Provable Gradient Editing of Deep Neural Networks

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Abstract

In explainable AI, DNN gradients are used to interpret the prediction; in safety-critical control systems, gradients could encode safety constraints; in scientific-computing applications, gradients could encode physical invariants. While recent work on provable editing of DNNs has focused on input-output constraints, the problem of enforcing hard constraints on DNN gradients remains unaddressed. We present ProGrad, the first efficient approach for editing the parameters of a DNN to provably enforce hard constraints on the DNN gradients. Given a DNN $\mathcal{N}$ with parameters θ, and a set $\mathcal{S}$ of pairs $(\mathbf{x}, \mathrm{Q})$ of input $\mathbf{x}$ and corresponding linear gradient constraints Q, ProGrad finds new parameters $\widehat{\boldsymbol{\theta}}$ such that $\bigwedge_{(\mathbf{x},\mathrm{Q})\in\mathcal{S}} \frac{\partial}{\partial\mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathrm{Q}$ while minimizing the changes $\|\widehat{\boldsymbol{\theta}} - \theta\|$. The key contribution is a novel *conditional variable gradient* of DNNs, which relaxes the NP-hard provable gradient editing problem to a linear program (LP), enabling ProGrad to use an LP solver to efficiently and effectively enforce the gradient constraints. We experimentally evaluated ProGrad via enforcing **(i)** hard Grad-CAM constraints on IMAGENET ResNet DNNs; **(ii)** hard Integrated Gradients constraints on Llama 3 and Qwen 3 LLMs; **(iii)** hard gradient constraints in training a function-approximation DNN as a proxy for safety constraints in control systems and physical invariants in scientific applications. The results highlight the unique capability of ProGrad in enforcing hard constraints on DNN gradients.

1 Introduction

Incorporating constraints into deep neural networks (DNNs) can enable learning with less data (e.g., in scientific domains) and provide guarantees about their behavior (e.g., in safety-critical applications). This has led to many recent works on provable editing of DNNs [41, 40], which enforce hard constraints on input-output behavior of DNNs. However, the problem of enforcing hard constraints on the gradients of DNNs remains unaddressed. This paper presents ProGrad, which addresses the provable gradient editing problem defined below:

Definition 1.1. Given a DNN $\mathcal{N} : \mathbb{R}^n \to \mathbb{R}^m$ with parameters θ, a set $\mathcal{S} \subseteq \left\{\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^n\right\} \times \left\{\mathrm{Q} \mid \mathrm{Q} \subseteq \mathbb{R}^{m\times n}\right\}$ of pairs $(\mathbf{x}, \mathrm{Q})$, where $\mathbf{x} \in \mathbb{R}^n$ is an input and $\mathrm{Q} \stackrel{\text{def}}{=} \left\{\mathbf{J} \in \mathbb{R}^{m\times n} \mid \mathbf{A}\,\mathrm{vec}(\mathbf{J}) \le \mathbf{b}\right\}$ is the corresponding linear constraints on the Jacobian $\frac{\partial}{\partial\mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathbb{R}^{m\times n}$ of the DNN $\mathcal{N}$ with respect to the input $\mathbf{x}$, we use $\mathrm{vec}(\mathbf{J})$ to denote the Jacobian matrix $\mathbf{J}$ flattened as a vector. The **provable gradient editing problem** is to find new parameters $\widehat{\boldsymbol{\theta}}$ such that

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \text{s.t.} \quad \bigwedge_{(\mathbf{x},\mathrm{Q})\in\mathcal{S}} \frac{\partial}{\partial\mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathrm{Q} \tag{1}$$ ■

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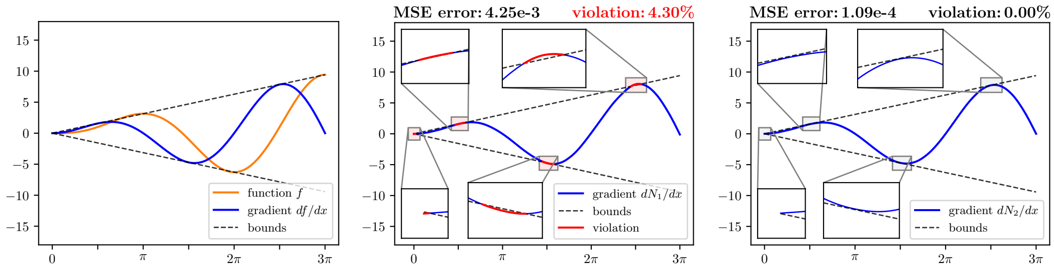

(a) Target function f, whose gradient $\frac{d}{dx}f$ is bounded.

(b) Unsafe DNN $\mathcal{N}_1$, whose gradient $\frac{d}{dx}\mathcal{N}_1$ is *not bounded*.

(c) Safe $\mathcal{N}_2$ repaired by ProGrad, whose gradient $\frac{d}{dx}\mathcal{N}_2$ is *bounded*.

Figure 1: **Enforcing hard constraints on the gradient of a DNN. (Left) 1(a)** shows the target function $f(x) = -x\cos(x) + \sin(x)$ over the input domain $[0, 3\pi]$, whose gradient $\frac{d}{dx}f(x) = x\sin(x)$ is bounded by $g_u(x) = x$ and $g_l(x) = -x$. **(Middle) 1(b)** shows a DNN $\mathcal{N}_1$ trained on both the output and the gradient of f. Although $\mathcal{N}_1$ has good (low) output and gradient errors, its gradient $\frac{d}{dx}\mathcal{N}_1$ violates the hard constraints—as shown in the zoom-ins, its gradient $\frac{d}{dx}\mathcal{N}_1$ is *not bounded* by g_u and g_l. **(Right) 1(c)** shows a DNN $\mathcal{N}_2$ edited by ProGrad to satisfy the hard gradient constraints – its gradient $\frac{d}{dx}\mathcal{N}_2$ is *bounded* by g_u and g_l. DNN $\mathcal{N}_2$ also achieves better (lower) output and gradient errors. See Section 5.3 for more details.

(a) Original image.

(b) Reference Grad-CAM on the original image.

(c) Misclassified Gaussian-noise corrupted image.

(d) Deviated Grad-CAM on the corrupted image.

(e) Edited Grad-CAM on the corrupted image.

Figure 2: **Enforcing hard Grad-CAM constraints on an IMAGENET ResNet152 DNN.** Figure 2(a) shows a correctly-classified image with an appropriate Grad-CAM (2(b)) focusing on the object of interest. Figure 2(c) shows a Gaussian-noise-corrupted version of the original image, which is misclassified by the DNN, and the focus of its Grad-CAM (2(d)) deviates from the object of interest. We use ProGrad to edit the DNN to enforce the reference Grad-CAM (2(b)) on the corrupted image (2(c)). Figure 2(e) shows the Grad-CAM of the corrupted image on the edited DNN, which is now aligned with the reference Grad-CAM (2(b)). See Section 5.1 for more details.

In other words, provable gradient editing aims to make minimal changes to the parameters of a DNN to ensure that the DNN is guaranteed to satisfy any affine constraints involving the gradients of the DNN with respect to its input. Hard constraints on the gradient of a function with respect to its input are common in many scientific applications and safety-critical control systems. As an illustrative example, consider the function $f(x)$ in Figure 1(a) whose gradient $\frac{d}{dx}f$ should be bounded by $g_u(x) = x$ and $g_l(x) = -x$ over the domain $[0, 3\pi]$. Prior regularization-based training approaches can be used to enforce soft constraints on the gradient. However, as shown in Figure 1(b), although such a DNN $\mathcal{N}_1$ achieves good (low) output and gradient errors, its gradient $\frac{d}{dx}\mathcal{N}_1$ exceeds the bounds g_u and g_l and violates the hard gradient constraints, hence *unsafe*. In contrast, Figure 1(c) shows a *safe* DNN $\mathcal{N}_2$ edited by our method ProGrad to satisfy the hard constraints on the gradient, which also achieves better (lower) output and gradient errors.

Another natural application of gradient constraints is to ensure that the DNN has the appropriate gradient-based interpretation for a given input, which is important for explainable AI. Figure 2 shows a use case where we enforce an expected Grad-CAM attribution (Definition 3.5) for an IMAGENET ResNet-152 DNN; Figure 3 shows a use case where we enforce an expected Integrated Gradients attribution (Definition 3.4) for a Llama 3 LLM [9].

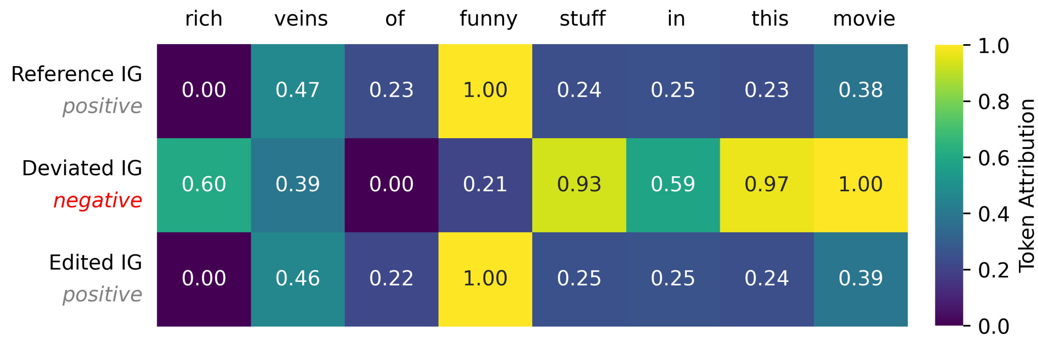

Figure 3: **Enforcing hard Integrated Gradients (IG) constraints on a Llama 3 LLM [9].** The sentence is from the Stanford Sentiment Treebank 2 (SST-2) dataset [36]. **The first row** shows the *reference IG* from a larger LLM, which correctly classifies the sentiment of the sentence as *positive*. **The second row** shows the *deviated IG* from the smaller LLM, which *misclassifies* the sentiment of the sentence as *negative*. **The third row** shows the *edited IG* from the repaired smaller LLM edited by `ProGrad`, whose IG is enforced to be close to the reference IG from the larger LLM, and correctly classifies the sentiment of the sentence as *positive*. See Section 5.2 for more details.

To the best of our knowledge, `ProGrad` is the *first* efficient approach for enforcing hard constraints on the gradients of a DNN that runs in polynomial time in the size of the edited layers (Theorem 4.3). Our **key contribution** is a novel *conditional variable gradient* of DNNs (Definition 4.2), which relaxes the NP-hard provable gradient editing problem to a **linear programming (LP)** problem, enabling `ProGrad` to use an LP solver to efficiently and effectively enforce the gradient constraints.

We evaluate `ProGrad` by enforcing **(i)** hard Grad-CAM constraints on IMAGENET ResNet DNNs; **(ii)** hard Integrated Gradients constraints on Llama 3 and Qwen 3 LLMs; **(iii)** hard gradient constraints in training a function-approximation DNN, which acts as a proxy for safety constraints in control systems and physical invariants in scientific applications. *The results highlight the unique capability of* `ProGrad` *in enforcing hard constraints on DNN gradients and gradient-based explanations.*

2 Related Work

There have been many recent works on incorporating constraints into deep learning. These can be categorized into four categories based on *whether they treat constraints as soft or hard constraints*, and *whether they support input-output constraints or gradient constraints*.

For **soft constraints**, regularized training modifies the loss function to incorporate constraints as regularization and does not guarantee constraint satisfaction. There have been many recent such approaches for incorporating *input-output constraints* [14, 45, 23, 5, 12, 17, 47, 38]. Certified training [21, 7, 31, 1, 24, 22, 20] is a type of regularized training geared towards adversarial robustness. For *gradient constraints*, Park et al. [25] present a technique for preserving the Grad-CAM attribution when performing network compression. They proposed a new loss function that incorporates the match between the attribution maps during the fine-tuning stage of compression, and present three variations of this matching loss function: `EWA`, `SWA` and `SSWA`. Similar approaches are also used in visual grounding for visual question answering tasks [30]. Physics-informed neural networks (PINNs) [28, 3] is another type of regularized training that incorporates DNN gradients to encode physics constraints to solve differential equations using DNNs.

For **hard constraints**, directly using an SMT solver to incorporate *input-output constraints* is inefficient and does not scale beyond small DNNs [6, 19, 8]. More efficient approaches are based on relaxing the problem to solving an LP problem [41, 37, 40]. `APRNN` [41] is efficient in enforcing arbitrary affine output constraints for input points. The state-of-the-art provable editing approaches `APRNN` and `PREPARED` [40] are also able to handle affine output constraints for input polytopes. However, they do not handle gradient constraints.

To the best of our knowledge, ours is the first approach to efficiently enforce hard constraints on the gradients of DNNs. Though the current work focuses on handling input points, future work could enforce gradient constraints on input polytopes by adapting ideas from APRNN and PREPARED.

DNN verification aims to determine whether a DNN satisfies a given input-output [34, 35, 50, 43, 33, 49, 46, 4, 2, 44] or gradient property such as monotonicity and Lipschitz robustness [15, 16, 32, 13].

3 Preliminaries

We use $\boldsymbol{x} \in \mathbb{R}$ to denote a scalar, $\mathbf{x} \in \mathbb{R}^m$ to denote a column vector, and $\mathbf{W} \in \mathbb{R}^{n\times m}$ to denote a matrix. Variables in blue with a hat denote LP decision variables, e.g., $\widehat{\mathbf{x}}$, $\widehat{\mathbf{z}}$, $\widehat{\mathbf{W}}$. Variables in blue with a tilde denote the conditional variables, e.g., $\widetilde{\mathbf{x}}$, $\widetilde{\mathbf{z}}$.

Definition 3.1 (DNN)**.** Consider an L-layer feed-forward ReLU deep neural network (DNN) $\mathcal{N}$ with parameters $\theta \overset{\text{def}}{=} \{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L-1)}, \mathbf{b}^{(0)}, \mathbf{b}^{(1)}, \dots, \mathbf{b}^{(L-1)}\}$. For each layer $0 \le \ell < L$, we use

$$\mathbf{z}^{(\ell)} \overset{\text{def}}{=} \mathbf{W}^{(\ell)}\mathbf{x}^{(\ell)} + \mathbf{b}^{(\ell)} \tag{2}$$

to denote the pre-activation output $\mathbf{z}^{(\ell)}$ after the affine transformation. For a non-last layer $\ell < L-1$,

$$\mathbf{x}^{(\ell+1)} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \mathbf{z}^{(\ell)} \tag{3}$$

denotes the layer output $\mathbf{x}^{(\ell+1)}$ after the ReLU activation, where $\operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)$ is a diagonal matrix of the indicator vector $\mathbf{1}_{\mathbf{z}^{(\ell)}>0}$, whose i-th element is 1 if $\mathbf{z}_i^{(\ell)} > 0$, or 0 otherwise. For the last layer $\ell = L-1$, we assume no ReLU activation and use $\mathbf{x}^{(L)} \overset{\text{def}}{=} \mathbf{z}^{(L-1)}$ to denote the layer output. Given the DNN input $\mathbf{x} \in \mathbb{R}^n$, we have the first-layer input $\mathbf{x}^{(0)} \overset{\text{def}}{=} \mathbf{x}$ and the network output $\mathcal{N}(\mathbf{x};\theta) \overset{\text{def}}{=} \mathbf{x}^{(L)}$. ■

Definition 3.2 (Gradient of DNNs)**.** For an L-layer ReLU DNN $\mathcal{N} : \mathbb{R}^n \to \mathbb{R}^m$ with parameters θ, the gradient (Jacobian) $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\theta)$ of the DNN output $\mathcal{N}(\mathbf{x};\theta) \in \mathbb{R}^m$ with respect to the input $\mathbf{x} \in \mathbb{R}^n$ is defined by the chain rule as

$$\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\theta) \overset{\text{def}}{=} \prod_{\ell=L-1}^{0} \frac{\partial \mathbf{x}^{(\ell+1)}}{\partial \mathbf{z}^{(\ell)}}\frac{\partial \mathbf{z}^{(\ell)}}{\partial \mathbf{x}^{(\ell)}} \tag{4}$$

For the ReLU activation $\mathbf{x}^{(\ell+1)} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \mathbf{z}^{(\ell)}$ of a non-last layer $\ell < L-1$, the gradient $\frac{\partial \mathbf{x}^{(\ell+1)}}{\partial \mathbf{z}^{(\ell)}}$ of the ℓ-th layer post-activation output $\mathbf{x}^{(\ell+1)}$ with respect to the pre-activation output $\mathbf{z}^{(\ell)}$ is

$$\frac{\partial \mathbf{x}^{(\ell+1)}}{\partial \mathbf{z}^{(\ell)}} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big) \tag{5}$$

and for the last layer $\ell = L-1$ without ReLU activation, $\frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{z}^{(L-1)}} \overset{\text{def}}{=} \operatorname{diag}(\mathbf{1})$ is the identity matrix.

For the affine transformation $\mathbf{z}^{(\ell)} \overset{\text{def}}{=} \mathbf{W}^{(\ell)}\mathbf{x}^{(\ell)} + \mathbf{b}^{(\ell)}$, the gradient $\frac{\partial \mathbf{z}^{(\ell)}}{\partial \mathbf{x}^{(\ell)}}$ of the pre-activation output $\mathbf{z}^{(\ell)}$ with respect to the ℓ-th layer input $\mathbf{x}^{(\ell-1)}$ is defined as

$$\frac{\partial \mathbf{z}^{(\ell)}}{\partial \mathbf{x}^{(\ell)}} \overset{\text{def}}{=} \mathbf{W}^{(\ell)} \tag{6}$$ ■

3.1 Conditional variable output of DNNs for provable output editing

Our method ProGrad extends the conditional variable output of DNNs, introduced by APRNN [41], to the conditional variable gradient of DNNs. We now present how APRNN focuses on the forward pass and constructs the conditional variable output of DNNs. For clarity, we assume the first-layer weight and all-layer biases are variables. In practice, APRNN can freeze the first few layers and only make the rest of the DNN have variable parameters.

Definition 3.3 (Conditional variable output of DNNs)**.** Consider an L-layer feed-forward ReLU DNN $\mathcal{N}$ with parameters $\widehat{\boldsymbol{\theta}} \overset{\text{def}}{=} \{\widehat{\mathbf{W}}^{(0)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L-1)}, \widehat{\mathbf{b}}^{(0)}, \widehat{\mathbf{b}}^{(1)}, \dots, \widehat{\mathbf{b}}^{(L-1)}\}$, where the first-layer weight $\widehat{\mathbf{W}}^{(0)}$ and all-layer biases $\widehat{\mathbf{b}}^{(\ell)}$ are variables. For an input $\mathbf{x} \in \mathbb{R}^n$, the conditional variable output $\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathbb{R}^m$ with linear activation condition $\widetilde{\varphi}$ is a linear expression over $\widehat{\boldsymbol{\theta}}$ that is sound if the condition $\widetilde{\varphi}$ is satisfied. In other words, for any assignment θ to the variable parameters $\widehat{\boldsymbol{\theta}}$ that satisfies the activation condition $\widetilde{\varphi}$, $\widetilde{\mathcal{N}}(\mathbf{x};\theta) = \mathcal{N}(\mathbf{x};\theta)$. Next we define the conditional variable output and condition $\widetilde{\varphi}^{(\ell)}$ for each layer ℓ.

The pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(0)}$ for the first layer $\ell = 0$ with variable weight is

$$\widetilde{\mathbf{z}}^{(0)} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)}\mathbf{x}^{(0)} + \widehat{\mathbf{b}}^{(0)} \tag{7}$$

The pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(\ell)}$ for other layers $0 < \ell < L$ with constant weight is

$$\widetilde{\mathbf{z}}^{(\ell)} \stackrel{\text{def}}{=} \mathbf{W}^{(\ell)}\widetilde{\mathbf{x}}^{(\ell)} + \widehat{\mathbf{b}}^{(\ell)} \tag{8}$$

The conditional variable layer output $\widehat{\mathbf{x}}^{(\ell+1)}$ for a non-last layer $\ell < L-1$ is defined as

$$\widetilde{\mathbf{x}}^{(\ell+1)} \stackrel{\text{def}}{=} \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\right) \widetilde{\mathbf{z}}^{(\ell)} \tag{9}$$

with the ℓ-th layer activation condition $\widetilde{\varphi}^{(\ell)}$

$$\widetilde{\varphi}^{(\ell)} \stackrel{\text{def}}{=} \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\right) \widetilde{\mathbf{z}}^{(\ell)} > 0 \ \wedge\ \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}\leq 0}\right) \widetilde{\mathbf{z}}^{(\ell)} \leq 0 \tag{10}$$

The activation condition $\widetilde{\varphi}^{(\ell)}$ is constraining the ReLU activation pattern of the pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(\ell)}$ to be the same as a constant pre-activation output $\mathbf{z}^{(\ell)}$, so that if $\widetilde{\varphi}^{(\ell)}$ is satisfied, $\operatorname{diag}\left(\mathbf{1}_{\widetilde{\mathbf{z}}^{(\ell)}>0}\right) = \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\right)$. The choice of the constant $\mathbf{z}^{(\ell)}$ is arbitrary, the default choice is the pre-activation output of the original DNN $\mathcal{N}$. For the last layer $\ell = L-1$ without ReLU activation, $\widetilde{\mathbf{x}}^{(L)} \stackrel{\text{def}}{=} \widetilde{\mathbf{z}}^{(L-1)}$ and $\widetilde{\varphi}^{(L-1)} \stackrel{\text{def}}{=} \top$.

Given the DNN input $\mathbf{x}^{(0)} \stackrel{\text{def}}{=} \mathbf{x}$, we have the conditional variable network output $\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \stackrel{\text{def}}{=} \widetilde{\mathbf{x}}^{(L)}$ with the activation condition $\widetilde{\varphi} \stackrel{\text{def}}{=} \bigwedge_\ell \widetilde{\varphi}^{(\ell)}$. ■

3.2 Gradient-based interpretation methods

Definition 3.4 (Integrated Gradients [39]). Given an input $\mathbf{x}$ and a baseline input $\mathbf{x}^0$. Let $\mathbf{x}^\alpha \stackrel{\text{def}}{=} \mathbf{x}^0 + \alpha\mathbf{d}$ be the linearly interpolated points between the baseline $\mathbf{x}^0$ and the input $\mathbf{x}$, where $\alpha \in [0,1]$ and $\mathbf{d} \stackrel{\text{def}}{=} \mathbf{x} - \mathbf{x}^0$. The *integrated gradients* (IG) from $\mathbf{x}^0$ to $\mathbf{x}$ is defined as the integral of the gradients $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}^\alpha)$ along the path, then multiplied by the difference vector $\mathbf{d}$:

$$\mathtt{IG}(\mathbf{x}) \stackrel{\text{def}}{=} \mathbf{d} \odot \int_{\alpha=0}^{1} \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}^\alpha) d\alpha \tag{11}$$

where $\odot$ denotes the element-wise product. In practice, this integral is approximated by a left-Riemann sum with m steps:

$$\mathtt{IG}^{\text{approx}}(\mathbf{x}) \stackrel{\text{def}}{=} \mathbf{d} \odot \frac{1}{m}\sum_{k=0}^{m} \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}^{\frac{k}{m}}) \tag{12}$$ ■

Definition 3.5 (Grad-CAM [29]). Given a convolutional DNN $\mathcal{N}$ and input $\mathbf{x}$, let $\mathbf{y} \in \mathbb{R}^C$ denote the DNN output, and $\mathbf{z} \in \mathbb{R}^{K\times H\times W}$ denote the pre-activation output of the last convolutional layer of the DNN where K is the number of channels, and H and W are the height and width of the feature map. The Grad-CAM localization map $\mathbf{L}^c \in \mathbb{R}^{H\times W}$ is defined as

$$\mathbf{L}^c \stackrel{\text{def}}{=} \sum_k \boldsymbol{\alpha}_k^c \mathbf{z}_k \quad \text{where} \quad \boldsymbol{\alpha}_k^c \stackrel{\text{def}}{=} \frac{1}{H\times W}\sum_i\sum_j \frac{\partial \mathbf{y}_c}{\partial \mathbf{z}_{k,i,j}} \tag{13}$$

where the neuron importance weights $\boldsymbol{\alpha}^c \in \mathbb{R}^K$ for $\mathbf{z}$ is the average gradient of the output class c with respect to each channel k of the pre-activation output $\mathbf{z}$. Optionally, one can simplify the Grad-CAM localization map $\mathbf{L}^c$ by applying a ReLU activation to ignore the negative attributions. In this paper, we consider the Grad-CAM attribution with any sign, hence don't apply the ReLU activation to $\mathbf{L}^c$. ■

4 Approach

This section presents ProGrad, which solves the provable gradient editing problem of DNNs using linear programming (LP). For ease of exposition, we consider the following provable gradient editing problem for a scalar-valued DNN $\mathcal{N} : \mathbb{R}^n \to \mathbb{R}$ with gradient $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\theta) \in \mathbb{R}^n$, and assume the first-layer weight and all-layer biases are variables. *In practice,* ProGrad *allows editing only the last few layers and freezing the rest of the DNN, enabling efficient editing because the size of the LP only depends on the edited layers instead of the entire DNN.* We defer the extension to the general provable editing problem of Definition 1.1 for vector-valued DNNs, as well as handling multiple inputs and editing only the last few layers to Appendix B. The proofs for all theorems can be found in Appendix A.

Definition 4.1. Given a DNN $\mathcal{N} : \mathbb{R}^n \to \mathbb{R}$ with parameters θ, and an input $\mathbf{x} \in \mathbb{R}^n$. The **provable gradient editing problem** is to find new parameters $\widehat{\boldsymbol{\theta}}$ that

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \text{s.t.} \quad \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathrm{Q} \tag{14}$$

where $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathbb{R}^n$ denotes the gradient of the scalar output of $\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \in \mathbb{R}$ with respect to the input $\mathbf{x}$ with new parameters $\widehat{\boldsymbol{\theta}}$. $\mathrm{Q} \stackrel{\text{def}}{=} \left\{\mathbf{z} \in \mathbb{R}^n \mid \mathbf{Az} \leq \mathbf{b}\right\}$ is a convex polytope denoting the linear constraints for the gradient $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}})$.

4.1 Conditional variable gradient of DNNs

Consider a DNN $\mathcal{N}$ with variable parameters $\widehat{\boldsymbol{\theta}}$ and input $\mathbf{x}$. The *exact* variable gradient $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ of $\mathcal{N}$ is *highly non-linear*, involving quadratic terms from the multiplication between weights and disjunctions from the ReLU activation. Our **key insight** is to relax the non-linear $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ to a *linear conditional variable gradient* $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ that is sound under a *linear activation condition* $\widetilde{\boldsymbol{\varphi}}$.

Definition 4.2. The conditional variable gradient $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ of a DNN $\mathcal{N}$ in terms of $\widehat{\boldsymbol{\theta}}$ with respect to the input $\mathbf{x}$, under a *poly-size linear* activation condition $\widetilde{\boldsymbol{\varphi}}$, is a *poly-size linear expression* that equals the exact variable gradient $\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ if the activation condition $\widetilde{\boldsymbol{\varphi}}$ is satisfied.

In other words, for any assignment θ to the variable parameters $\widehat{\boldsymbol{\theta}}$ that satisfies the activation condition $\widetilde{\boldsymbol{\varphi}}$, $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\theta) = \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x};\theta)$. The size of the condition $\widetilde{\boldsymbol{\varphi}}$ and the expression $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ is polynomial in the size of the *edited layers* of the DNN, i.e., the number of edited layers, parameters, and the input and output dimensions of each edited layer. In practice, ProGrad allows editing only the last few layers of a DNN. We defer the construction of such conditional variable gradient $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ of $\mathcal{N}$ to Section 4.3, and first show how it can be used to solve the provable gradient editing problem.

4.2 Provable gradient editing via conditional variable gradient of DNNs

The following theorem shows how the conditional variable gradient of DNNs can be used to solve the provable gradient editing problem.

Theorem 4.3. *Given a provable gradient editing problem (Definition 4.1) for DNN $\mathcal{N}$ and parameters θ with input $\mathbf{x}$ and a gradient constraint $\mathrm{Q} \stackrel{\text{def}}{=} \left\{\mathbf{z} \in \mathbb{R}^n \mid \mathbf{Az} \leq \mathbf{b}\right\}$. Let $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}})$ be the conditional variable gradient of the DNN $\mathcal{N}$ with respect to the input $\mathbf{x}$, under the activation condition $\widetilde{\boldsymbol{\varphi}}$. The following linear program can be solved in polynomial time in the size of the edited layers of the DNN $\mathcal{N}$, and its solution is a solution to the provable gradient editing problem.*

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \textit{s.t.} \quad \widetilde{\boldsymbol{\varphi}} \wedge \mathbf{A}\,\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x};\widehat{\boldsymbol{\theta}}) \leq \mathbf{b} \tag{15}$$

4.3 Conditional variable gradient of fully-connected ReLU DNN

This section presents how ProGrad focuses on the backward pass and constructs the conditional variable gradient of a fully-connected ReLU DNN $\mathcal{N}$ with respect to the input $\mathbf{x}$ and its parameters $\widehat{\boldsymbol{\theta}}$.

Definition 4.4. Consider an L-layer feed-forward ReLU DNN $\mathcal{N}$ (Definition 3.1) with parameters $\widehat{\boldsymbol{\theta}} \stackrel{\text{def}}{=} \{\widehat{\mathbf{W}}^{(0)}, \mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L-1)}, \widehat{\mathbf{b}}^{(0)}, \widehat{\mathbf{b}}^{(1)}, \ldots, \widehat{\mathbf{b}}^{(L-1)}\}$, where the first-layer weight $\widehat{\mathbf{W}}^{(0)}$ and all-layer biases $\widehat{\mathbf{b}}^{(\ell)}$ are variables. For an input $\mathbf{x} \in \mathbb{R}^n$, the conditional variable gradient $\frac{\partial}{\partial \mathbf{x}} \widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ of a DNN $\mathcal{N}$ in terms of $\widehat{\boldsymbol{\theta}}$ with respect to the input $\mathbf{x}$ is defined by the chain rule as

$$\frac{\partial}{\partial \mathbf{x}} \widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \stackrel{\text{def}}{=} \prod_{\ell=L-1}^{0} \frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} \frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} \tag{16}$$

with the activation condition $\widetilde{\boldsymbol{\varphi}} \stackrel{\text{def}}{=} \bigwedge_\ell \widetilde{\boldsymbol{\varphi}}^{(\ell)}$ defined from each layer ℓ.

For the conditional ReLU activation $\widetilde{\mathbf{x}}^{(\ell+1)} \stackrel{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \widetilde{\mathbf{z}}^{(\ell)}$ of non-last layer $\ell < L-1$, the conditional variable gradient $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ of the ℓ-th layer post-activation output $\widetilde{\mathbf{x}}^{(\ell+1)}$ with respect to the pre-activation output $\widetilde{\mathbf{z}}^{(\ell)}$ is

$$\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} \stackrel{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big) \tag{17}$$

with the ℓ-th layer activation condition $\widetilde{\boldsymbol{\varphi}}^{(\ell)}$

$$\widetilde{\boldsymbol{\varphi}}^{(\ell)} \stackrel{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \widetilde{\mathbf{z}}^{(\ell)} > 0 \;\wedge\; \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}\leq 0}\big)\, \widetilde{\mathbf{z}}^{(\ell)} \leq 0 \tag{18}$$

The activation condition $\widetilde{\boldsymbol{\varphi}}^{(\ell)}$ is constraining the ReLU activation pattern of the pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(\ell)}$ to be the same as a constant pre-activation output $\mathbf{z}^{(\ell)}$, so that if $\widetilde{\boldsymbol{\varphi}}^{(\ell)}$ is satisfied, $\operatorname{diag}\big(\mathbf{1}_{\widetilde{\mathbf{z}}^{(\ell)}>0}\big) = \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)$. The choice of the constant $\mathbf{z}^{(\ell)}$ is arbitrary, the default choice is the pre-activation output of the original DNN $\mathcal{N}$. For the last layer $\ell = L-1$ without ReLU activation, $\frac{\partial \widetilde{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}} \stackrel{\text{def}}{=} \operatorname{diag}(\mathbf{1})$ is the identity matrix.

As seen in Equations 18 and 10, `ProGrad` and `APRNN` share the same idea of using activation condition to constrain each input in the edit set to lie on a specific linear piece of the edited DNN. Note that the linear piece is not fixed but variable, because it is expressed as a closed-form linear expression in terms of the editable DNN parameters.

For the conditional affine transformation $\widetilde{\mathbf{z}}^{(\ell)} \stackrel{\text{def}}{=} \mathbf{W}^{(\ell)} \widetilde{\mathbf{x}}^{(\ell)} + \widehat{\mathbf{b}}^{(\ell)}$ of the non-first layer $\ell > 0$ with constant weight $\mathbf{W}^{(\ell)}$ and conditional variable input $\widetilde{\mathbf{x}}^{(\ell)}$, the conditional variable gradient $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}}$ of the pre-activation output $\widetilde{\mathbf{z}}^{(\ell)}$ with respect to the layer input $\widetilde{\mathbf{x}}^{(\ell)}$ is

$$\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} \stackrel{\text{def}}{=} \mathbf{W}^{(\ell)} \tag{19}$$

For the conditional affine transformation $\widetilde{\mathbf{z}}^{(0)} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)} \mathbf{x}^{(0)} + \widehat{\mathbf{b}}^{(0)}$ of the first layer $\ell = 0$ with variable weight $\widehat{\mathbf{W}}^{(0)}$ and constant input $\mathbf{x}^{(0)}$, the conditional variable gradient $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$ of the pre-activation output $\widetilde{\mathbf{z}}^{(0)}$ with respect to the layer input $\mathbf{x}^{(0)}$ is

$$\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)} \tag{20}$$ ■

Theorem 4.5. *The conditional variable gradient constructed in Definition 4.4 is valid and satisfies the conditions stated in Definition 4.2.*

5 Experimental Evaluation

We have implemented `ProGrad` in `PyTorch` [26] and use `Gurobi` [10] as the LP solver. All experiments were run on a machine with dual Intel Xeon Platinum 8362 Processors, 32-Core 2.8GHz with 1.5 TB of memory, SSD, and NVIDIA H100 GPU with 80 GB of GPU memory running Ubuntu 22.04. Additional details can be found in Appendix C.

Table 1: **Enforcing hard Grad-CAM constraints on ResNet DNNs.** Comparison of the (pixel-level) Grad-CAM constraint satisfaction rate (Constr. Sat.), minimum cosine similarity (Min. Cos.) and minimum intersection over union (Min. IoU) between the expected and edited Grad-CAMs, and the top-1 accuracy (Acc.) of the edited DNNs on the ILSVRC 2012 IMAGENET validation set.

(a) Enforcing hard Grad-CAM constraints on `ResNet152`

Method	100 images with ε=1e-2				1,000 images with ε=5e-2			
	Constr. Sat.	Min. Cos.	Min. IoU	Acc.	Constr. Sat.	Min. Cos.	Min. IoU	Acc.
Original	7.06%	34.66%	4.35%	78.31%	30.85%	24.51%	0.00%	78.31%
`EWA`	6.61%	73.53%	20.00%	77.27%	30.47%	26.31%	0.00%	73.32%
`SWA`	6.27%	49.95%	71.43%	77.79%	34.34%	65.56%	4.35%	76.55%
`SSWA`	6.37%	56.54%	71.43%	77.79%	34.32%	65.36%	4.35%	76.56%
`ProGrad`	**100.00%**	**99.97%**	**84.62%**	**78.08%**	**100.00%**	**99.44%**	**50.00%**	**77.43%**

(b) Enforcing hard Grad-CAM constraints on `ResNet50`

Method	100 images with ε=1e-2				1,000 images with ε=5e-2			
	Constr. Sat.	Min. Cos.	Min. IoU	Acc.	Constr. Sat.	Min. Cos.	Min. IoU	Acc.
Original	7.35%	24.15%	0.00%	76.13%	31.21%	-68.81%	0.00%	76.13%
`EWA`	5.39%	65.44%	0.00%	73.42%	23.84%	37.95%	0.00%	65.86%
`SWA`	6.80%	83.25%	50.00%	75.24%	31.64%	-1.84%	4.35%	73.67%
`SSWA`	6.71%	83.01%	41.18%	75.25%	31.67%	-1.00%	4.35%	73.72%
`ProGrad`	**100.00%**	**99.96%**	**84.62%**	**75.38%**	**100.00%**	**99.31%**	**50.00%**	**74.33%**

5.1 Enforcing hard Grad-CAM constraints on ResNet DNNs for IMAGENET

In this experiment, we edit `ResNet152` and `ResNet50` DNNs from `torchvision` [18] so that the Grad-CAM attributions [29] for a set of images are ε-close to their expected attributions. We compare `ProGrad` to the state-of-the-art Grad-CAM fine-tuning methods `EWA`, `SWA` and `SSWA` [25].

Edit set. The edit set consists of *misclassified* images that have *deviated* Grad-CAM attributions for their expected class. These images are from the IMAGENET-C dataset [11] that are corrupted with Gaussian noise, whose original uncorrupted version is correctly classified. For each misclassified image in the edit set, we take the Grad-CAM attribution of the corresponding original correctly-classified image as the expected Grad-CAM. For each DNN, we construct two such edit sets: **(i)** 100 images from the first 50 classes with ε=1e-2; **(ii)** 1,000 images from the first 200 classes with ε=5e-2.

Grad-CAM constraints. For each image $\mathbf{x}$ in the edit sets and its expected Grad-CAM $\mathbf{L}$ for the expected class, let $\mathbf{L}'$ denote the Grad-CAM on the edited DNN $\mathcal{N}'$; let $\mathbf{L}_\mathrm{n}$ and $\mathbf{L}'_\mathrm{n}$ be the min-max-normalized expected and edited Grad-CAMs; we use $\|\mathbf{L}_\mathrm{n} - \mathbf{L}'_\mathrm{n}\|_\infty \leq \varepsilon$ as the constraint.

Results. As shown in Table 1, `ProGrad` *is the only method able to enforce the hard Grad-CAM constraints, achieving a 100% constraint satisfaction rate (Constr. Sat.), and it achieves the best accuracy (Acc.).* `ProGrad` also achieves the best similarity between the edited and expected Grad-CAM as measured by cosine similarity (Min. Cos.) and intersection over union (Min. IoU). In the `ResNet152` experiment, `ProGrad` took 22 minutes for 100 images and 3 hours 51 minutes for 1,000 images; in the `ResNet50` experiment, `ProGrad` took 25 minutes for 100 images and 3 hours 37 minutes for 1,000 images. For each baseline, we performed a grid search over hyperparameters with a time limit of 12 hours, and report the best results with the highest constraint satisfaction rate (Constr. Sat.). Although the baselines (`EWA`, `SWA` and `SSWA`) can improve these similarity metrics, they are unable to enforce the hard constraints.

Table 2: **Enforcing hard Integrated Gradients (IG) constraints on Llama 3 and Qwen 3 LLMs.** Comparison of the (token-level) IG constraint satisfaction rate (Constr. Sat.), cosine similarity (Cos.) and intersection over union (IoU) between the expected and edited IG, and the accuracy (Acc.) of the edited LLMs on the SST-2 validation set.

(a) Enforce hard IG constraints on `Llama-3.2-1b-Instruct`

Method	100 samples with ε=5e-2				200 samples with ε=1e-1			
	Constr. Sat.	Cos.	IoU	Acc.	Constr. Sat.	Cos.	IoU	Acc.
Original	25.45%	71.26%	32.34%	60.55%	38.15%	70.07%	30.83%	60.55%
`SFT`	52.67%	51.29%	32.17%	49.08%	67.07%	87.20%	37.14%	50.92%
`DPO`	51.70%	64.20%	23.73%	50.92%	65.88%	66.15%	35.81%	50.92%
`ProGrad`	**100.00%**	**99.69%**	**84.10%**	**60.67%**	**100.00%**	**98.82%**	**71.50%**	**59.63%**

(b) Enforce hard IG constraints on `Qwen3-1.7B`

Method	100 samples with ε=5e-2				200 samples with ε=1e-1			
	Constr. Sat.	Cos.	IoU	Acc.	Constr. Sat.	Cos.	IoU	Acc.
Original	26.55%	64.70%	26.27%	85.89%	35.73%	64.81%	26.77%	85.89%
`SFT`	29.51%	63.09%	25.37%	**89.22%**	37.75%	58.64%	29.52%	51.03%
`DPO`	32.18%	56.52%	30.18%	50.92%	37.72%	60.12%	31.18%	50.92%
`ProGrad`	**100.00%**	**99.75%**	**84.59%**	88.19%	**100.00%**	**99.05%**	**74.00%**	**88.07%**

5.2 Enforcing hard Integrated Gradients constraints on LLMs for SST-2

In this experiment, we edit `Llama-3.2-1b-Instruct` [9] and `Qwen3-1.7B` [48] LLMs so that the Integrated Gradients (IG) attributions [39] for a set of sentences are ε-close to their expected IG attributions as determined by the corresponding teacher LLMs `Llama-3.1-8b-Instruct` and `Qwen3-8B`. We compare `ProGrad` against supervised fine-tuning (`SFT`) and direct preference optimization (`DPO`) [27] as baselines.

Edit set. The edit set consists of *misclassified* sentences that have *deviated* IG attributions for the expected answer token. These sentences are *misclassified* samples from the Stanford Sentiment Treebank 2 (SST-2)[36] training set, but are correctly classified by the corresponding teacher LLM. For each sentence in the edit set, we take the corresponding IG from the teacher LLM as the expected IG attribution. For each LLM, we construct two such edit sets: **(i)** the first 100 misclassified sentences from SST-2 with ε=5e-2; **(ii)** the first 200 misclassified sentences from SST-2 with ε=1e-1.

IG constraints. For each sentence $\mathbf{x}$ in the edit set and the corresponding expected IG $\mathbf{L}$ for the expected answer token, let $\mathbf{L}'$ denote the IG on the edited LLM $\mathcal{N}'$; let $\mathbf{L}_\mathtt{n}$ and $\mathbf{L}'_\mathtt{n}$ denote the min-max-normalized expected and edited IGs. We use $\|\mathbf{L}_\mathtt{n} - \mathbf{L}'_\mathtt{n}\|_\infty \leq \varepsilon$ as the IG constraint.

Results. As shown in Table 2, `ProGrad` *is the only method able to enforce the hard IG constraints and achieves the best accuracy in three out of four experiments.* `ProGrad` also achieves the best similarity between the edited and expected IG as measured by cosine similarity (Cos.) and intersection over union (IoU). In the `Llama-3.2-1b-Instruct` experiment, `ProGrad` took 9 minutes for 100 samples, and 10 minutes for 200 samples. In the `Qwen3-1.7B` experiment, `ProGrad` took 28 minutes for 100 samples, and 32 minutes for 200 samples. For each baseline, we performed a grid search over hyperparameters with a time limit of 4 hours, and report the best results with the highest constraint satisfaction rate (Constr. Sat.). The baselines (`SFT` and `DPO`) failed to enforce the hard constraints, barely improved the similarity metrics, and in most cases decreased the accuracy of the edited LLM on the SST-2 validation set.

Table 3: **Enforce hard gradient constraints on a function approximation DNN.** Comparison of the gradient constraints violation rate (Grad. Violation), as well as the MSE error on the gradient (Grad. Error) and output (Output Error). The GD baseline is regularization-based training on both the DNN output and gradient. The GD + ProGrad method applies ProGrad after the regularization-based training to enforce the hard gradient constraints and minimize the gradient and output errors.

Method	Grad. Violation	Grad. Error	Output Error
GD	4.30%	4.25e-03	1.74e-03
GD + ProGrad	**0.00%**	**1.09e-04**	**1.50e-05**

5.3 Enforce gradient constraints in training a DNN to approximate a target function

In this experiment, we aim to enforce hard gradient constraints on a DNN that approximates a target function. The gradient constraints are derived from the gradient of the target function. This experiment acts as a proxy for safety constraints in control systems and physical invariants in scientific applications. We compare ProGrad against regularized-based training method, which incorporates the DNN gradients in the loss function.

Setup. We use a 4-layer fully-connected DNN $\mathcal{N} : \mathbb{R} \to \mathbb{R}$ with 100 hidden neurons per layer and Tanh activation function. Over the domain $[0, 3\pi]$, the DNN $\mathcal{N}$ is trained to approximate the following function $f : \mathbb{R} \to \mathbb{R}$

$$f(x) = -x\cos(x) + \sin(x) \tag{21}$$

and the gradient $\frac{d\mathcal{N}}{dx}$ of DNN $\mathcal{N}$ approximates the gradient $\frac{df}{dx} : \mathbb{R} \to \mathbb{R}$ of the target function f:

$$\frac{d}{dx} f(x) = x\sin(x) \tag{22}$$

Gradient constraints. The target gradient function $\frac{d}{dx} f(x) = x\sin(x)$ is bounded by the upper bound function $g_u(x) = x$ and the lower bound function $g_l(x) = -x$, and we aim to enforce this hard constraint on the DNN gradient $\frac{d}{dx}\mathcal{N}$ for all training samples $\forall x \in \mathcal{D}$, $-x \le \frac{d}{dx}\mathcal{N}(x) \le x$.

Results. Table 3 presents the results of the experiment. Although regularization-based training on both the DNN output and gradient can achieve good (low) errors, the trained DNN is not free of the gradient constraints violations. Applying ProGrad after the regularization-based training to enforce the hard gradient constraints as well as minimize the gradient and output errors can achieve 0% gradient constraints violation and further improve (decrease) the gradient and output errors. ProGrad took 10 seconds to edit this DNN.

6 Conclusion

We have presented ProGrad, the first efficient approach for provable gradient editing of DNNs that runs in polynomial time in the size of the edited layers. We presented a novel method for constructing conditional variable gradient of DNNs, enabling ProGrad to use an LP solver to find an edit. To demonstrate the effectiveness of ProGrad, we evaluated ProGrad in enforcing hard Grad-CAM constraints on ResNet DNNs for IMAGENET, enforcing hard Integrated Gradients constraints on Llama 3 and Qwen 3 LLMs, and enforcing hard gradient constraints in training a function-approximation DNN. The results highlight the unique capability of ProGrad in enforcing hard constraints on DNN gradients.

Societal Impacts The use of hard constraints to edit DNNs enables learning with fewer data points, and guaranteeing the safety of DNNs. ProGrad can be used to make DNNs safer, trustworthy, and interpretable. However, because ProGrad is a general technique for editing the gradients of DNNs, it could also be misused, for instance, to tamper with the interpretation of a DNN.

Limitations ProGrad is currently limited to enforcing gradient constraints for a (finite) set of input points. Future work could extend ProGrad to enforce gradient constraints for input polytopes by adapting ideas from APRNN [41] and PREPARED [40].

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A Proofs

Theorem 4.3. *Given a provable gradient editing problem (Definition 4.1) for DNN $\mathcal{N}$ and parameters θ with input $\mathbf{x}$ and a gradient constraint $\mathrm{Q} \stackrel{\text{def}}{=} \{\mathbf{z} \in \mathbb{R}^n \mid \mathbf{A}\mathbf{z} \leq \mathbf{b}\}$. Let $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ be the conditional variable gradient of the DNN $\mathcal{N}$ with respect to the input $\mathbf{x}$, under the activation condition $\widetilde{\varphi}$. The following linear program can be solved in polynomial time in the size of the edited layers of the DNN $\mathcal{N}$, and its solution is a solution to the provable gradient editing problem.*

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \textit{s.t.} \quad \widetilde{\varphi} \ \wedge \ \mathbf{A}\,\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \leq \mathbf{b} \tag{15}$$

Proof. We first show that **Equation 15 is a linear program that can be solved in polynomial time in the size of the DNN**. By the definition of conditional variable gradient (Definition 4.2), **(i)** $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ is a linear expression and $\widetilde{\varphi}$ is a linear formula, hence Equation 15 is a linear program; **(ii)** the sizes of both $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ and $\widetilde{\varphi}$ are polynomial in the size of the DNN, i.e., the number of parameters, layers, and the input and output dimensions of each layer, hence Equation 15 can be solved in polynomial time in the size of the DNN.

We then show that **any solution to Equation 15 is a solution to the provable gradient editing problem (Equation 14 in Definition 4.1)**. By the definition of conditional variable gradient (Definition 4.2), for any solution θ' to the variable parameters $\widehat{\boldsymbol{\theta}}$ that satisfies the activation condition $\widetilde{\varphi}$, $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \theta') = \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}; \theta')$, hence $\mathbf{A}\frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}; \theta') \leq \mathbf{b}$ holds and Equation 14 is satisfied. ☐

Theorem 4.5. *The conditional variable gradient constructed in Definition 4.4 is valid and satisfies the conditions stated in Definition 4.2.*

Proof. We will recall Definition 4.4 and prove this theorem step by step. Consider an L-layer feed-forward ReLU deep neural network (DNN) $\mathcal{N}$ with parameters $\widehat{\boldsymbol{\theta}} \stackrel{\text{def}}{=} \{\widehat{\mathbf{W}}^{(0)}, \mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(L-1)}, \widehat{\mathbf{b}}^{(0)}, \widehat{\mathbf{b}}^{(1)}, \ldots, \widehat{\mathbf{b}}^{(L-1)}\}$, where the first-layer weight $\widehat{\mathbf{W}}^{(0)}$ and all-layer biases $\widehat{\mathbf{b}}^{(\ell)}$ are variables. For an input $\mathbf{x} \in \mathbb{R}^n$, the conditional variable gradient $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ of a DNN $\mathcal{N}$ in terms of $\widehat{\boldsymbol{\theta}}$ with respect to the input $\mathbf{x}$ is defined by the chain rule as

$$\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \stackrel{\text{def}}{=} \prod_{\ell=L-1}^{0} \frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} \frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} \tag{23}$$

with the activation condition $\widetilde{\varphi} \stackrel{\text{def}}{=} \bigwedge_\ell \widetilde{\varphi}^{(\ell)}$ defined from each layer ℓ.

We will show below that **(i) except for $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$ for the first layer $\ell = 0$ is a linear expression, all other $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ and $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}}$ are *constant* matrices (ii) $\widetilde{\varphi}^{(\ell)}$ for each layer ℓ are linear formulas, $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$ is a linear expression, and their sizes are polynomial in the number of input and output neurons as well as parameters of the layer ℓ; (iii) for each layer ℓ, $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} = \frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}}$, and $\widetilde{\varphi}^{(\ell)}$ implies $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} = \frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$.** Consequently, we can conclude that **(i)** $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ is a linear expression, because it is a product of one linear expression ($\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$) and many constant matrices (all other $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ and $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}}$); **(ii)** $\widetilde{\varphi} \stackrel{\text{def}}{=} \bigwedge_\ell \widetilde{\varphi}^{(\ell)}$ is a linear formula, the sizes of $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ and $\widetilde{\varphi}$ are polynomial in the size of the DNN $\mathcal{N}$, i.e., the number of parameters, layers, and the input and output dimensions of each layer; **(iii)** by induction, $\widetilde{\varphi}$ implies $\frac{\partial}{\partial \mathbf{x}}\widetilde{\mathcal{N}}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) = \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$. Hence, the conditional variable gradient constructed in Definition 4.4 is valid and satisfies the conditions stated in Definition 4.2.

We first prove those conditions for the affine transformation. For the conditional affine transformation $\widetilde{\mathbf{z}}^{(0)} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)}\mathbf{x}^{(0)} + \widehat{\mathbf{b}}^{(0)}$ of the first layer $\ell = 0$ with variable weight $\widehat{\mathbf{W}}^{(0)}$ and constant input $\mathbf{x}^{(0)}$, the conditional variable gradient $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$ of the pre-activation output $\widetilde{\mathbf{z}}^{(0)}$ with respect to the layer input $\mathbf{x}^{(0)}$ is

$$\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)} \tag{24}$$

which **(i) is a matrix of variable weights whose size is the same as $\mathbf{W}^{(\ell)}$, hence linear; (ii) unconditionally equals to the exact gradient $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}} \overset{\text{def}}{=} \widehat{\mathbf{W}}^{(0)}$.**

For the conditional affine transformation $\widetilde{\mathbf{z}}^{(\ell)} \overset{\text{def}}{=} \mathbf{W}^{(\ell)} \widetilde{\mathbf{x}}^{(\ell)} + \widehat{\mathbf{b}}^{(\ell)}$ of the non-first-layer $\ell > 0$ with constant weight $\mathbf{W}^{(\ell)}$ and conditional variable input $\widetilde{\mathbf{x}}^{(\ell)}$, the conditional variable gradient $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}}$ of the pre-activation output $\widetilde{\mathbf{z}}^{(\ell)}$ with respect to the layer input $\widetilde{\mathbf{x}}^{(\ell)}$ is

$$\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} \overset{\text{def}}{=} \mathbf{W}^{(\ell)} \tag{25}$$

which **(i) is a constant matrix, hence linear; (ii) unconditionally equals to the exact gradient $\frac{\partial \widetilde{\mathbf{z}}^{(\ell)}}{\partial \widetilde{\mathbf{x}}^{(\ell)}} \overset{\text{def}}{=} \mathbf{W}^{(\ell)}$.**

For the conditional ReLU activation $\widetilde{\mathbf{x}}^{(\ell+1)} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \widetilde{\mathbf{z}}^{(\ell)}$ of non-last layer $\ell < L-1$, let p be the number of output neurons of the layer ℓ. **We first show that $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ is a constant matrix, and $\widetilde{\varphi}^{(\ell)}$ is a linear formula whose size is polynomial in the number of output neurons p of the layer ℓ.** Recall that the conditional variable gradient $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ of the ℓ-th layer post-activation output $\widetilde{\mathbf{x}}^{(\ell+1)}$ with respect to the pre-activation output $\widetilde{\mathbf{z}}^{(\ell)}$ is

$$\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big) \tag{26}$$

with the ℓ-th layer activation condition $\widetilde{\varphi}^{(\ell)}$

$$\widetilde{\varphi}^{(\ell)} \overset{\text{def}}{=} \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big)\, \widetilde{\mathbf{z}}^{(\ell)} > 0 \;\wedge\; \operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}\leq 0}\big)\, \widetilde{\mathbf{z}}^{(\ell)} \leq 0 \tag{27}$$

$\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} \in \mathbb{R}^{p\times p}$ is a constant matrix of size $p \times p$, and $\widetilde{\varphi}^{(\ell)}$ is a conjunction of p linear inequalities, hence $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ is a constant matrix, $\widetilde{\varphi}^{(\ell)}$ is a linear formula whose size is polynomial in the number of output neurons p of the layer ℓ.

We then show that $\widetilde{\varphi}^{(\ell)}$ implies $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} = \frac{\partial \widehat{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$ where $\widehat{\mathbf{x}}^{(\ell+1)} \overset{\text{def}}{=} \mathtt{ReLU}(\widetilde{\mathbf{z}}^{(\ell)})$. The activation condition $\widetilde{\varphi}^{(\ell)}$ constrains the ReLU activation pattern of the pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(\ell)}$ to be the same as a constant pre-activation output $\mathbf{z}^{(\ell)}$. Hence, if $\widetilde{\varphi}^{(\ell)}$ is satisfied, then **(i)** for any $\mathbf{z}_i^{(\ell)} > 0$, we have the conditional variable $\widetilde{\mathbf{z}}_i^{(\ell)} > 0$, hence $\widehat{\mathbf{x}}_i^{(\ell+1)} = \widetilde{\mathbf{z}}_i^{(\ell)}$ and $\mathbf{1}_{\widetilde{\mathbf{z}}_i>0} = 1$; **(ii)** for any $\mathbf{z}_i^{(\ell)} \leq 0$, we have the conditional variable $\widetilde{\mathbf{z}}_i^{(\ell)} \leq 0$, hence $\widehat{\mathbf{x}}_i^{(\ell+1)} = 0$ and $\mathbf{1}_{\widetilde{\mathbf{z}}_i>0} = 0$. Therefore, we proved that $\widetilde{\varphi}^{(\ell)}$ implies $\operatorname{diag}\big(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\big) = \operatorname{diag}\big(\mathbf{1}_{\widetilde{\mathbf{z}}^{(\ell)}>0}\big)$, which is our goal $\frac{\partial \widetilde{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}} = \frac{\partial \widehat{\mathbf{x}}^{(\ell+1)}}{\partial \widetilde{\mathbf{z}}^{(\ell)}}$.

For the last layer $\ell = L-1$ without ReLU activation, $\frac{\partial \widetilde{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}} = \frac{\partial \widehat{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}} = \operatorname{diag}(\mathbf{1})$ is an identity matrix and $\widetilde{\varphi}^{(L-1)} = \top$ has a constant size. Hence, **for the last layer $\ell = L-1$, $\frac{\partial \widetilde{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}}$ is a constant matrix, $\widetilde{\varphi}^{(L-1)}$ is a linear formula of constant size, and $\widetilde{\varphi}^{(L-1)}$ trivially implies $\frac{\partial \widetilde{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}} = \frac{\partial \widehat{\mathbf{x}}^{(L)}}{\partial \widetilde{\mathbf{z}}^{(L-1)}}$.** $\square$

B General provable gradient editing of DNNs

In this section, we present the extension of our approach presented in Section 4 to solve the general provable gradient editing, which handles **(i) efficient editing**: our approach allows editing only the last few layers of the DNN while keeping the rest of the DNN unchanged, which enables efficient editing of large DNNs; **(ii) general DNN architectures**: the editing is not restricted to multi-layer perceptron (MLP) fully-connected ReLU DNNs, but applies to DNNs of any architecture with an MLP ReLU DNN as the last few layers; **(iii) set of inputs**: our approach can edit the DNN for a set of inputs at the same time, guaranteeing constraint satisfaction for all of them; **(iv) general linear constraints**: our approach allows any linear constraints over the set of inputs, as well as their corresponding DNN outputs and gradients, not restricted to constraints that only talk about individual inputs. *The effectiveness and efficiency of our approach for solving the general provable gradient editing problem is demonstrated in our experiments (Section 5).*

Definition B.1. Given a DNN $\mathcal{N} \stackrel{\text{def}}{=} \mathcal{N}^{(\text{up})} \circ \mathcal{N}^{(\text{down})}$, which is a composition of a *general* DNN $\mathcal{N}^{(\text{up})}\colon \mathbb{R}^p \to \mathbb{R}^n$ of *any differentiable architecture*, and an L-layer fully-connected ReLU DNN $\mathcal{N}^{(\text{down})}\colon \mathbb{R}^n \to \mathbb{R}^m$ with parameters $\theta \stackrel{\text{def}}{=} \{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L-1)}, \mathbf{b}^{(0)}, \mathbf{b}^{(1)}, \dots, \mathbf{b}^{(L-1)}\}$ as defined in Definition 3.1. Let $\widehat{\boldsymbol{\theta}} \stackrel{\text{def}}{=} \{\widehat{\mathbf{W}}^{(0)}, \mathbf{W}^{(1)}, \dots, \mathbf{W}^{(L-1)}, \widehat{\mathbf{b}}^{(0)}, \widehat{\mathbf{b}}^{(1)}, \dots, \widehat{\mathbf{b}}^{(L-1)}\}$ be the new parameters of $\mathcal{N}^{(\text{down})}$. Given a set $\mathcal{S} \subseteq \{\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^n\} \times \{\mathrm{Q} \mid \mathrm{Q} \subseteq \mathbb{R}^{m\times n}\}$ of pairs $(\mathbf{x}, \mathrm{Q})$, where $\mathbf{x} \in \mathbb{R}^n$ is a DNN input, and $\mathrm{Q} \stackrel{\text{def}}{=} \{\mathbf{J} \in \mathbb{R}^{m\times n} \mid \mathbf{A}\,\mathrm{vec}(\mathbf{J}) \le \mathbf{b}\}$ is the corresponding linear constraints on the Jacobian $\mathbf{J} \stackrel{\text{def}}{=} \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \in \mathbb{R}^{m\times n}$ of the DNN $\mathcal{N}$ with respect to the input $\mathbf{x} \in \mathbb{R}^n$, we use $\vec{\mathbf{J}}$ to denote the Jacobian matrix $\mathbf{J}$ flattened as a vector. The **provable gradient editing problem** is to find new parameters $\widehat{\boldsymbol{\theta}}$ that

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \text{s.t.} \quad \bigwedge_{(\mathbf{x},\mathrm{Q})\in\mathcal{S}} \frac{\partial}{\partial \mathbf{x}}\mathcal{N}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \in \mathrm{Q} \tag{28}$$

The problem above can be solved using conditional variable gradient of DNNs defined in Definition 4.4:

$$\min \|\widehat{\boldsymbol{\theta}} - \theta\| \quad \text{s.t.} \quad \bigwedge_{(\mathbf{x},\mathrm{Q})\in\mathcal{S}} \widetilde{\varphi}_{\mathbf{z}^{(\text{up})}} \wedge \mathbf{A}\frac{\partial \mathbf{z}^{(\text{up})}}{\partial \mathbf{x}} \frac{\partial}{\partial \mathbf{z}^{(\text{up})}} \widetilde{\mathcal{N}}^{(\text{down})}(\mathbf{z}^{(\text{up})}; \widehat{\boldsymbol{\theta}}) \le \mathbf{b} \tag{29}$$

where $\mathbf{z}^{(\text{up})} \stackrel{\text{def}}{=} \mathcal{N}^{(\text{up})}(\mathbf{x})$ denotes the input to $\mathcal{N}^{(\text{down})}$, $\widetilde{\varphi}_{\mathbf{z}^{(\text{up})}}$ denotes the activation condition constraint for $(\mathbf{x}, \mathrm{Q}) \in \mathcal{S}$, $\frac{\partial \mathbf{z}^{(\text{up})}}{\partial \mathbf{x}}$ denotes the Jacobian matrix of $\mathbf{z}^{(\text{up})}$ with respect to $\mathbf{x}$. ■

B.1 Analysis of the LP Size

First, we would like to emphasize that the size of the formulated linear program (LP) *does not* necessarily depend on the size (depth and width) of the entire DNN; viz., the size of the LP does not necessarily grow with the size of the DNN. Because `ProGrad` *does not require editing from the first layer; in practice,* `ProGrad` *allows editing only the last few layers ($\mathcal{N}^{(\text{down})}$) of the DNN, while keeping the rest of the DNN ($\mathcal{N}^{(\text{up})}$) unchanged, enabling efficient editing of large DNNs.*

In this section, we analyze the size of the LP for formulating the conditional variable gradient for one input in terms of the depth and width of the *non-frozen editing-layers* $\mathcal{N}^{(\text{down})}$, which are the the last L layers of an arbitrarily large DNN. For ease of presentation, we assume $\mathcal{N}$ is a feed-forward ReLU DNN as defined in Definition 3.1. Let n_ℓ and $n_{\ell+1}$ for $0 \le \ell < L$ be the input and output widths of the ℓ-th layer, viz., $\mathbf{x}^{(\ell)} \in \mathbb{R}^{n_\ell}$, $\mathbf{z}^{(\ell)} \in \mathbb{R}^{n_{\ell+1}}$, $\mathbf{W}^{(\ell)} \in \mathbb{R}^{n_{\ell+1}\times n_\ell}$ and $\mathbf{b}^{(\ell)} \in \mathbb{R}^{n_{\ell+1}}$. We will show that the size of the formulated LP for each edited layer is polynomial in the input and output widths of that layer, hence the LP size for encoding the conditional variable gradient of a large DNN $\mathcal{N}$ for one input is polynomial only in the size of the last L edited layers $\mathcal{N}^{(\text{down})}$.

LP size for encoding the pre-activation conditional variable output. For the first layer $\ell = 0$, encoding the pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(0)}$ (Equation 7)

$$\widetilde{\mathbf{z}}^{(0)} \stackrel{\text{def}}{=} \widehat{\mathbf{W}}^{(0)}\mathbf{x}^{(0)} + \widehat{\mathbf{b}}^{(0)} \tag{7}$$

uses $\left|\widetilde{\mathbf{z}}^{(0)}\right| = n_1$ constraints, $\left|\widetilde{\mathbf{z}}^{(0)}\right| + \left|\widehat{\mathbf{W}}^{(0)}\right| + \left|\widehat{\mathbf{b}}^{(0)}\right| = n_1 + n_0 n_1 + n_1 = n_0 n_1 + 2n_1$ variables and less than $\left|\widetilde{\mathbf{z}}^{(0)}\right| \times (1 + \left|\widehat{\mathbf{W}}^{(0)}\right| + 1) = n_0 n_1^2 + 2n_1$ non-zero entries in the formulated LP.

For other layers $0 < \ell < L$, encoding the pre-activation conditional variable output $\widetilde{\mathbf{z}}^{(\ell)}$ (Equation 8)

$$\widetilde{\mathbf{z}}^{(\ell)} \overset{\text{def}}{=} \mathbf{W}^{(\ell)} \widetilde{\mathbf{x}}^{(\ell)} + \widehat{\mathbf{b}}^{(\ell)} \tag{8}$$

uses $\left|\widetilde{\mathbf{z}}^{(\ell)}\right| = n_{\ell+1}$ constraints, $\left|\widetilde{\mathbf{z}}^{(\ell)}\right| + \left|\widetilde{\mathbf{x}}^{(\ell)}\right| + \left|\widehat{\mathbf{b}}^{(\ell)}\right| = n_{\ell+1} + n_\ell + n_{\ell+1} = n_\ell + 2n_{\ell+1}$ variables and less than $\left|\widetilde{\mathbf{z}}^{(\ell)}\right| \times (1 + \left|\widetilde{\mathbf{x}}^{(\ell)}\right| + 1) = n_\ell n_{\ell+1} + 2n_{\ell+1}$ non-zero entries in the formulated LP.

LP size for encoding the post-activation conditional layer output. For any layer $0 \leq \ell < L$, encoding the ℓ-th layer post-activation conditional variable layer output $\widetilde{\mathbf{x}}^{(\ell+1)}$ (Equation 9)

$$\widetilde{\mathbf{x}}^{(\ell+1)} \overset{\text{def}}{=} \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\right) \widetilde{\mathbf{z}}^{(\ell)} \tag{9}$$

uses $\left|\widetilde{\mathbf{x}}^{(\ell+1)}\right| = n_{\ell+1}$ constraints, $\left|\widetilde{\mathbf{x}}^{(\ell+1)}\right| + \left|\widetilde{\mathbf{z}}^{(\ell)}\right| = n_{\ell+1} + n_{\ell+1} = 2n_{\ell+1}$ variables and less than $2 \times \left|\widetilde{\mathbf{x}}^{(\ell+1)}\right| = 2n_{\ell+1}$ non-zero entries in the formulated LP.

LP size for encoding the activation condition. For any non-last layer $0 \leq \ell < L-1$, encoding the ℓ-th layer activation condition $\widetilde{\varphi}^{(\ell)}$ (Equation 10)

$$\widetilde{\varphi}^{(\ell)} \overset{\text{def}}{=} \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}>0}\right) \widetilde{\mathbf{z}}^{(\ell)} > 0 \ \wedge \ \operatorname{diag}\left(\mathbf{1}_{\mathbf{z}^{(\ell)}\leq 0}\right) \widetilde{\mathbf{z}}^{(\ell)} \leq 0 \tag{10}$$

uses $2 \times \left|\widetilde{\mathbf{z}}^{(\ell)}\right| = 2n_{\ell+1}$ constraints, $\left|\widetilde{\mathbf{z}}^{(\ell)}\right| = n_{\ell+1}$ variables and less than $2 \times \left|\widetilde{\mathbf{z}}^{(\ell)}\right| = 2n_{\ell+1}$ non-zero entries in the formulated LP.

For the last layer $\ell = L-1$, there is no ReLU activation, hence no activation condition to encode.

LP size for encoding the conditional variable gradient. Encoding the conditional variable gradient for the first editing layer $\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}$ (Equation 20)

$$\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}} \overset{\text{def}}{=} \widehat{\mathbf{W}}^{(0)} \tag{20}$$

uses $\left|\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}\right| = n_1 n_0$ constraints, $\left|\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}\right| + \left|\widehat{\mathbf{W}}^{(0)}\right| = n_0 n_1 + n_0 n_1$ variables, and less than $2 \times (\left|\frac{\partial \widetilde{\mathbf{z}}^{(0)}}{\partial \mathbf{x}^{(0)}}\right| + \left|\widehat{\mathbf{W}}^{(0)}\right|) = 2n_0 + 2n_1$ non-zero entries in the formulated LP.

Because the gradient for $\mathcal{N}^{(\text{down})(1:L)}$ is constant, encoding the variable gradient for $\frac{\partial}{\partial \mathbf{x}} \widetilde{\mathcal{N}}^{(\text{down})}(\mathbf{x}; \widehat{\boldsymbol{\theta}})$ uses $n_0 n_L$ constraints, $n_0 n_L + n_1 n_L$ variables, and less than $n_0 n_1 \times n_0 n_L + n_0 n_L$ non-zero entries in the formulated LP.

Because the gradient for the frozen layers $\mathcal{N}^{(\text{up})}$ is constant, let n denote the input width to $\mathcal{N}$, encoding the variable gradient for $\mathcal{N}$ uses $n n_L$ constraints, $n n_L + n_0 n_L$ variables, and less than $n n_0 \times n n_L + n n_L$ non-zero entries in the formulated LP.

Therefore, by induction, we have that the size of the formulated LP for encoding the conditional variable gradient for one input is polynomial in the input and output widths of each edited layer, hence polynomial in the size of the last L edited layers $\mathcal{N}^{(\text{down})}$ instead of the entire DNN $\mathcal{N}$. When editing the DNN gradients for a set of inputs, the size of the formulated LP grows linearly with the number of inputs in the set.

C Evaluation Details

C.1 Enforcing hard Grad-CAM constraints on ResNet DNNs for IMAGENET.

In this section we present the experiment details for Section 5.1.

Setup details. For the two edit sets, (**i**) the 100 images with ε=1e-2 edit set consists of the first 100 images from the first 50 classes of the IMAGENET-C dataset with Gaussian noise and severity 1, for which the original uncorrupted images are correctly classified, while the corrupted images are top-1 misclassified but top-5 correctly classified; (**ii**) the 1,000 images with ε=5e-2 edit set consists of the first 1,000 images from the first 200 classes of the IMAGENET-C dataset with Gaussian noise and severity 1, for which the original uncorrupted images are correctly classified, while the corrupted images are top-1 misclassified but top-5 correctly classified. Both cosine similarity and IoU are computed on the min-max-normalized Grad-CAM attributions, where IoU uses a 75% percentile threshold.

The `ResNet152` DNN is from `torchvision` with the pre-trained weights `ResNet152_Weights.IMAGENET1K_V1`: `https://docs.pytorch.org/vision/main/models/generated/torchvision.models.resnet152.html#torchvision.models.ResNet152_Weights`. The `ResNet50` DNN is from `torchvision` with the pre-trained weights `ResNet50_Weights.IMAGENET1K_V1`: `https://docs.pytorch.org/vision/main/models/generated/torchvision.models.resnet50.html#torchvision.models.ResNet50_Weights`.

For each gradient-descent-based baseline, we perform a grid search over the learning rate, batch size, number of epochs, and transfer weight hyperparameters, with a time limit of 12 hours, and report the best results with the best constraint satisfaction rate.

Setup for `EWA` baseline. The hyperparameters are taken from the original `EWA` experiments. We use the SGD optimizer with learning rate $1e-3$, momentum 0.9 and weight decay $1e-4$. We fine-tune the last layer of `ResNet152` for 300 epochs with a batch size of 100. For the 100 images with $\varepsilon = 1e-2$ experiment, we use the transfer weight $1e4$; for the 1000 images with $\varepsilon = 5e-2$ experiment, we use the transfer weight $1e3$.

Setup for `SWA` baseline. The hyperparameters are taken from the original `SWA` experiments. We use the SGD optimizer with learning rate $1e-3$, momentum 0.9 and weight decay $1e-4$. We fine-tune the last layer of `ResNet152` for 300 epochs with a batch size of 100. For the 100 images with $\varepsilon = 1e-2$ experiment, we use the transfer weight $1e4$; for the 1000 images with $\varepsilon = 5e-2$ experiment, we use the transfer weight $1e3$.

Setup for `SSWA` baseline. The hyperparameters are taken from the original `SSWA` experiments. We use the SGD optimizer with learning rate $1e-3$, momentum 0.9 and weight decay $1e-4$. We use the `SSWA` erase rate 0.3, and fine-tune the last layer of `ResNet152` for 300 epochs with a batch size of 100. For the 100 images with $\varepsilon = 1e-2$ experiment, we use the transfer weight $1e4$; for the 1000 images with $\varepsilon = 5e-2$ experiment, we use the transfer weight $1e3$.

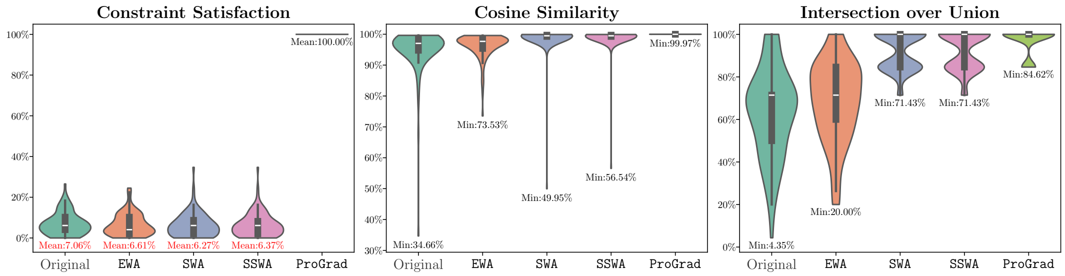
Setup for `ProGrad`. We edit the last layer of both ResNet DNNs, with the changes to the parameters bounded by $[-3, 3]$.

Additional statistics for Grad-CAM similarity metrics. Figure 4 shows the statistics of various Grad-CAM similarity metrics, viz., the constraint satisfaction rate (Constr. Sat.), cosine similarity (Cos.) and intersection over union (IoU) between the expected and edited Grad-CAM attributions for the `ResNet152` experiments.

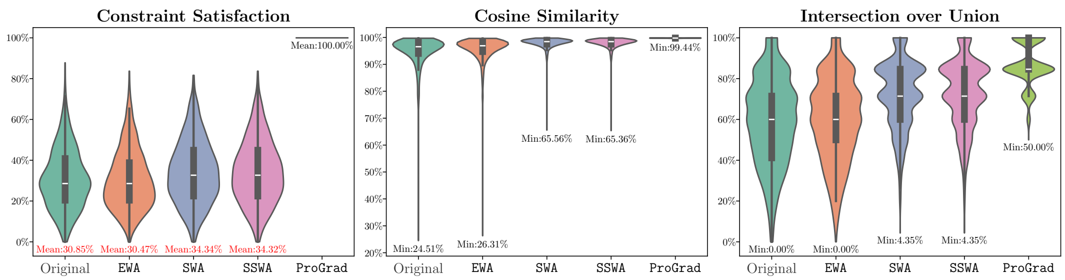
Additional generalization results. In Table 4 we present additional generalization results for the `ResNet152` experiment on enforcing hard Grad-CAM constraints with 1000 samples in Section 5.1. As evidenced by the results, `ProGrad` improves those metrics comparing to the original model, and achieves the best generalization comparing to the baselines.

C.2 Enforce hard Integrated Gradients constraint for SST-2 Llama LLM.

In this section we present the experiment details for Section 5.2.



(a) Statistics of the 100 images with ε=1e-2 experiment on `ResNet152`.



(b) Statistics of the 1,000 images with ε=5e-2 experiment on `ResNet152`.

Figure 4: Additional statistics for Grad-CAM similarity metrics of Table 1 in the main paper (Section 5.1), viz., the (pixel-level) Grad-CAM constraint satisfaction rate (Constr. Sat.), cosine similarity (Cos.) and intersection over union (IoU) between the expected and edited Grad-CAMs.

Table 4: Additional generalization results for the `ResNet152` experiment on enforcing hard Grad-CAM constraints with 1000 samples in Section 5.1. For a generalization set consisting of 4,000 images that's similar to the 1,000-image edit set but with different corruption levels, we present the constraint satisfaction rate (Constr. Sat.) with ε=1e-1, cosine similarity (Cos.) and intersection over union (IoU) on the generalization set, as well as the top-1 accuracy (Acc.) of the edited DNN on the ILSVRC 2012 ImageNet validation set. As evidenced by the results, `ProGrad` improves those metrics comparing to the original model, and achieves the best generalization comparing to the baselines.

Method	Constr. Sat.	Min. Cos.	Min. IoU	Acc.
Original	32.98%	77.53%	39.42%	78.31%
`EWA`	35.71%	82.41%	39.89%	73.32%
`SWA`	36.15%	84.74%	45.28%	76.55%
`SSWA`	36.16%	84.74%	45.26%	76.56%
`ProGrad`	**42.35%**	**85.75%**	**47.43%**	**77.43%**

Setup details. For both constant and conditional variable integrated gradients, we use Gauss-Legendre quadrature to approximate the integral with 25 steps in `bfloat16` precision. Following the common practice, we use the zero point in the token space as the baseline, i.e., a vector of token ID 0. We apply hard constraints and evaluate IG similarity metrics on the IG of the actual sentences from the SST-2 dataset, ignoring the template and special tokens. Both cosine similarity and IoU are computed on the min-max-normalized IG attributions, where IoU uses a 50% percentile threshold. The `Llama-3.2-1b-Instruct` LLM for editing is from `https://huggingface.co/meta-llama/Llama-3.2-1B-Instruct`; The teacher `Llama-3.1-8b-Instruct` LLM for computing the expected IG is from `https://huggingface.co/meta-llama/Llama-3.1-8B-Instruct`. The `Qwen3-1.7B` LLM for editing is from `https://huggingface.co/Qwen/Qwen3-1.7B`; The teacher `Qwen3-8B` LLM for computing the expected IG is from `https://huggingface.co/Qwen/Qwen3-8B`.

For each gradient-descent-based baseline, we perform a grid search over the learning rate, batch size, number of epochs, and trainable parameters, with a time limit of 4 hours, and report the best results with the best constraint satisfaction rate.

Setup for `SFT` baselines. We use `trl` [42] with a learning rate from {1e-3, 1e-4}, epochs from $\{1, 2, 3, 4, 5\}$, `bfloat16` precision, and trainable parameters from the language modelling head (`lm_head`) only or all layers. In Table 2 we report the best results among all hyperparameter combinations with the highest constraint satisfaction rate. For the Llama 3 experiment with 100 samples, the best result uses a learning rate of 1e-3, fine-tunes all layers for 1 epoch; for the Llama 3 experiment with 200 samples, the best result uses a learning rate of 1e-3, fine-tunes all layers for 3 epochs; for the Qwen 3 experiment with 100 samples, the best result uses a learning rate of 1e-4, fine-tunes all layers for 5 epochs; for the Qwen 3 experiment with 200 samples, the best result uses a learning rate of 1e-3, fine-tunes all layers for 3 epochs.

Setup for `DPO` baselines. We use `trl` [42] with a learning rate from {1e-3, 1e-4}, epochs from $\{1, 2, 3, 4, 5\}$, `bfloat16` precision, and trainable parameters from the language modelling head (`lm_head`) only or all layers. In Table 2 we report the best results among all hyperparameter combinations with the highest constraint satisfaction rate. For the Llama 3 experiment with 100 samples, the best result uses a learning rate of 1e-3, fine-tunes all layers for 1 epoch; for the Llama 3 experiment with 200 samples, the best result uses a learning rate of 1e-3, fine-tunes all layers for 1 epoch; for the Qwen 3 experiment with 100 samples, the best result uses a learning rate of 1e-3, fine-tunes `lm_head` for 1 epoch; for the Qwen 3 experiment with 200 samples, the best result uses a learning rate of 1e-3, fine-tunes `lm_head` for 1 epoch.

Setup for `ProGrad`. For both LLMs, we edit the language modelling head (`lm_head`) with the changes to the parameters bounded by $[-10, 10]$.

C.3 Enforce gradient constraints in training a DNN to approximate a target function

Setup. We use a 4-layer fully-connected DNN $\mathcal{N} : \mathbb{R} \to \mathbb{R}$ with 100 hidden neurons per layer and Tanh activation function. Over the domain $[0, 3\pi]$, we uniformly sample 2,048 points as the dataset $\mathcal{D}$. The DNN $\mathcal{N}$ is trained to approximate the following function $f : \mathbb{R} \to \mathbb{R}$

$$f(x) = -x\cos(x) + \sin(x) \tag{30}$$

and the gradient $\frac{d\mathcal{N}}{dx}$ of DNN $\mathcal{N}$ approximates the gradient $\frac{df}{dx} : \mathbb{R} \to \mathbb{R}$ of the target function f:

$$\frac{d}{dx}f(x) = x\sin(x) \tag{31}$$

Gradient constraint. The target gradient function $\frac{d}{dx}f(x) = x\sin(x)$ is bounded by the upper bound function $g_u(x) = x$ and the lower bound function $g_l(x) = -x$, and we aim to enforce this hard constraint on the DNN gradient $\frac{d}{dx}\mathcal{N}$: for all training samples $\forall x \in \mathcal{D}$, $-x \leq \frac{d}{dx}\mathcal{N}(x) \leq x$.

Setup for `GD` baseline. We use the Adam optimizer with learning rate 0.01, and exponential learning rate decay with $\gamma = 0.997$. We train the DNN for 300 epochs with a batch size of 64, using the following loss function to learn both the DNN output and the gradient:

$$\mathcal{L}(x) = \mathtt{MSE}\big(\mathcal{N}(x), f(x)\big) + \mathtt{MSE}\big(\frac{d}{dx}\mathcal{N}(x), \frac{d}{dx}f(x)\big) \tag{32}$$

Setup for `ProGrad`. We edit the last layer of the `GD` trained DNN, with the following hard constraints

$$\forall \mathbf{x} \in \mathcal{D}.\ -\mathbf{x} \leq \frac{d}{d\mathbf{x}}\mathcal{N}(\mathbf{x}; \widehat{\boldsymbol{\theta}}) \leq \mathbf{x}$$

while minimizing the difference between the DNN outputs and gradients with the reference outputs and gradients.

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