Machine Learning for Graphs and Sequential Data

Robustness of Machine Learning Models

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Data Analytics and
Machine Learning

Roadmap

1. **Introduction**
2. Construction of adversarial examples
3. Improving robustness
4. Certifiable robustness
   - Exact certification
   - Convex relaxations
   - Lipschitz-continuity
   - Randomized smoothing

Introduction

- Often ML models and algorithms are optimized w.r.t. simple metrics
  - e.g. misclassification rate, reconstruction error, etc.
- As ML/AI is becoming more widespread and is used in critical applications (e.g. autonomous driving, algorithmic decision-making involving humans) we must consider further aspects
- As ML models get deployed in the real-world they create feedback loops which can have potentially unintended consequences

- One important aspect: Are the ML models reliable?
  - How do they behave in the wild? When your data might, e.g., be corrupted?

What Are Adversarial Examples?

Predicted class:

“pig”

+ 0.005 x

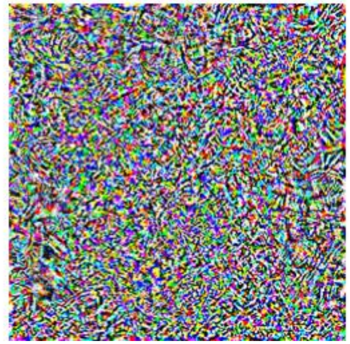

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Image from http://gradientscience.org/intro_adversarial/

What Are Adversarial Examples?

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“pig”

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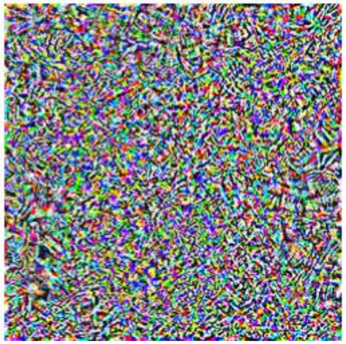

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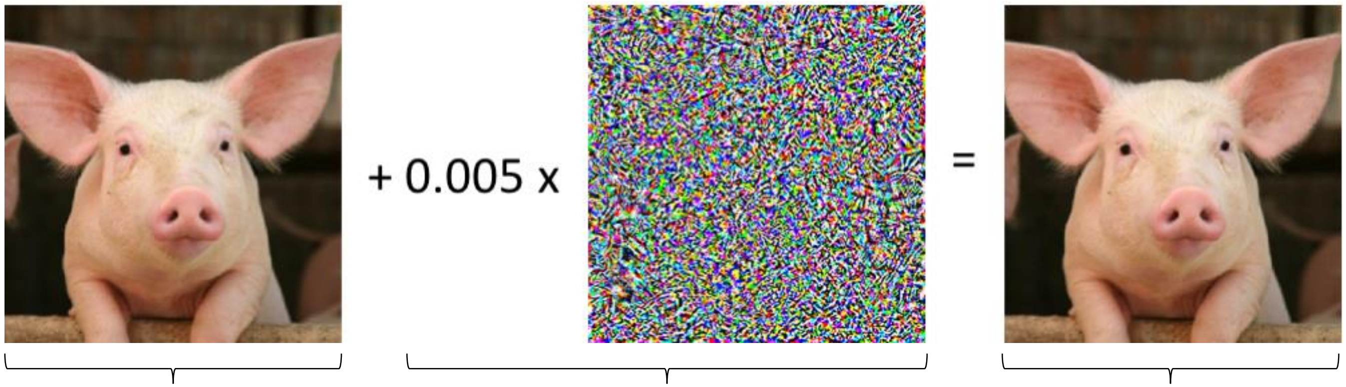
“airliner”

Image from http://gradientscience.org/intro_adversarial/

What Are Adversarial Examples?

Predicted class:

“pig” + 0.005 x = “airliner”



Original (clean) sample

Adversarial perturbation

Adversarial example

Small (imperceptible) but **specifically crafted perturbations** lead to **false predictions** in machine learning models.

- Why should we care about adversarial examples?
- What does ”small“ mean?
- How are adversarial examples created?
- How to protect against adversarial examples?

Image from http://gradientscience.org/intro_adversarial/

Why We (Should) Care About Adversarial Examples

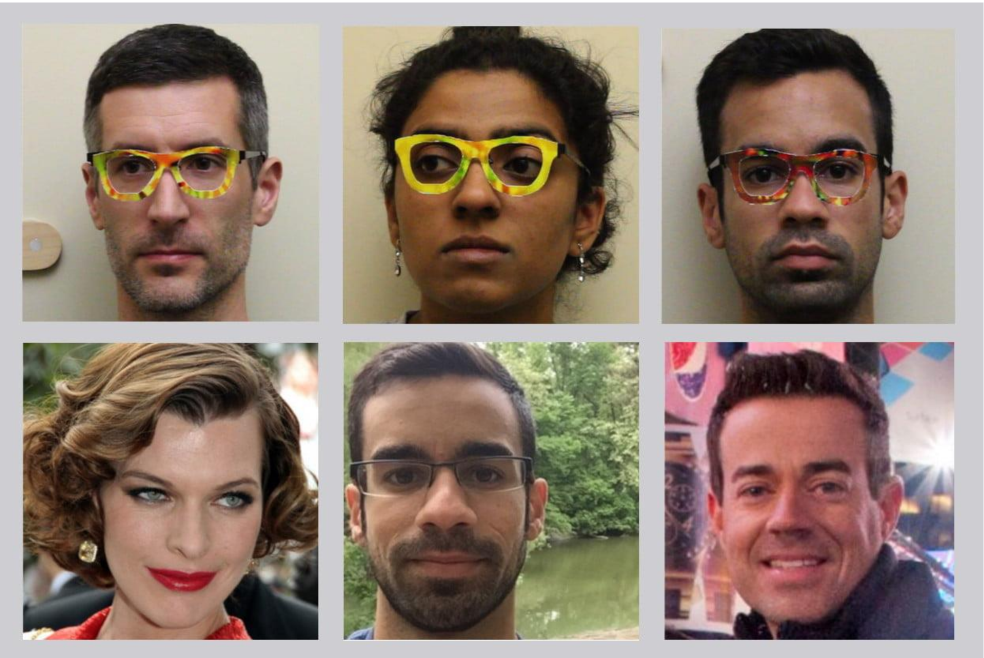
Real-world risks

- Adversarial examples are an obvious security threat for many real-world applications, e.g. self-driving cars.
- Adversarial examples also exist in the real world, e.g. 2D / 3D prints, special glasses to disturb face recognition, etc.

Conceptual gaps

- Neural networks are hypothesized to learn meaningful representations that capture semantic understanding of the domain and task.
  - Adversarial examples are counterexamples to this hypothesis: the semantic content of the samples in unchanged but the network is fooled.
- Nature as an adversary: Even if there is no adversary in our use-case, we should quantify robustness to **worst-case noise**

Adversarial Examples



Adversarial glasses fool facial recognition systems into classifying the wearer as someone else, [Sharif et al., 2016]

ML systems classify the adversarially modified STOP sign as a speed limit sign, [Eykholt et al., 2018]

Adversarial Examples – Definition

Classification task:

- Dataset: $(\mathbf{x}_{\boldsymbol{i}}, y_i) \sim \mathbb{P}_{\text{data}}$, $\quad (\mathbf{x}_{\boldsymbol{i}}, y_i) \in \mathbb{R}^d \times \mathcal{Y}$
- Classifier: $f\colon \mathbb{R}^d \to \mathcal{Y}$

- Specify a perturbation set $\mathcal{P}(\mathbf{x})$, i.e. a set of perturbations which when applied to $\mathbf{x}$ do not change it‘s semantic
  - and, thus, should also not change it‘s classification
- We say that a point $\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})$ is an adversarial example for f at $(\mathbf{x}, y)$
  - if $f(\mathbf{x}) = y$, i.e., f correctly classifies $\mathbf{x}$
  - but $f(\tilde{\mathbf{x}}) \neq y$, i.e. fails to correctly classify $\tilde{\mathbf{x}}$

On “small” Perturbations

- Perturbations should not change the **semantic content** of a sample.
- This is often translated into L_p constraints with some small ϵ
- L_p norm: $\mathcal{P}_{\epsilon,p}(\mathbf{x}) = \{\tilde{\mathbf{x}}\colon \|\tilde{\mathbf{x}} - \mathbf{x}\|_p < \epsilon\}$, typically $p \in \{1, 2, \infty\}$
- While mathematically convenient, L_p norms with small ϵ do not contain **all** semantically meaningless perturbations.
- For example, a **small rotation** does typically not change the meaning of a picture but often corresponds to **large changes** in L_p norm.

Attack Variants

- **Evasion attacks**: given a **fixed**, trained classifier f, the attacker aims to find an adversarial perturbation (at test time)
- **Poisoning attacks**: the adversary aims to modify the **training dataset** such that a classifier trained on the dataset has properties desired by the attacker.
  - i.e. the manipulation/corruption is done **before** training

  ➔ **Not covered in this course.**

- **Targeted attacks**: the attacker aims to have a certain sample classified as a specific class (e.g. speed limit 100 km/h sign).
- **Untargeted attacks**: the attacker aims to have a sample misclassified as **any class** different than the correct one.

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Adversarial Attacks: Objective Function

Construction of adversarial examples can be phrased as an optimization problem. For example:

$$\tilde{\mathbf{x}}_{\mathbf{x}}^* = \underset{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})}{\arg\max} \ \ell_{0/1}(f(\tilde{\mathbf{x}}), y)$$

- **Recall:** $\ell_{0/1}$ is the zero/one loss (0 if correct, 1 if incorrect).
- **However**: $\ell_{0/1}$ has either zero or undefined gradient.
- Therefore, the **cross-entropy loss** $\mathcal{L}$ is often used as a surrogate:

$$\tilde{\mathbf{x}}_{\mathbf{x}}^* = \underset{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})}{\arg\max} \ \mathcal{L}(f(\tilde{\mathbf{x}}), y)$$

Projected Gradient Descent

$$\tilde{\mathbf{x}}^*_{\mathbf{x}} = \underset{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})}{\arg\max} \; \mathcal{L}\left(f(\tilde{\mathbf{x}}), y\right)$$

- One common method is **Projected gradient descent** (PGD): after each gradient step on the objective, project onto the valid domain.
- $\mathbf{x}_{t+1} = \Pi(\mathbf{x}_t + \eta_t \nabla_{\mathbf{x}} \mathcal{L}(f(\mathbf{x}_t), y))$
- Like training the model but **updating the data instead of the weights**.
- Note: since $f(\tilde{\mathbf{x}})$ is **not convex**, in general we cannot find the global optimum.

Fast Gradient-Sign Method (FGSM):

- $\tilde{\mathbf{x}} = \Pi(\mathbf{x} + \eta \cdot \mathrm{sign}\left(\nabla_{\mathbf{x}} \mathcal{L}(f(\mathbf{x}), y)\right))$
- When $\mathcal{P}(\mathbf{x})$ is a ball with radius ϵ measured by the L_∞ norm, setting $\eta = \epsilon$ yields valid perturbations with only a single step and without projection.

Alternative Optimization Problem

- An alternative formulation is to optimize:

$$\min_{\tilde{\mathbf{x}}} \mathcal{D}(\mathbf{x}, \tilde{\mathbf{x}}) \quad \text{subject to } \ell_{0/1}(f(\tilde{\mathbf{x}}), \mathrm{y}) > 0$$

- Here, $\mathcal{D}$ is a term that is large when $\tilde{\mathbf{x}}$ is far from $\mathbf{x}$ (e.g., an L_p distance)
- [Carlini and Wagner, 2017] convert this constrained into an **unconstrained** optimization problem:

$$\min_{\tilde{\mathbf{x}}} \mathcal{D}(\mathbf{x}, \tilde{\mathbf{x}}) + \lambda \cdot L(\tilde{\mathbf{x}}, \mathrm{y}),$$

- A very effective **loss function** is

$$L(\tilde{\mathbf{x}}, \mathrm{y}) = \left[Z(\tilde{\mathbf{x}})_y - \max_{i \neq y} (Z(\tilde{\mathbf{x}})_i) \right]_+$$

  - y is the original class we want $\tilde{\mathbf{x}}$ to deviate from
  - $[\mathbf{x}]_+ = \max(\mathbf{x}, 0)$
  - $Z(\tilde{\mathbf{x}})_i = \log \mathrm{f}(\tilde{\mathbf{x}})_\mathrm{i}$ (log probability of class i)
  - The loss L is positive if $\tilde{\mathbf{x}}$ is classified as y and 0 otherwise.

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Introduction

- Most ML models (trained and/or applied in the traditional way) are vulnerable to adversarial examples

- How to defend against adversarial examples?
- Can we prevent them?
- Can we improve the robustness of our models?

What does not seem to work

- **Post-hoc prevention of attacks**
  E.g. gradient obfuscation, i.e. randomizing or shattering gradients of the model in order to prevent gradient-based attacks. So far, these defenses have all been broken by stronger attacks.
- **Detection of adversarial examples**
  E.g. out-of-distribution shift: since the adversarial examples come from a different distribution as the natural images, we could try to distinguish the two distributions or perform outlier / anomaly detection. While some of these methods work against "vanilla" PGD attacks, targeted attacks are very successful against these defenses.

- Fixing a "bad" model seems not to be the solution

Robust Training

Robust training refers to training procedures aimed at producing models that are robust to adversarial (and/or other) perturbations.

A **common theme** is to optimize a 'worst-case' loss (also called robust loss), i.e. the loss achieved under the worst-case perturbation.

- Let $\ell(\hat{y}, y)$ be some loss, e.g. cross-entropy loss

- The (non-robust) training tries to find an f that minimizes the expected loss
$$R = \mathop{\mathbb{E}}_{(\mathbf{x}, y) \in \mathbb{P}_{\text{data}}} [\ell(f(\mathbf{x}), y)]$$

- The robust version of this problem is
$$R_{\text{rob}} = \mathop{\mathbb{E}}_{(\mathbf{x}, y) \in \mathbb{P}_{\text{data}}} \left[\boxed{\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f(\tilde{\mathbf{x}}), y\right)} \right]$$

Loss achieved by the worst-case perturbation in $\mathcal{P}(\mathbf{x})$

Robust Training

Robust training refers to training procedures aimed at producing models that are robust to adversarial (and/or other) perturbations.

A **common theme** is to optimize a ‘worst-case’ loss (also called robust loss), i.e. the loss achieved under the worst-case perturbation.

- **Adversarial training** is an easy-to-implement robust training procedure that uses adversarial examples as a proxy for the ‘worst-case’ perturbation.
- In the next chapter, we will cover **robustness certification** techniques. Some of these can also be used for robust training.

Adversarial Training

Idea: perform stochastic gradient descent (SGD) on the **robust loss** R_{rob} :

$$R_{\text{rob}} = \mathop{\mathbb{E}}_{(\mathbf{x}, y) \in \mathbb{P}_{\text{data}}} \left[\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f(\tilde{\mathbf{x}}), y\right) \right]$$

For $f = f_\theta$ being a **neural network** parameterized by weights θ, we can write

$$\nabla_\theta R_{\text{rob}} = \nabla_\theta \left(\mathop{\mathbb{E}}_{(\mathbf{x}, y) \in \mathbb{P}_{\text{data}}} \left[\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f_\theta(\tilde{\mathbf{x}}), y\right) \right] \right)$$

$$= \mathop{\mathbb{E}}_{(\mathbf{x}, y) \in \mathbb{P}_{\text{data}}} \left[\boxed{\nabla_\theta \left(\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f_\theta(\tilde{\mathbf{x}}), y\right) \right)} \right]$$

How to take the gradient of the **worst-case loss** w.r.t. the weights θ?

Adversarial Training: Danskin‘s Theorem

- How to obtain $\nabla_\theta L = \nabla_\theta \left(\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f_\theta(\tilde{\mathbf{x}}), y\right) \right)$?
- That is, the **gradient** of the **worst-case loss** w.r.t. the model parameters.

- **Danskin's Theorem***: Let $\Delta(\theta)$ be the set of $\tilde{\mathbf{x}}$ for which the supremum is obtained. If $\Delta(\theta)$ contains only a single element, i.e. $\Delta(\theta) = \{\tilde{\mathbf{x}}_\theta^*\}$, then the sup is differentiable at θ and

$$\nabla_\theta \left(\sup_{\tilde{\mathbf{x}} \in \mathcal{P}(\mathbf{x})} \ell\left(f_\theta(\tilde{\mathbf{x}}), y\right) \right) = \nabla_\theta\, \ell\left(f_\theta\left(\tilde{\mathbf{x}}_\theta^*\right), y\right)$$

* Technically, the theorem requires some conditions which might not hold in our case; e.g., that $\ell\left(f_\theta(\tilde{\mathbf{x}}), y\right)$ is convex in θ.

Adversarial Training: Algorithm

- Using **Danskin's theorem** we can compute the gradient of the worst-case loss given the corresponding perturbation.
- **Problem**: finding the **worst-case** perturbed example $\tilde{\mathbf{x}}$ is **intractable**; if we could find it efficiently, we would have solved the **exact verification** problem.
- **Idea**: Create any adversarial example as a proxy of the worst-case perturbation, e.g. via the fast gradient-sign method (FGSM).
- Adversarial training algorithm outline:
  1. Sample $(\mathbf{x}_i, y_i) \sim \mathbb{P}_{\text{data}}$
  2. Using an adversarial attack procedure, find an $\tilde{\mathbf{x}}_i$ with high loss $\ell(f_\theta(\tilde{\mathbf{x}}_i), y_i)$
  3. Update weights via gradient descent: $\theta \leftarrow \theta - \eta \nabla_\theta \ell(f_\theta(\tilde{\mathbf{x}}_i), y_i)$

- In step 2, we must trade off the strength of the attack with its computational cost.

Adversarial Training: Summary

Pro:

- It empirically increases robustness of the resulting models.
- It is easy to implement.

Con:

- If we want to use a powerful attack on the inner optimization, the slowdown is about 10x compared to standard training.
- The resulting models typically have lower accuracy on clean data.
- We don’t get any theoretical guarantees of the model’s robustness

Questions – Rob1

1. Given an arbitrary binary classifier f for an input domain $\mathbb{R}^d$ and the perturbation set $\mathcal{P}_{\epsilon,p}(\mathbf{x})$ as defined before. Is it possible that every $\mathbf{x} \in \mathbb{R}^d$ is "robust", i.e. no adversarial example exists?

2. Will the fast gradient-sign method (FGSM) always find an adversarial example (assuming there exist some in the set of perturbations $\mathcal{P}_{\epsilon,\infty}(\mathbf{x})$)?

Recommended Reading

- Lecture 09: Introduction to adversarial examples and
  Lecture 10: Empirical defenses for adversarial examples
  of Jerry Li‘s course on Robustness in Machine Learning (CSE 599-M),
  https://jerryzli.github.io/robust-ml-fall19.html

References

- Carlini, Nicholas, and David Wagner. "Towards evaluating the robustness of neural networks." *2017 ieee symposium on security and privacy (sp)*. IEEE, 2017.
- Eykholt, Kevin, et al. "Robust physical-world attacks on deep learning visual classification." *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2018.
- Sharif, Mahmood, et al. "Accessorize to a crime: Real and stealthy attacks on state-of-the-art face recognition." *Proceedings of the 2016 acm sigsac conference on computer and communications security*. 2016.