorem 4      |
| Classification         | Hinge loss    | Any norm        | None          | Closed form, Theorem 5      |
| Graphical Models       | Log-likelihood| Euclidean       | None          | 1-D optimization, Theorem 7 |
| Graphical Models       | Log-likelihood| Entry-wise $\ell_\infty$ | None          | Semidefinite programming, Theorem 8 |
| Matrix Completion (MC) | Squared loss  | Frobenius       | None          | Closed form, Theorem 9      |
| Matrix Completion (MC) | Squared loss  | Entry-wise $\ell_\infty$ | None          | Closed form, Corollary 10   |
| Max-Margin MC          | Hinge loss    | Frobenius       | None          | Sorting based algorithm, Theorem 11 |
| Max-Margin MC          | Hinge loss    | Entry-wise $\ell_\infty$ | None          | Closed form, Corollary 12   |

Figure 1: Figure 1a shows the domain for clean training points while the dashed cube in Figure 1b shows the worst case adversarial attack domain (slightly bigger than original training domain). Each new worst case adversarially attacked point is judiciously picked from within the green spheres around the corresponding clean training point with radius $\epsilon$ in a predefined norm.

regression, classification, two-layer neural networks, graphical models and matrix completion. The solutions are either in closed-form, 1-D optimization, semidefinite programming, difference of convex programming or a sorting based algorithm.

- **Plug-and-play solution:** We provide a plug-and-play solution which can be easily integrated with existing training algorithms. This is a boon for practitioners who can incorporate our method in their existing models with minimal changes. As a conscious design choice, we provide computationally cheap solutions for our optimization problems.

- **Theoretical analysis:** On the theoretical front, we provide a systematic analysis for several loss functions and norm constraints which are commonly used in applications across various domains. Table 1 provides a summary of our findings in a concise manner.

- **Real world applications:** We further validate our results by conducting extensive experiments on several real world applications. We show that our plug-and-play solution performs better in problems such as blog feedback prediction using linear regression [8], classification using logistic regression and hinge loss on the ImageNet dataset [10], graphical models on the
cancer genome atlas (TCGA) dataset, matrix completion on the Netflix Prize dataset [7], and max-margin matrix completion on the House of Representatives (HouseRep) voting records.

2 Preliminaries

For any general prediction problem in machine learning (ML), consider we have $n$ samples of $(x, y)$, where we try to predict $y \in Y$ from $x \in X$ using the function $f : X \to Y$. Assuming that the function $f$ can be parameterized by some parameter $w$, we minimize a loss function $l(x, y, w)$ to obtain an estimate of $w$ from $n$ samples:

$$\hat{w} = \arg \min_w \frac{1}{n} \sum_{i=1}^{n} l(x^{(i)}, y^{(i)}, w)$$

(1)

where $(x^{(i)}, y^{(i)})$ represents the $i^{th}$ sample. This basic formulation will be used in the later section to describe the proposed method. Before proceeding to the main discussion, we briefly discuss the notations and basic mathematical definitions used in the paper.

Notation: We use a lowercase alphabet such as $x$ to denote a scalar, a lowercase bold alphabet such as $x$ to denote a vector and an uppercase bold alphabet such as $X$ to denote a matrix. The $i^{th}$ entry of the vector $x$ is denoted by $x_i$. The superscript star on a vector or matrix such as $x^*$ denotes it is the optimal solution for some optimization problem. A general norm for a vector is denoted by $\|x\|$ and its dual norm is indicated by a subscript asterisk, such as $\|x\|_*$. The set $\{1, 2, \ldots, n\}$ is denoted by $[n]$. A set is represented by capital calligraphic alphabet such as $\mathcal{P}$, and its cardinality is represented by $|\mathcal{P}|$. For a scalar $x$, $|x|$ represents its absolute value.

Definition 1. The dual norm of a vector, $\| \cdot \|_*$ is defined as:

$$\|z\|_* = \sup\{z^T x \mid \|x\| \leq 1\}$$

(2)

Definition 2. The sub-differential of a norm is defined as:

$$\partial \|x\| = \{v : v^T x = \|x\|, \|v\|_* \leq 1\}$$

(3)

where $\|\|_*$ is the dual norm to $\|\|$.

In this work, we propose plug-and-play solutions for various ML problems to enable out-of-distribution generalization. By plug-and-play solution, we mean that any addition to the existing algorithm comes in terms of a closed-form equation or as a solution to an easy-to-solve optimization problem. Such a solution can be integrated with the existing algorithm with very minimal changes.

3 Main Results

In this section, we formally discuss our proposed approach of adversarially robust training for out-of-distribution generalization. We consider a wide variety of well known ML problems. The classical approach to estimate model parameters in various ML problems is to minimize a loss function using an optimization algorithm such as gradient descent [11] or variants [9, 3]. In order to prepare the model for the out-of-distribution scenario, we consider training with perturbed data that increases the loss function to a extent possible within the bounds of a given norm constraint. The worst case additive error is a function of the model parameters and each data sample at hand. As the model
parameters are not known before training, we estimate them iteratively by adding the worst case adversarial error in each gradient descent iteration for every sample.

Turning the focus to adversarially robust training, we work with the following optimization problem:

\[
\hat{w} = \arg\min_w \frac{1}{n} \sum_{i=1}^{n} \sup_{\|\Delta\| \leq \epsilon} l(x^{(i)} + \Delta, y^{(i)} , w) \tag{4}
\]

The optimization problem (4) depends on two variables: the adversarial perturbation \(\Delta\) and the model parameter \(w\). We solve for one variable assuming the other is given iteratively as illustrated in Algorithm 1. Specifically, we estimate \(\Delta^{\star}\) for robust learning by defining the worst case adversarial attack for a given parameter vector \(w^{(j-1)}\) (\(j\) denotes the iteration number in gradient descent) and sample \(\{x^{(i)}, y^{(i)}\}\) as follows:

\[
\Delta^{\star} = \arg\sup_{\|\Delta\| \leq \epsilon} l(x^{(i)} + \Delta, y^{(i)} , w^{(j-1)})
\]

For brevity, we drop the subscript \(j-1\) from the parameter \(w\) when it is clear from the context that the optimization problem is being solved for a particular iteration. Naturally, computing \(\Delta^{\star}\) by solving another maximization problem every time might not be necessarily efficient. To tackle this issue, we provide plug-and-play solutions of \(\Delta^{\star}\) for a given \((x^{(i)}, y^{(i)}, w^{(j)})\) where \(i \in [n]\) and \(j \in [T]\) for various widely-used ML problems.

### 3.1 Linear Regression

We start with a linear regression model which is used in various applications across numerous domains such as biology [43], econometrics, epidemiology, and finance [34]. The optimal parameter is estimated by solving the following minimization problem.

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} \left( w^\top x^{(i)} - y^{(i)} \right)^2
\]

As discussed in the previous sub-section, the adversary tries to perturb each sample to the maximum possible extent using the budget \(\epsilon\) by solving the following maximization problem for each sample:

\[
\Delta^{\star} = \arg\sup_{\|\Delta\| \leq \epsilon} \left( w^\top (x^{(i)} + \Delta) - y^{(i)} \right)^2, \tag{5}
\]

**Algorithm 1:** Plug and play algorithm

\[
\begin{align*}
\text{Input:} & \quad \{x^{(i)}, y^{(i)}\} \text{ for } i \in [n], T: \text{number of iterations, } \eta: \text{step size} \\
& \quad w^{(0)} \leftarrow \text{initial value} \; ; \\
& \quad \text{for } j = 1 \text{ to } T \text{ do} \\
& \qquad \text{gradient} \leftarrow 0 \; ; \\
& \qquad \text{for } i = 1 \text{ to } n \text{ do} \\
& \qquad \qquad \Delta^{\star} = \arg\sup_{\|\Delta\| \leq \epsilon} \left( l(x^{(i)} + \Delta, y^{(i)} , w^{(j-1)}) \right) \; ; \\
& \qquad \qquad \text{gradient} \leftarrow \text{gradient} + \frac{\partial l(x^{(i)} + \Delta^{\star}, y^{(i)}, w^{(j-1)})}{\partial w} \; ; \\
& \qquad \text{end} \\
& \qquad w^{(j)} \leftarrow w^{(j-1)} - \eta \frac{1}{n} \text{gradient} \\
& \quad \text{end} \\
\end{align*}
\]

\[
\text{Output: } \hat{w} = w^{(T)}
\]
where \( y^{(i)} \in \mathbb{R}, x^{(i)}, \Delta \in \mathbb{R}^d \) and \( \|\Delta\| \) denotes any general norm. We provide the following theorem to compute \( \Delta^* \) in closed form.

**Theorem 3.** For any general norm \( \| \cdot \| \), the solution for the problem in equation (5) for a given \((x^{(i)}, y^{(i)})\) is:

\[
\Delta^* = \begin{cases} 
\pm \varepsilon \frac{v}{\|v\|}, & \text{if } w^T x^{(i)} - y^{(i)} = 0 \\
\text{sign}(w^T x^{(i)} - y^{(i)}) \varepsilon \frac{v}{\|v\|}, & \text{otherwise}
\end{cases}
\]

where \( v \in \partial \|w\|_* \) as specified in Definition 2.

### 3.2 Logistic Regression

Next, we tackle logistic regression which is widely used for classification tasks in many fields such as medical diagnosis [53], marketing [33] and biology [11]. Using previously introduced notations, we formulate logistic regression [22] with worst case adversarial attack in the following way:

\[
\Delta^* = \arg \sup_{\|\Delta\| \leq \varepsilon} \log \left( 1 + \exp \left( -y^{(i)} w^T (x^{(i)} + \Delta) \right) \right)
\]

where \( y^{(i)} \in \{ -1, 1 \} \) and \( x^{(i)}, \Delta \in \mathbb{R}^d \). The optimal solution for above optimization problem is provided in the following theorem.

**Theorem 4.** For any general norm \( \| \cdot \| \), and the problem specified in equation (6), the optimal solution is given by:

\[
\Delta^* = -\varepsilon y^{(i)} \frac{v}{\|v\|}
\]

where \( v \in \partial \|w\|_* \) as specified in Definition 2.

### 3.3 Hinge Loss

The hinge loss is another widely used loss function. Machine learning models such as support vector machines (SVM) utilize it for various applications involving classification such as text categorization [19] and fMRI image classification [12]. Again, using previously introduced notations, we formulate our problem as:

\[
\Delta^* = \arg \sup_{\|\Delta\| \leq \varepsilon} \max \left( 0, 1 - y^{(i)} w^T (x^{(i)} + \Delta) \right)
\]

where \( y^{(i)} \in \{ -1, 1 \} \) and \( x^{(i)}, \Delta \in \mathbb{R}^d \). The optimal solution to this problem is proposed in the following theorem.

**Theorem 5.** For any general norm \( \| \cdot \| \), and the problem specified in equation (8), the optimal solution is given by:

\[
\Delta^* = -\varepsilon y^{(i)} \frac{v}{\|v\|}
\]

where \( v \in \partial \|w\|_* \) as specified in Definition 2.
3.4 Two-Layer Neural Networks

Consider a two-layer neural network for a binary classification problem with any general activation function $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ in the first layer. As we work on the classification problem, we consider the log sigmoid activation function in the final layer. The general adversarial problem can be stated as:

$$\Delta^* = \arg \sup_{\|\Delta\| \leq \varepsilon} \log \left(1 + \exp \left(-y^{(i)} \mathbf{v}^\top \sigma_h \left(\mathbf{W}^\top (\mathbf{x}^{(i)} + \Delta)\right)\right)\right)$$

where $y^{(i)} \in \{1, -1\}$ for binary classification, $\mathbf{x}, \Delta \in \mathbb{R}^d$, and the weight parameters $\mathbf{W} \in \mathbb{R}^{h \times d}$, and $\mathbf{v} \in \mathbb{R}^h$. Note that $h$ denotes the number of hidden units in the first layer, and the output for the general activation function $\sigma_h : \mathbb{R}^h \rightarrow \mathbb{R}^h$ is obtained by applying $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ to each dimension independently. The optimal solution to the above problem is the following theorem.

**Theorem 6.** For any general norm $\| \cdot \|$, and any activation function, the optimal solution for the problem specified in Eq. (9) can be solved by following difference of convex functions.

**Proof.** As $\log(\cdot)$ and $\exp(\cdot)$ are monotonically increasing functions, the adversarial problem specified in Eq. (9) can be equivalently expressed as:

$$\Delta^* = \arg \min_{\|\Delta\| \leq \varepsilon} f(\Delta) = y\mathbf{v}^\top \sigma_h (\mathbf{W}^\top (\mathbf{x} + \Delta))$$

where we have dropped the subscript (i) for brevity, as it is clear that the above problem is solved for each sample. The objective function of the above problem can be equivalently represented as:

$$f(\Delta) = \sum_{i: y\mathbf{v}_i > 0} y\mathbf{v}_i \sigma (\mathbf{z}_i) - \sum_{i: y\mathbf{v}_i < 0} |y\mathbf{v}_i| \sigma (\mathbf{z}_i)$$

$$\mathbf{z}_i = \mathbf{W}_i^\top (\mathbf{x} + \Delta)$$

where $\mathbf{W}_i$ represents the $i^{th}$ row of matrix $\mathbf{W}$. Further, we express any general activation function $\sigma(\cdot)$ (which may be non-convex) as the difference of two convex functions:

$$\sigma(\Delta) = \sigma_1(\Delta) - \sigma_2(\Delta)$$

Using the above formulation, the objective function in Eq. (11) can be expressed as $f(\Delta) = g(\Delta) - h(\Delta)$, where $g(\Delta)$ and $h(\Delta)$ are convex functions defined as:

$$g(\Delta) = \sum_{i: y\mathbf{v}_i > 0} y\mathbf{v}_i \sigma_1 (\mathbf{z}_i) + \sum_{i: y\mathbf{v}_i < 0} |y\mathbf{v}_i| \sigma_2 (\mathbf{z}_i)$$

$$h(\Delta) = \sum_{i: y\mathbf{v}_i > 0} y\mathbf{v}_i \sigma_2 (\mathbf{z}_i) + \sum_{i: y\mathbf{v}_i < 0} |y\mathbf{v}_i| \sigma_1 (\mathbf{z}_i)$$

where $\mathbf{z}_i$ is defined in Eq. (12). It should be noted that $g(\Delta)$ and $h(\Delta)$ are convex functions as they are positive weighted combination of convex functions $\sigma_1(\cdot)$ and $\sigma_2(\cdot)$. As the objective function $f(\Delta)$ can be expressed as difference of convex functions for any activation function specified in Table 2, we can use difference of convex functions algorithms (DCA) [51].

If set $S = \{i \mid y\mathbf{v}_i < 0, i \in [h]\} = \emptyset$ and we have an activation function $\sigma(\Delta)$ such that $\sigma_2(\Delta) = 0$, then $h(\Delta) = 0$ and the problem in Eq. (9) reduces to a convex optimization problem. This may not be the case in general for two-layer neural networks. Therefore we use the difference of convex
programming approach \cite{51,48,60,11,27,58,20,35} which are proved to converge to the global minima.

The first step to solve this optimization problem is constructing the functions \(g(\Delta)\) and \(h(\Delta)\), which requires decomposing the activation functions as the difference of convex functions. In order to do this, we decompose various activation functions commonly used in the literature as a difference of two convex functions. The decomposition is done by constructing a linear approximation of the activation function around the point where it changes the curvature. These results are presented in Table 2. Activation functions like hyperbolic tangent, inverse tangent, sigmoid, inverse square root, and ELU change the curvature at \(z = 0\), and hence it is defined in piece-wise manner. Other functions like GELU, SiLU, and clipped ReLU change the curvature at two points and hence have three “pieces”.

It should be noted that \(\sigma_1(z)\) and \(\sigma_2(z)\) in Table 2 are proper continuous convex functions which allows us to use the difference of convex algorithms (DCA) \cite{51} and claim global convergence. Due to space constraints, we have omitted some of the commonly used activation functions. By ReLU and variants in Table 2 we refer to ReLU, leaky ReLU, parametrized ReLU, randomized ReLU, and shifted ReLU. The decomposition for scaled exponential linear unit (SELU) \cite{21} can be done as shown for ELU in Table 2.

The first five rows of Table 2 correspond to \(\sigma_2(\Delta) = 0\). It should be noted that \(h(\Delta) \neq 0\) even if \(\sigma_2(\Delta) = 0\), which is evident from Eq. (15). Hence the original problem may not be convex, and we may have to use the difference of convex programming approach even for activation functions with \(\sigma_2(\Delta) = 0\).

Further, we compute \(\Delta^*\) defined in Eq. (10) by expressing \(f(\Delta) = g(\Delta) - h(\Delta)\) and using concave-convex procedure (CCCP) \cite{48} or difference of convex function algorithm (DCA) \cite{51}. These algorithms are established to be globally convergent, and hence optimal \(\Delta^*\) is obtained and plugged in Algorithm 1.

3.5 Learning Gaussian Graphical Models

Next, we provide a robust adversarial training process for learning Gaussian graphical models. These models are used to study the conditional independence of jointly Gaussian continuous random variables. This can be analyzed by inspecting the zero entries in the inverse covariance matrix, popularly referred as the precision matrix and denoted by \(\Omega\) \cite{26,16}. The classical (non-adversarial) approach \cite{61} solves the following optimization problem to estimate \(\Omega\):

\[
\Omega^* = \arg \min_{\Omega > 0} -\log(\det(\Omega)) + \frac{1}{n} \sum_{i=1}^{n} x^{(i)\top} \Omega x^{(i)} + c \|\Omega\|_1
\]

where \(\Omega\) is constrained to be a symmetric positive definite matrix and \(c\) is a positive regularization constant. As the first term \(\log(\det(\Omega))\) in the above equation can not be influenced by adversarial perturbation in \(x^{(i)}\), we define the adversarial attack problem for this case as maximizing the second term by perturbing \(x^{(i)}\) for each sample:

\[
\Delta^* = \arg \sup_{\|\Delta\| \leq \varepsilon} \left( x^{(i)} + \Delta \right)^\top \Omega \left( x^{(i)} + \Delta \right)
\]

The optimization problem (16) can be defined for various norms. Here, we provide solutions for the \(\ell_2\) and \(\ell_\infty\) norms.
Table 2: Activation function decomposed as a difference of convex functions.

| Name                  | $\sigma(z)$ | $\sigma_1(z)$ | $\sigma_2(z)$ | Domain |
|-----------------------|-------------|---------------|---------------|--------|
| Linear                | $z$         | $z$           | 0             | R      |
| Softplus              | $\log(1 + e^z)$ | $\log(1 + e^z)$ | 0             | R      |
| ReLu & variants       | $\max(0, z)$ | $\max(0, z)$ | 0             | R      |
| Bent Identity         | $\frac{z}{\sqrt{z^2 + 1}} + x$ | $\frac{z}{\sqrt{z^2 + 1}} + x$ | 0             | R      |
| Inverse square root   | $\frac{z}{1 + az^2}$ | $\frac{z}{1 + az^2}$ | 0             | $z < 0$|
| linear unit           | $z$         | $z$           | $z > 0$       |        |
| Hyperbolic            | $\tanh(z)$  | $\tanh(z) - z$ | $z < 0$       |        |
| Tangent               | $\arctan(z)$ | $z - \tanh(z)$ | $z > 0$       |        |
| Inverse               | $\arctan(z)$ | $z - \arctan(z)$ | $z < 0$       |        |
| Tangent               | $\arctan(z)$ | $z - \arctan(z)$ | $z > 0$       |        |
| Sigmoid               | $\frac{1}{1 + \exp(-z)}$ | $\frac{1}{1 + \exp(-z)}$ | $\frac{\tanh(z/2) + 1 - z/2}{z/2 + 1}$ | $z < 0$|
| Gauss Error Function  | $\frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$ | $\frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$ | $\frac{-z}{\sqrt{\pi}}$ | $z > 0$|
| Gauss Error Linear    | $\frac{1}{2} \left( 1 + \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt \right)$ | $\frac{-0.13z - 0.29}{\sqrt{\pi}}$ | $\frac{0.13z - 0.29 - \sigma(z)}{\sqrt{\pi}}$ | $z < -\sqrt{2}$|
| (GELU)                | $\sigma(z)$  | $\sigma(z)$ | $\frac{-0.13z - 0.29 - \sigma(z)}{\sqrt{\pi}}$ | $-\sqrt{2} \leq z \leq \sqrt{2}$|
| Inverse square root   | $\frac{z}{\sqrt{1 + az^2}}$ | $\frac{z}{\sqrt{1 + az^2}}$ | $\frac{-z}{\sqrt{1 + az^2}}$ | $z < 0$|
| root Unit             | $z$         | $z$           | $z - \frac{1}{1 + az^2}$ | $z > 0$|
| Sigmoid Linear        | $\frac{z}{1 + \exp(-z)}$ | $\frac{\sigma(z)}{1 + \exp(-z)}$ | $\frac{\sigma(z) - \frac{1}{1 + az^2}}{1 + \exp(-z)}$ | $z < -2.4$|
| Unit (SiLU)           | $\frac{e^z - 1}{\alpha}$ | $\frac{e^z - 1}{\alpha}$ | $\frac{(\alpha - 1)z}{\alpha}$ | $z > 0$|
| Exponential Linear    | $\max(z, 0)$ | $\max(z, 0)$ | $\max(z - a, 0)$ | $0 \leq z \leq a$|
| Unit (ELU)            | $z$         | $z$           | $z \geq a$    |        |
| Clipped RELU          | $\max(z, 0)$ | $\max(z - a, 0)$ | $0 \leq z \leq a$ |        |

Theorem 7. The solution for the problem specified in equation (16) with $l_2$ constraint on $\Delta$ is given by

$$\Delta^* = (\mu^* I - \Omega)^{-1} \Omega x^{(i)}$$

where $\mu^*$ can be derived from the following one dimensional optimization problem:

$$\max \ - \frac{1}{2} x^{(i)\top} \Omega (\mu I - \Omega)^{-1} \Omega x^{(i)} - \frac{\mu \epsilon^2}{2}$$

such that $\mu I - \Omega \succeq 0$

Proof. The detailed proof is presented in Appendix A.4 due to space constraints. The proof sketch without intermediate steps is discussed here. First, we write the Lagrangian function for the optimization problem specified in Eq. (16):

$$L(\Delta, \mu) = \frac{1}{2} \Delta^\top (\mu I - \Omega) \Delta - \Delta^\top \Omega x^{(i)} - \frac{\mu \epsilon^2}{2}$$

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where $\mu$ is the dual variable. Further, we write all the Karush–Kuhn–Tucker (KKT) conditions to derive the dual function as:

$$g(\mu) = \begin{cases} -\frac{1}{2}x^{(i)^T} (\mu I - \Omega)^{-1} \Omega x^{(i)} - \frac{\mu^2}{2} & (\mu I - \Omega) \succeq 0 \\ -\infty & \text{otherwise} \end{cases}$$

which leads to the one dimensional optimization problem stated in equation (18).

**Theorem 8.** The solution for the problem specified in equation (16) with $\ell_\infty$ constraint on $\Delta \in \mathbb{R}^p$ can be derived from the last column/row of $Y$ obtained from the following optimization problem:

$$\max \left\langle \begin{bmatrix} \Omega \\ (\Omega x^{(i)})^T \\ 0 \end{bmatrix}, Y \right\rangle$$

such that

- $Y_{p+1,p+1} = 1$
- $Y_{ij} \leq 2\epsilon$, $\forall i, j \in [p]$
- $-Y_{ij} \leq 2\epsilon$, $\forall i, j \in [p]$
- $Y \succeq 0$

**Proof.** Please refer to Appendix A.5

The results in Theorem 7 and Theorem 8 do not have a closed form but can be computed easily by solving a standard one-dimensional optimization problem and a SDP respectively. Very efficient scalable SDP solvers exist in practice [62].

### 3.6 Matrix Completion

Recovering the entries of a partially observed matrix has various applications such as collaborative filtering [23], system identification [31], remote sensing [42] and hence, we use it as our next example for the robust adversarial training framework. Assume we are given a partially observed matrix $X$. Let $P$ be a set of indices where the entries of $X$ are observed (i.e., not missing). The classical (non-adversarial) matrix completion approach aims to find a low rank matrix [45] with small squared error in the observed entries. That is:

$$\min_Y \sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2 + c\|Y\|_{tr},$$

where $c$ is a positive regularization constant and $\|\cdot\|_{tr}$ denotes trace norm of matrix which ensures low-rankness. Note that regularization does not impact the adversarial training framework. We define the following worst-case adversarial attack problem:

$$\Delta^* = \arg \sup_{\|\Delta\| \leq \epsilon} \sum_{(i,j) \in P} (X_{ij} + \Delta_{ij} - Y_{ij})^2$$

The solution for the above problem for the Frobenius norm constraint and entry-wise $\ell_\infty$ constraint on $\Delta$ is proposed in Theorem 9 and Corollary 10.

**Theorem 9.** The optimal solution for the optimization in Eq. (19) with Frobenius norm constraint on $\Delta$ if $\exists (i, j) \in P$ such that $X_{ij} \neq Y_{ij}$ is given by

$$\Delta^*_{ij} = \begin{cases} \epsilon \frac{(X_{ij} - Y_{ij})}{\sqrt{\sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2}} & (i,j) \in P \\ 0 & (i,j) \notin P \end{cases}$$

If $X_{ij} = Y_{ij}, \forall (i, j) \in P$, then the optimal $\Delta^*$ can be any solution satisfying $\sum_{(i,j) \in P} \Delta_{ij}^2 = \epsilon$. 


Proof. The detailed proof is presented in the Appendix [A.6] but the proof sketch is discussed here.

First, we construct the Lagrangian for the optimization problem in equation (19):

\[
L(\Delta, \lambda) = -\frac{1}{2} \sum_{(i,j) \in \mathcal{P}} (X_{ij} + \Delta_{ij} - Y_{ij})^2 + \frac{\lambda}{2} \left( \sum_{(i,j) \in \mathcal{P}} \Delta_{ij}^2 - \epsilon^2 \right)
\]

where \( \lambda \) is the dual variable. Further, we write the KKT conditions and derive the dual function:

\[
g(\lambda) = \begin{cases} 
-\lambda (\lambda - 1) \sum_{(i,j) \in \mathcal{P}} (X_{ij} - Y_{ij})^2 - \frac{\lambda^2}{2} & \text{for } \lambda > 1 \\
-\frac{\epsilon^2}{2} & \text{for } \lambda = 1, X_{ij} = Y_{ij}, \forall (i, j) \in \mathcal{P} \\
-\infty & \text{otherwise}
\end{cases}
\]

The above dual problem has a closed form solution and can be used to derive the optimal solution for the primal problem mentioned in Theorem 9.

**Corollary 10.** The optimal solution for the optimization problem in equation (19) with the constraint \( |\Delta_{ij}| \leq \epsilon \) for all \((i, j) \in \mathcal{P}\) is given by \( \Delta_{ij} = \frac{(X_{ij} - Y_{ij})}{|X_{ij} - Y_{ij}|} \epsilon \).

Proof. For this case with \( |\Delta_{ij}| \leq \epsilon \) for all \((i, j) \in \mathcal{P}\), the problem can be solved for each \( \Delta_{ij} \) separately. The problem for each \( \Delta_{ij} \) separately reduces to a particular case of Lemma 14.

### 3.7 Max-Margin Matrix Completion

Our next example is max-margin matrix completion which is closely related to matrix completion. It is also heavily used for collaborative filtering [39, 54]. We start the discussion from the problem under the classical (non-adversarial) setting. Consider a partially observed label matrix where the observed entries are +1 or -1. Let \( \mathcal{P} \) be the indices of the observed entries. The problem of max-margin matrix completion [47] is defined as follows:

\[
\min_Y \sum_{(i,j) \in \mathcal{P}} \max(0, 1 - X_{ij} Y_{ij}) + c ||Y||_{\text{tr}}
\]

where \( c \) is a positive regularization constant and ||·||_{\text{tr}} represents the trace norm [5]. As the second term, ||\(Y||_{\text{tr}}\) in the above optimization problem can not be affected by the adversary, we define the worst-case adversarial attack problem as the maximization of the first term with \( \epsilon \) radius around \( X \):

\[
\Delta^* = \arg \sup_{||\Delta|| \leq \epsilon} \sum_{(i,j) \in \mathcal{P}} \max(0, 1 - (X_{ij} + \Delta_{ij}) Y_{ij})
\]

(20)

The optimal \( \Delta^* \) for the above problem is proposed in the following theorem for the Frobenius norm constraint on \( \Delta \).

**Theorem 11.** For the problem in equation (20) with Frobenius norm constraint on \( \Delta \), the solution is given by

\[
\Delta_{ij} = \begin{cases} 
-\frac{Y_{ij}}{\sqrt{|\mathcal{P}|}} & \text{for } (i,j) \in \mathcal{P}_1 \\
0 & \text{for } (i,j) \notin \mathcal{P}_1
\end{cases}
\]

where \( \mathcal{P}_1 \subseteq \mathcal{P} \) is chosen by sorting \( X_{ij} Y_{ij} \) and selecting indices which satisfy \( X_{ij} Y_{ij} < 1 + \frac{\epsilon}{\sqrt{|\mathcal{P}_1|}} \).
Table 3: Error metrics on real-world data sets for various supervised and unsupervised ML problems. Notice that the proposed approach outperforms the baselines (“No error” and “Random”).

| Problem                | Loss function | Dataset       | Metric | Norm     | No error | Random | Proposed |
|------------------------|---------------|---------------|--------|----------|----------|--------|----------|
| Regression             | Squared loss  | BlogFeedback  | MSE    | Euclidean | 11.66    | 11.66  | 11.18    |
| Regression             | Squared loss  | BlogFeedback  | MSE    | $\ell_\infty$ | 11.66   | 11.66  | 11.20    |
| Classification         | Logistic loss | ImageNet      | Accuracy | Euclidean | 49.80     | 48.13  | 56.75    |
| Classification         | Logistic loss | ImageNet      | Accuracy | $\ell_\infty$ | 49.80   | 45.46  | 55.34    |
| Classification         | Hinge loss    | ImageNet      | Accuracy | Euclidean | 47.89     | 46.66  | 52.31    |
| Classification         | Hinge loss    | ImageNet      | Accuracy | $\ell_\infty$ | 47.89   | 45.99  | 52.30    |
| Classification         | Two-layer NN (ReLU) | ImageNet  | Accuracy | Euclidean | 70.74    | 70.66  | 75.86    |
| Classification         | Two-layer NN (Sigmoid) | ImageNet | Accuracy | Euclidean | 63.73    | 59.97  | 71.86    |
| Graphical Model        | Log-likelihood | TCGA       | Likelihood | Euclidean | -7984.8  | -7980.6 | -7406.1 |
| Graphical Model        | Log-likelihood | TCGA       | Likelihood | $\ell_\infty$ | -7984.8 | -7810.7 | -3571.9 |
| Matrix Completion (MC) | Squared loss  | Netflix      | MSE    | Frobenius | 4.783    | 4.894  | 3.2      |
| Matrix Completion      | Squared loss  | Netflix      | MSE    | Entry-wise $\ell_\infty$ | 4.783 | 4.783  | 3.869    |
| Max-Margin MC          | Squared loss  | HouseRep     | Accuracy | Frobenius | 94.9     | 79.1   | 95.2     |
| Max-Margin MC          | Squared loss  | HouseRep     | Accuracy | Entry-wise $\ell_\infty$ | 92.4 | 60.7   | 92.5     |

Similarly, the solution for the problem specified in equation (20) for the entry-wise $\ell_\infty$ norm is proposed in the following corollary.

**Corollary 12.** For the problem in equation (20) with the constraint $|\Delta_{ij}| \leq \epsilon$ for all $(i, j) \in \mathcal{P}$, the optimal solution is given by $\Delta_{ij} = -Y_{ij}\epsilon$.

**Proof.** This is a particular case of Lemma 14. As all the entries $(i, j) \in \mathcal{P}$ of $\Delta$ can use the budget $\epsilon$ independently, the problem can be solved for each $\Delta_{ij}$ separately. □

A concise summary of all our results is available in Table 1. In the next section, we proceed to validate our approach with experiments on real-world data sets.

### 4 Real-World Experiments

In this section, we validate the proposed method for various ML problems discussed in the previous section on real-world datasets. We compare the proposed approach against two training approaches. The first baseline is the classical (non-adversarial) approach of setting $\Delta^* = 0$ and the second baseline is the approach of choosing $\Delta^*$ randomly as in [13, 36]. We ran the experiments on various supervised and unsupervised ML problems described below:

1. **Regression**: We consider the BlogFeedback dataset [8] to predict the number of comments on a post. We chose the first 5000 samples for training and the last 5000 samples for testing.

2. **Classification**: For this task, we use the ImageNet dataset [10] which is available publicly. The dataset contains 1000 bag-of-words features. We perform experiments for logistic regression, hinge loss, and two-layer neural networks using ReLU and sigmoid activation.

3. **Gaussian Graphical models**: For this task, we use the publicly available cancer genome atlas (TCGA) dataset. The dataset contains gene expression data for 171 genes. We chose breast cancer (590 samples) for training and ovarian cancer (590 samples) for testing to create an out-of-distribution scenario.
4. **Matrix Completion**: For this problem, we use the publicly available Netflix Prize dataset [7]. We chose the 1500 users and 500 movies with most ratings. We randomly assigned the available user/movie ratings to the training and testing sets. As the users can be from any location, age, gender, nationality and movies can also have different genres, language, or actors, this generates an instance of the out-of-distribution scenario.

5. **Max-margin matrix completion**: We used the votes in the House of Representatives (HouseRep) for the first session of the 110th U.S. congress. The HouseRep dataset contains 1176 votes for 435 representatives. A “Yea” vote was considered +1, a “Nay” vote was considered -1. We randomly assigned the available votes to the training and testing sets.

The results are summarized in Table 3 and it can be clearly observed that the proposed method outperforms the baselines. Please refer to Appendix A.8 for more details.

5 **Concluding Remarks**

As robust adversarial training is not limited only to the problems covered in this work, it can be extended to other problems such as clustering, discrete optimization problems, and randomized algorithms in the future.

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A Appendix

A.1 Proof of Theorem 3

Proof. Please refer to Lemma 13 and Lemma 14 for the case of \( w^\top x^{(i)} - y^{(i)} = 0 \) and \( w^\top x^{(i)} - y^{(i)} \neq 0 \) respectively. The proof relies on norm duality and sub-differentials.

Lemma 13. For the problem specified in equation (5), the optimal solution for the case when \( w^\top x^{(i)} - y^{(i)} = 0 \) is given by \( \Delta^* = \pm \epsilon \frac{v}{\|v\|} \) where \( v \in \partial \|w\|_* \) as specified in Definition 2.

Proof. The problem specified in equation (5) reduces to the dual norm problem for \( w^\top x^{(i)} - y^{(i)} = 0 \):

\[
\sup_{\|\Delta\| \leq \epsilon} w^\top \Delta
\]

Using the Holder’s inequality, we can claim:

\[
w^\top \Delta \leq \|w\| \|\Delta\| \leq \epsilon \|w\|_*
\]

Therefore to compute \( \Delta^* \), we need to find the solution for

\[
\Delta^* = \{ \Delta : \langle \Delta, w \rangle = \|w\|, \|\Delta\|_* \leq 1 \}
\]

To compute the optimal point, we use the sub-differential of a norm in Definition 2 and claim that \( \Delta^* \in \partial \|w\|_* \). The scaling is done to maintain \( \|\Delta^*\| \leq \epsilon \). As the original objective function is quadratic, \( -\Delta^* \) can also be a solution.

Lemma 14. For the problem specified in equation (5), the optimal solution for the case when \( w^\top x^{(i)} - y^{(i)} \neq 0 \) is:

\[
\Delta^* = \epsilon \text{sign}(w^\top x^{(i)} - y^{(i)}) \frac{v}{\|v\|}
\]

where \( v \in \partial \|w\|_* \) as specified in Definition 2.

Proof. Assume \( w^\top x^{(i)} - y^{(i)} > 0 \), so the objective function to maximize \( (w^\top x^{(i)} - y^{(i)} + w^\top \Delta)^2 \) can be expressed as maximizing \( w^\top \Delta \) because \( w^\top x^{(i)} - y^{(i)} \) is a positive constant and not a function of \( \Delta \). Further, we use Lemma 13 to derive the solution as \( \epsilon \frac{v}{\|v\|} \).

Similarly for the other case, assuming \( w^\top x^{(i)} - y^{(i)} < 0 \), our objective is to minimize \( w^\top \Delta \) and hence using Lemma 13 or norm duality, the optimal solution is \( -\epsilon \frac{v}{\|v\|} \). Combining the results from the two cases, we complete the proof of this lemma.

A.2 Proof of Theorem 4

Proof. The objective function can be seen as maximizing \( \log(1 + \exp(-f(\Delta))) \), where \( f(\Delta) = y^{(i)}w^\top (x^{(i)} + \Delta) \). It should be noted that \( \log(\cdot) \) and \( 1 + \exp(\cdot) \) are strictly monotonically increasing functions and hence maximizing \( \log(1 + \exp(-f(\Delta))) \) is equivalent to minimizing \( f(\Delta) \). This is equivalent to minimizing \( y^{(i)}w^\top \Delta \). Using Lemma 13, the solution can be stated as \( \Delta^* = -\epsilon y^{(i)} \frac{v}{\|v\|} \) where \( v \in \partial \|w\|_* \).
Thus, we have \( \Delta \) which gives the optimal solution: 
\[
- \epsilon \frac{\|v\|}{\|w\|} \nabla \nabla \Delta.
\]
Due to the presence of the max function in the hinge loss, \((x^{(i)}, y^{(i)})\) satisfying 
\[
y^{(i)}w^T x^{(i)} - cw^T v \geq 1
\]
does not affect the objective function.

\[\square\]

### A.3 Proof of Theorem 5

**Proof.** Define the function \( f(\Delta) = y^{(i)}w^T (x^{(i)} + \Delta) \). Hence the optimization problem can be seen as the maximization of \( \max(0, 1 - f(\Delta)) \). If we had the maximization problem of \( 1 - f(\Delta) \) instead of \( \max(0, 1 - f(\Delta)) \), the solution would be simple. This can be seen as maximization of \( 1 - y^{(i)}w^T (x^{(i)} + \Delta) \), which is equivalent to minimizing \( y^{(i)}w^T \Delta \). Using Lemma 13, the solution can be claimed as 
\[
- \epsilon \frac{\|v\|}{\|w\|} \nabla \nabla \Delta.
\]

### A.4 Proof of Theorem 7

**Proof.** First we drop the superscript from \( x^{(i)} \) for clarity. For the problem in Eq. (16) with constraint \( \|\Delta\|_2 \leq \epsilon \), we write the Lagrangian function:
\[
L(\Delta, \mu) = -\frac{1}{2} (\Delta^T \Omega + 2\Delta^T \Omega x) + \frac{\mu}{2} (\Delta^T \Delta - \epsilon^2)
\]
\[
= \frac{1}{2} \Delta^T (\mu I - \Omega) \Delta - \Delta^T \Omega x - \frac{\mu \epsilon^2}{2}
\]
Note that we need \((\mu I - \Omega) \geq 0\) for the problem to be convex. If \((\mu I - \Omega) \geq 0\) does not hold, then \((\mu I - \Omega) \) has at least one negative eigenvalue. Let \( \nu \) and \( \mathbf{u} \) be the associated eigenvalue and eigenvector. Therefore, the Lagrangian can be simplified to 
\[
L(\Delta, \mu) = \nu^2 - \nu t^T \Omega x + c,
\]
where \( c \) is a constant by choosing \( \Delta = tu \). Further, we can set \( t \rightarrow \infty \) if \( u^T \Omega x > 0 \), or \( t \rightarrow -\infty \) otherwise. Thus \( g(\mu) = \inf_{\Delta} L(\Delta, \mu) = -\infty \).

Assume \((\mu I - \Omega) \geq 0\), then by the first order stationarity condition:
\[
\frac{\partial L}{\partial \Delta} = (\mu I - \Omega) \Delta - \Omega x = 0
\]
which gives the optimal solution: 
\[
\Delta^* = (\mu I - \Omega)^{-1} \Omega x.
\]

The dual function, assuming \((\mu I - \Omega) \geq 0\) is:
\[
g(\mu) = L(\Delta^*, \mu)
\]
\[
= \frac{1}{2} x^T \Omega (\mu I - \Omega)^{-1} (\mu I - \Omega) (\mu I - \Omega)^{-1} \Omega x - x^T \Omega (\mu I - \Omega)^{-1} \Omega x - \frac{\mu \epsilon^2}{2}
\]
\[
= \frac{1}{2} x^T \Omega (\mu I - \Omega)^{-1} \Omega x - x^T \Omega (\mu I - \Omega)^{-1} \Omega x - \frac{\mu \epsilon^2}{2}
\]
\[
= -\frac{1}{2} x^T \Omega (\mu I - \Omega)^{-1} \Omega x - \frac{\mu \epsilon^2}{2}
\]
Thus, we have
\[
g(\mu) = \begin{cases} 
-\frac{1}{2} x^T \Omega (\mu I - \Omega)^{-1} \Omega x - \frac{\mu \epsilon^2}{2} & \text{if } (\mu I - \Omega) \geq 0 \\
-\infty & \text{otherwise}
\end{cases}
\]

Hence the dual problem is:
\[
\max \quad -\frac{1}{2} x^T \Omega (\mu I - \Omega)^{-1} \Omega x - \frac{\mu \epsilon^2}{2}
\]
such that \( \mu I - \Omega \geq 0 \)

This is a one dimensional optimization problem, which can be solved easily. 

\[\square\]
A.5 Proof of Theorem 8

Proof. First we drop the superscript from $x^{(i)}$ for clarity. The constraint $\|\Delta\|_\infty \leq \epsilon$ can be expressed as $\max_{i \in [p]} |\Delta_i| \leq \epsilon$, which implies $\max_{i,j \in [p]} |\Delta_i \Delta_j| \leq \epsilon^2$.

The objective function can be expressed as follows by using the notation for inner products of matrices:

$$L(\Delta) = (\Delta^\top \Omega \Delta + 2\Delta^\top \Omega x)$$

$$= \left\langle \begin{bmatrix} \Omega & \Omega x \\ (\Omega x)^\top & 0 \end{bmatrix}, \begin{bmatrix} \Delta \Delta^\top \Delta \\ \Delta^\top 1 \end{bmatrix} \right\rangle$$

$$= \left\langle \begin{bmatrix} \Omega & \Omega x \\ (\Omega x)^\top & 0 \end{bmatrix}, \begin{bmatrix} \Delta \end{bmatrix} \begin{bmatrix} \Delta \end{bmatrix}^\top \right\rangle$$

(22)

Hence the above problem can be formulated as an SDP:

$$\max \left\langle \begin{bmatrix} \Omega & \Omega x \\ (\Omega x)^\top & 0 \end{bmatrix}, Y \right\rangle$$

such that $Y_{p+1,p+1} = 1$

$Y_{ij} \leq \epsilon^2, \quad \forall i, j \in [p]$

$-Y_{ij} \leq \epsilon^2, \quad \forall i, j \in [p]$

$Y \succeq 0$

The optimal $\Delta$ can be obtained from the last column/row of the optimal solution $Y$ for the above problem. \qed

A.6 Proof of Theorem 9

Proof. The function is maximized if the adversary spend the budget on the entries in $\mathcal{P}$. First, we write the Lagrangian for Eq. (19):

$$L(\Delta, \lambda) = -\frac{1}{2} \sum_{(i,j) \in \mathcal{P}} (X_{ij} + \Delta_{ij} - Y_{ij})^2 + \frac{\lambda}{2} \left( \sum_{(i,j) \in \mathcal{P}} \Delta_{ij}^2 - \epsilon^2 \right)$$

$$= -\frac{1}{2} \sum_{(i,j) \in \mathcal{P}} (X_{ij} - Y_{ij})^2 - \sum_{(i,j) \in \mathcal{P}} \Delta_{ij} (X_{ij} - Y_{ij}) + \frac{1 + \lambda}{2} \left( \sum_{(i,j) \in \mathcal{P}} \Delta_{ij}^2 \right) - \frac{\epsilon^2}{2}$$

For $\lambda < 1$, we can set $\Delta_{ij} = t \text{sign}(X_{ij} - Y_{ij})$, then the Lagrangian simplifies to:

$$L(\Delta, \lambda) = -\frac{1}{2} \sum_{(i,j) \in \mathcal{P}} (X_{ij} - Y_{ij})^2 - \sum_{(i,j) \in \mathcal{P}} t |X_{ij} - Y_{ij}| + \frac{1 + \lambda}{2} \left( \sum_{(i,j) \in \mathcal{P}} t^2 \right) - \frac{\epsilon^2}{2}$$

Then we can take $t \to \infty$ and therefore $g(\lambda) = \inf_\Delta L(\Delta, \lambda) = -\infty$.

For $\lambda > 1$, the first order derivative of the Lagrangian is:

$$\frac{\partial L}{\partial \Delta_{ij}} = -(X_{ij} + \Delta_{ij} - Y_{ij}) + \lambda \Delta_{ij} = 0$$
and thus:
\[ \Delta^*_{ij} = \frac{(X_{ij} - Y_{ij})}{\lambda - 1} \quad \text{if } \lambda > 1 \]

Hence, the dual function can be derived assuming \( \lambda > 1 \):
\[
g(\lambda) = L(\Delta^*, \lambda) = -\frac{1}{2} \lambda \sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2 - \frac{\lambda \epsilon^2}{2}
\]

For \( \lambda = 1 \), the Lagrangian \( L \) is:
\[
L(\Delta, 1) = -\frac{1}{2} \sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2 - \sum_{(i,j) \in P} \Delta_{ij} (X_{ij} - Y_{ij}) - \frac{\epsilon^2}{2}
\]

Note that \( g(1) = \inf_{\Delta} L(\Delta, 1) = -\infty \) if there exists \((i, j) \in P\) such that \( X_{ij} \neq Y_{ij} \), since we can set \( \Delta_{ij} = t \text{sign}(X_{ij} - Y_{ij}) \) and take \( t \to \infty \).

Thus we have the dual function as:
\[
g(\lambda) = \begin{cases} 
\frac{1}{2} \lambda \sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2 - \frac{\lambda \epsilon^2}{2} & \lambda > 1 \\
\frac{\epsilon^2}{2} & \lambda = 1 \text{ and } X_{ij} = Y_{ij}, \forall (i,j) \in P \\
-\infty & \text{otherwise}
\end{cases}
\]

The optimal \( \lambda \) can be derived by taking the first order derivative
\[
\frac{1}{\epsilon^2} \sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2 = (\lambda - 1)^2
\]

Therefore
\[
\lambda^* = 1 + \frac{1}{\epsilon} \sqrt{\sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2}
\]

Hence \( \Delta^*_{ij} \) is given by
\[
\Delta^*_{ij} = \epsilon \frac{(X_{ij} - Y_{ij})}{\sqrt{\sum_{(i,j) \in P} (X_{ij} - Y_{ij})^2}}
\]

If \( X_{ij} = Y_{ij}, \forall (i,j) \in P \), then the optimal \( \Delta^* \) can be any solution satisfying \( \sum_{(i,j) \in P} \Delta^2_{ij} = \epsilon \). \( \square \)

### A.7 Proof of Theorem 11

**Proof.** The problem without the max function in the objective function is equivalent to:
\[
\sup_{\|\Delta\|^2 \leq \epsilon^2} -\sum_{(i,j) \in P} \Delta_{ij} Y_{ij}
\]

The optimal solution for above problem is
\[
\Delta_{ij} = -Y_{ij} \frac{\epsilon}{\sqrt{|P|}}
\]
for \((i, j) \in \mathcal{P}\). But the optimal solution changes with the introduction of the max term in equation \([20]\). Few of the terms with indices \((i, j) \in \mathcal{P}\) do not affect the objective function if

\[
X_{ij}Y_{ij} > 1 + \frac{\epsilon}{\sqrt{|\mathcal{P}|}}
\]

Hence the budget should be spent on the indices satisfying \(X_{ij}Y_{ij} < 1 + \frac{\epsilon}{\sqrt{|\mathcal{P}|}}\), where \(\mathcal{P}_1 \subseteq \mathcal{P}\) is the modified set. Note that the set \(\mathcal{P}_1\) can be derived by sorting \(X_{ij}Y_{ij}\) for \((i, j) \in \mathcal{P}\), which takes \(O(|\mathcal{P}| \log(|\mathcal{P}|))\) time.

We further describe the method to compute \(\mathcal{P}_1\). Let \(Z = X \odot Y\) denote the Hadamard product of \(X\) and \(Y\). We define the mapping \(\Pi : \{1, 2, \ldots, |\mathcal{P}|\} \to \mathcal{P}\) which sorts the terms \(X_{ij}Y_{ij}\) for \((i, j) \in \mathcal{P}\) in ascending order, i.e. \(Z_{\Pi(1)} \leq Z_{\Pi(2)} \leq \ldots Z_{\Pi(n)}\), where \(n = |\mathcal{P}|\).

Now consider the three cases:

1. Case 1: Assume \(Z_{\Pi(i)} \geq 1 + \epsilon\). Therefore, \(Z_{\Pi(i)} \geq 1 + \epsilon\) for all \(i \in [n]\). Hence, any change in \(X_{ij}Y_{ij}\) does not make any change in the objective function. Therefore, \(\Delta_{ij} = 0\) for all \((i, j) \in \mathcal{P}\) and \(\mathcal{P}_1 = \emptyset\).

2. Case 2: Assume \(Z_{\Pi(n)} \leq 1\). All the \(X_{ij}Y_{ij}\) can be decreased to increase the objective function value. Thus, \(\Delta_{ij} = -\epsilon Y_{ij}/\sqrt{n}\) and \(\mathcal{P}_1 = \mathcal{P}\).

3. Case 3: Other cases which are not satisfied in the above two cases are discussed here. We define the left set \(\mathcal{S}_l = \{\Pi(i) : Z_{\Pi(i)} \leq 1, i \in [n]\}\). We also define the middle set \(\mathcal{S}_m = \{\Pi(i) : Z_{\Pi(i)} \in (1, 1 + \epsilon), i \in [n]\}\) and let \(k = |\mathcal{S}_l| > 0\). A few elements of the set \(\mathcal{S}_m\) will contribute in decreasing the objective function and we discuss the approach to compute those terms.

Consider two sub-cases:

(a) If \(Z_{\Pi(k+1)} > 1 + \frac{\epsilon}{k+1}\), then \(\Pi(k+1)\) should not be included and hence \(\mathcal{P}_1 = \mathcal{S}_l\) and each \(\Delta_{ij} = -Y_{ij}/\sqrt{k}\).

(b) If \(Z_{\Pi(k+1)} \leq 1 + \frac{\epsilon}{k+1}\), then \(\Pi(k+1)\) should be included in \(\mathcal{P}_1\). Assume such \(i^*\) elements can be included in \(\mathcal{P}_1\). This can be computed by finding the largest index \(i^* \in \{k+1, k+2, \ldots, k+|\mathcal{S}_m|\}\) such that \(Z_{\Pi(i)} \leq 1 + \frac{\epsilon}{\sqrt{i}}\).

Further, we compute \(\mathcal{P}_1 = \{\Pi(i) : i \in \{1, 2, \ldots, i^*\}\}\) and \(\Delta_{ij}\) can be computed as \(-Y_{ij}/\sqrt{|\mathcal{P}_1|}\).

\[\square\]

### A.8 Experiments

In this section, we validate the proposed method for various ML problems. Our intention in this work is not motivated towards designing the most optimal algorithm which solves all the ML problems discussed previously. Rather, we demonstrate the practical utility of our novel approach that can integrate our plug-and-play solution with widely accepted ML models. As a generic optimization algorithm, we chose to work with projected gradient descent in all the experiments, which can be replaced with any other variant of the user’s choice.

We compare our proposed approach with two other training approaches. The first baseline is the classical approach of training without any perturbation, meaning \(\Delta^* = 0\) in Algorithm \([1]\). The second approach is to directly use a random \(\Delta^*\) without solving the optimization problem. These two baselines are referred as “No error” and “Random” in the columns of Table \([8]\) and Table \([4]\). Our proposed approach is referred as “Proposed”. As there are different ML problems, we use different performance metrics for comparison.
Table 4: Running time (in seconds) for experiments on real-world data sets for various supervised and unsupervised ML problems. Note that the running times of the proposed approach is comparable to the baselines (“No error” and “Random”).

| Problem               | Loss function | Dataset         | Norm   | No error | Random  | Proposed |
|-----------------------|---------------|-----------------|--------|----------|---------|----------|
| Regression            | Squared loss  | BlogFeedback    | Euclidean | 5.66     | 19.41   | 6.03     |
| Regression            | Squared loss  | BlogFeedback    | $\ell_\infty$ | 5.76     | 19.64   | 6.15     |
| Classification        | Logistic loss | ImageNet        | Euclidean | 22.69    | 64.12   | 21.8     |
| Classification        | Logistic loss | ImageNet        | $\ell_\infty$ | 22.64    | 64.39   | 21.75    |
| Classification        | Hinge loss    | ImageNet        | Euclidean | 20.03    | 59.82   | 18.29    |
| Classification        | Hinge loss    | ImageNet        | $\ell_\infty$ | 20.52    | 59.5    | 18.06    |
| Graphical Model       | Log-likelihood| TCGA            | Euclidean | 5.1      | 5.43    | 5.82     |
| Graphical Model       | Log-likelihood| TCGA            | $\ell_\infty$ | 4.64     | 5.14    | 8.73     |
| Matrix Completion (MC)| Squared loss  | Netflix         | Frobenius | 9.85     | 10.93   | 10.94    |
| Matrix Completion     | Squared loss  | Netflix         | Entry-wise $\ell_\infty$ | 9.82     | 10.42   | 10.54    |
| Max-Margin MC         | Hinge loss    | HouseRep        | Frobenius | 6.84     | 7.68    | 8.05     |
| Max-Margin MC         | Hinge loss    | HouseRep        | Entry-wise $\ell_\infty$ | 6.99     | 7.46    | 6.72     |

**Regression:** We consider the BlogFeedback dataset [8] to predict the number of comments on a post. We chose the first 5000 samples for training and the last 5000 samples for testing. We perform training using the three approaches. In our method, we plug $\Delta^*$ using Theorem 3. We use mean square error (MSE) to evaluate the performance on a test set, which is reported to be the lowest for our proposed approach for the Euclidean and $\ell_\infty$ norm constraints.

**Classification:** For this task, we use the ImageNet dataset [10] which is available publicly. The dataset contains 1000 bag-of-words features. For training, we used “Hungarian pointer” having 2334 samples versus “Lion” with 1795 samples. For testing, we used “Siamese cat” with 1739 samples versus “Tiger” having 2086 samples. Hence the data set is constructed for the out-of-distribution scenario. We train the model with the logistic loss by supplying $\Delta^*$ from Theorem 4 for our algorithm. We use the accuracy metric to evaluate the performance on a test set, and it was observed to be the best for our proposed algorithm. The same procedure was applied to test the hinge loss function by supplying $\Delta^*$ from Theorem 5 and we note that our proposed algorithm outperforms the other approaches for the Euclidean and $\ell_\infty$ norm constraints.

**Gaussian Graphical models:** For this task, we use the publicly available Cancer Genome Atlas (TCGA) dataset. The dataset contains gene expression data for 171 genes. We chose breast cancer (590 samples) for training and ovarian cancer (590 samples) for testing to create an out-of-distribution scenario. The adversarial perturbation for robust learning in the proposed method was supplied from Theorem 7 and Theorem 8. We compare the training approaches based on the log-likelihood of a test set from the learned precision matrices. The log-likelihood is reported to be the largest for our proposed approach for the Euclidean and $\ell_\infty$ norm constraints.

**Matrix Completion:** For this problem, we use the publicly available Netflix Prize dataset [7]. We chose the 1500 users and 500 movies with most ratings. We randomly assigned the available user/movie ratings to the training and testing sets. As the users can be from any location, age, gender, nationality and movies can also have different genres, language, or actors, this generates an instance of the out-of-distribution scenario. Training was performed using the three approaches.
In our method, $\Delta^*$ was chosen using Theorem 9 and Corollary 10. We use the MSE metric on the test set which is reported to be the lowest for our proposed method.

**Max-Margin Matrix Completion:** We used the votes in the House of Representatives (HouseRep) for the first session of the 110th U.S. congress. The HouseRep dataset contains 1176 votes for 435 representatives. A “Yea” vote was considered +1, a “Nay” vote was considered -1. We randomly assigned the available votes to the training and testing sets. Further, we trained the model using the three approaches. In our method, $\Delta^*$ was chosen using Theorem 11 and Corollary 12. We use the percentage of correctly recovered votes on a test set as the metric to compare the three training approaches.

All the codes were ran on a machine with an 2.2 GHz Quad-Core Intel Core i7 processor with RAM of 16 GB. The running times for the three training approaches is compared in Table 4. It can be seen that the running time for the proposed approach is comparable to the other training approaches for most of the ML problems discussed above.