Yale

Introduction to Trustworthy AI

CPSC 471/571: Trustworthy Deep Learning

Rex Ying

CPSC 471 / 571 Course Logistics

- **Welcome to CPSC 471 / 571**
- **The class meets Monday and Wednesday 2:30 PM-3:45 PM**
  - This is still a **seminar-like, graduate-level** course
    - Students are expected to master the background of deep learning, and are expected to have the ability to explore cutting-edge research topics on their own
  - Most of the lectures will be in-person
  - There will be a few guest lectures, some of which might be held remotely.
- **This is a relatively new course, and feedbacks are especially welcomed!**
  - It's also a course that can benefit a lot from discussions

Course Outline

- **Introduction** (3 lectures)
  - Trustworthy AI intro; preliminaries of deep neural networks
- **Explainable AI** (3-4 lectures)
  - Model interpretability and explainability; evaluation of explainable models
- **Adversarial Robustness** (4 lectures)
  - Evasion attacks; poisoning attacks; defense against adversarial attacks; verification
- **Fairness** (2 lectures)
  - Biases in deep learning models; fairness algorithms in deep learning models
- **Privacy** (3 lectures)
  - Privacy attacks; differentially private deep models; federated learning; unlearning
- **Efficient Deep Learning** (2-3 lectures)
  - Model pruning; sparse transformers; efficient LLM; Quantization
- **Trustworthy LLM** (1-2 lectures)
  - Hallucination; retrieval-augmented generation (RAG); various aspects of trustworthy AI in LLMs

Logistics: Canvas

- **Check Canvas often for course materials and communications**
  - Slides will be posted before or shortly after the class
- **Readings:**
  - Pre-reading for next lecture will be announced at the end of the previous class
- **Optional readings:**
  - Papers and pointers to additional literature (suggested on slides)
  - **These will be very useful for course projects**
- **Student presentations:**
  - Presenter(s) will post the slides on canvas after the presentation

Logistics: Communication

- **Canvas has a discussion panel:**
  - **Please participate and help each other!**
  - **It's also a great way to show engagement and understanding in case you missed classes or didn't join discussions in class**
  - Search for answers before you ask
- **Mailing list:**
  - Teaching staff: cpsc471_staff@googlegroups.com
  - Send email to the mailing list if you have requests or questions (not individual instructor / TA)
  - Only email the instructor if the message is highly private / not related to teaching in general
- **Office Hours:**
  - Instructor: Monday 1:30 – 2:30 pm
  - TAs: see canvas announcements

Work for the Course & Grading (1)

- **Final grade will be composed of course project, discussions, exams**
- **Course project: 50% (Code and Report to be submitted on Canvas)**
  - In-class discussion session: 5%
  - Proposal: 5%
  - In-class “Hackathon”: 5%
  - Milestone: 15%
  - Final report: 20%
  - Consistent work is valued the most

Work for the Course & Grading (2)

- **Final grade will be composed of course project, discussions, exams**
- **4 Assignments**
  - Written assignment 1 – Explainability
  - Coding assignment 1 – Explainability
  - Written assignment 2 – Adversarial Robustness
  - Coding assignment 2 – Adversarial Robustness

Work for the Course & Grading (3)

- **In-class Exam (last lecture)**
- **Will potentially cover all content taught in this class**
  - Close-book but we will provide all necessary knowledge in the exam
  - No memorization of complex equations needed
  - I will highlight the parts that are important to prepare
  - We do assume all pre-requisites (multi-variable calculus, linear algebra) in the exam. They should be the second instinct for an ML student imo

Honor Code

- **We strictly enforce the Yale Honor Code**
  - Violations of the Honor Code include:
    - Copying or allowing another to copy from one's own paper
    - Unpermitted collaboration
    - Plagiarism
    - Giving or receiving unpermitted aid on an examination
    - Representing as one's own work the work of another
    - Giving or receiving aid on an assignment under circumstances in which a reasonable person should have known that such aid was not permitted
  - The sanction for even a first offense is severe

Course Projects

- **Course project:**
  - Development of methods related to trustworthy AI and perform benchmarking
  - Propose new trustworthy DL models and validate on non-trivial datasets
- **Performed in groups of up to 3 students:**
  - Fine to have groups of 1 or 2. The team size will be taken under consideration when evaluating the scope of the project in breadth and depth.
  - Project is the **important work** for the class
  - Can be very beneficial if you aim to work on research in this topic
  - Graduate and undergraduate students will have the same criteria
  - **Even for group projects each student needs to submit their own separate method and experiment sections**
- **More information will be posted on Canvas in 3 weeks**

Student Participation

- Trustworthy AI is both about people and machine learning
- **Participation** (5% of overall grade) is highly encouraged
- I will likely also pick different students to ask questions or give answers each lecture
- The two in-class discussion and work sessions are mandatory

Course Schedule

Week	Milestones	Due on (11:59pm ET)
3	**Finalize project groups**	Fri, Feb 2rd
5	**In-class project discussions**	Fri, Feb 14th
7	**Project proposal**	Fri, March 1st
8	**In-class work session**	Wed, March 6th
12	**Project milestone**	Fri, April 5th
15	**Exam**	Wed, April 24th
	Project Report	Fri, May 5th 11:59pm

Prerequisites

- **The course has relevance to a wide range of topics and background in DL is needed!**
- Trustworthy DL for different architectures will all be in scope of the class
  - However, although beneficial, students are not required to understand all model architectures
  - **The course will give a brief overview on common model architectures**
- **Minimum Pre-requisites**
  CPSC 201, 223 and one of S&DS 265a, 381/581 or 452
  - **Familiarity with Linear algebra**
  - **Familiarity with Multi-variable calculus**

Machine Learning Tools

- PyTorch
- There are many libraries for specific architectures
  - Hugging Face is a good place to check out the tools
  - Most papers have associated codebase on GitHub so check out what tools / libraries that the researchers use
    (in fact, I do not recommend presenting a paper that does not have open-source implementation)
- Computational resource from YCRC can be utilized
  - I will follow up with more information about computation resources after the proposals are submitted

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Readings

- Readings are updated on the website (syllabus page)

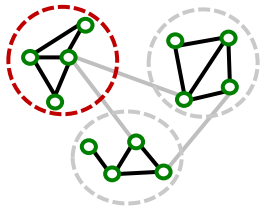
- **Lecture 1 readings**: AI Sustainability

What Deep Learning Looks Like

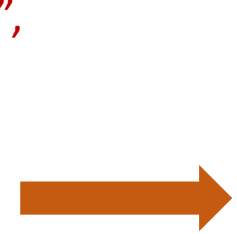
Why do we need Trustworthy AI?

Input

Sentence: [SOS, “graph”, “neural”, “networks”, “are”, “powerful”, EOS]



None / Noise

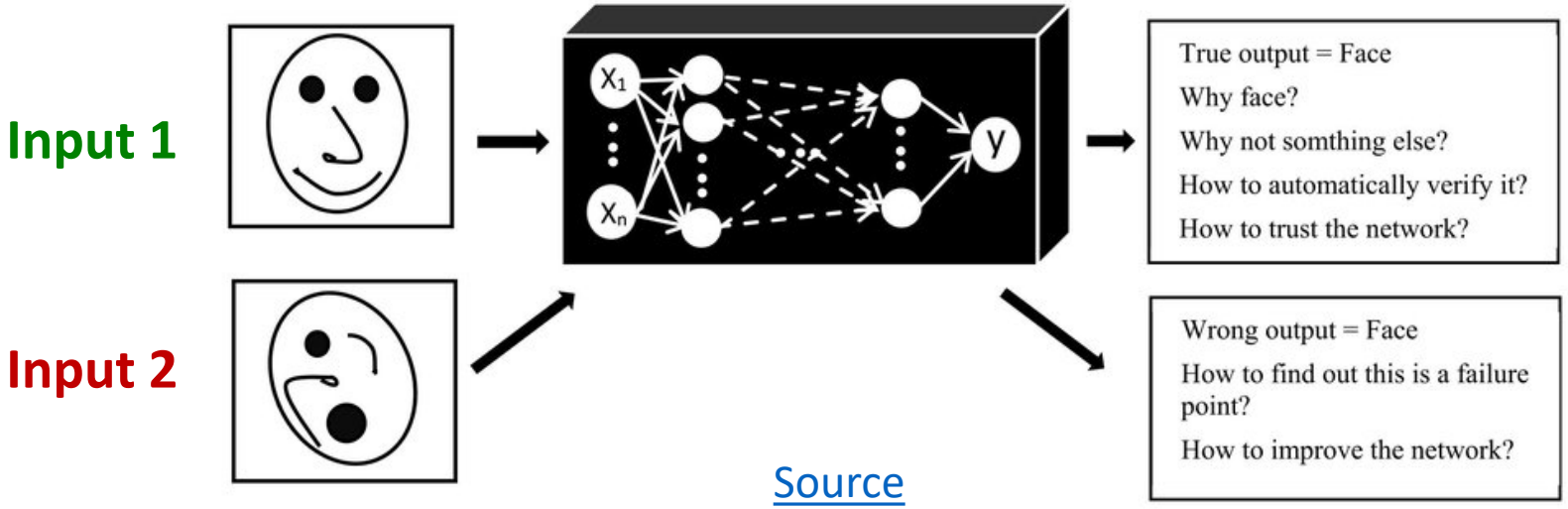


Neural network architecture

Labels,
generated content,
agent decision
etc.

What People Want

- **Model debugging**
- **Phenomenon understanding**
- **Robustness and consistency**
- **Efficiency and human-like behavior**



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Trustworthy Graph Learning

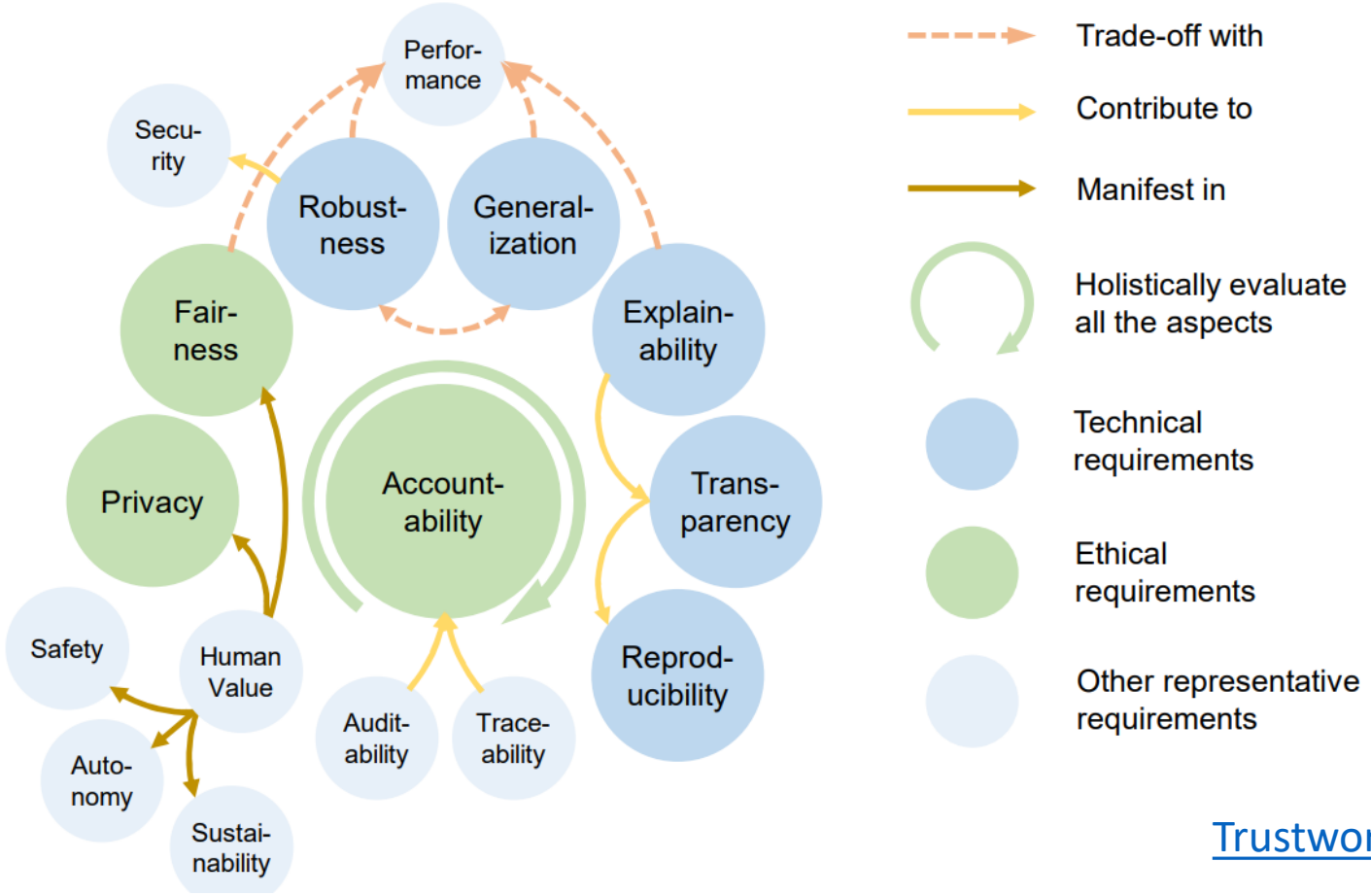
Trustworthy AI includes many components

- Explainability, fairness, robustness, privacy, efficiency …
- The goal is to develop algorithms to tackle one or a combination of these aspects

Challenges

- Deep learning is typically regarded as blackbox
  - High dimensionality, multimodal data, larger and larger parameter space
- Trustworthiness is defined by human, and in particular, domain experts in many applications
- Sometimes performance and runtime tradeoffs seem inevitable

Trustworthy DL Topics



[Trustworthy AI: From Principles to Practices]

Aspects of Trustworthy Deep Learning

- **Robustness** (often against adversarial attacks)
- **Explainability**
- Privacy
- Fairness
- Efficiency / Environmental well-being
- Others

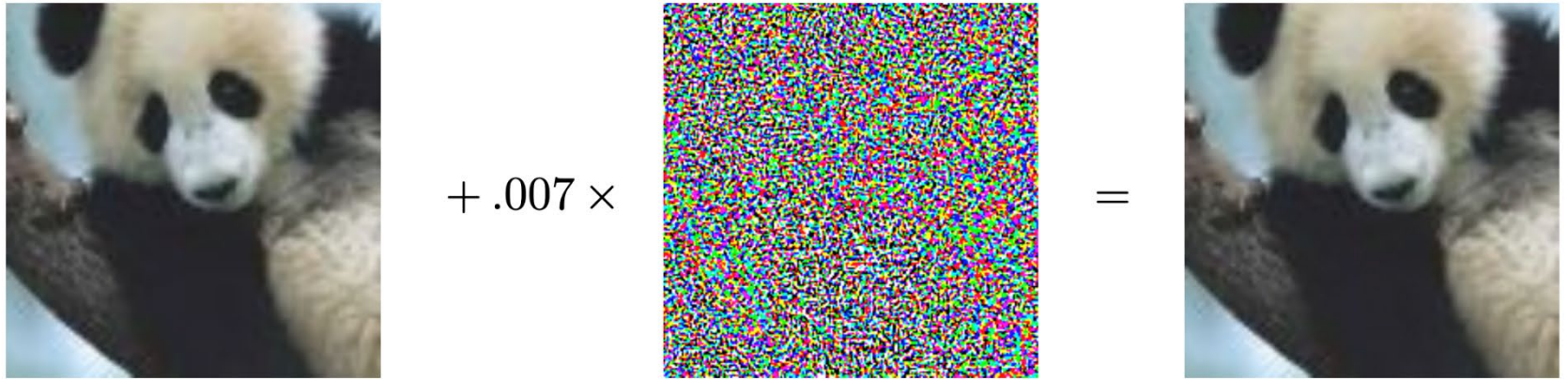
How does each aspect play a role in gaining trust from users of machine learning models?

Deep Learning Performance

- Recent years have seen **impressive performance of deep learning models in a variety of applications.**
  - Deep generative models (e.g. diffusion models)
  - AlphaFold
  - Language models
  - Multi-modal models
- **Are these models ready to be deployed in real world?**

Adversarial Examples

- Deep convolutional neural networks are vulnerable to **adversarial attacks:**
  - Imperceptible noise changes the prediction.

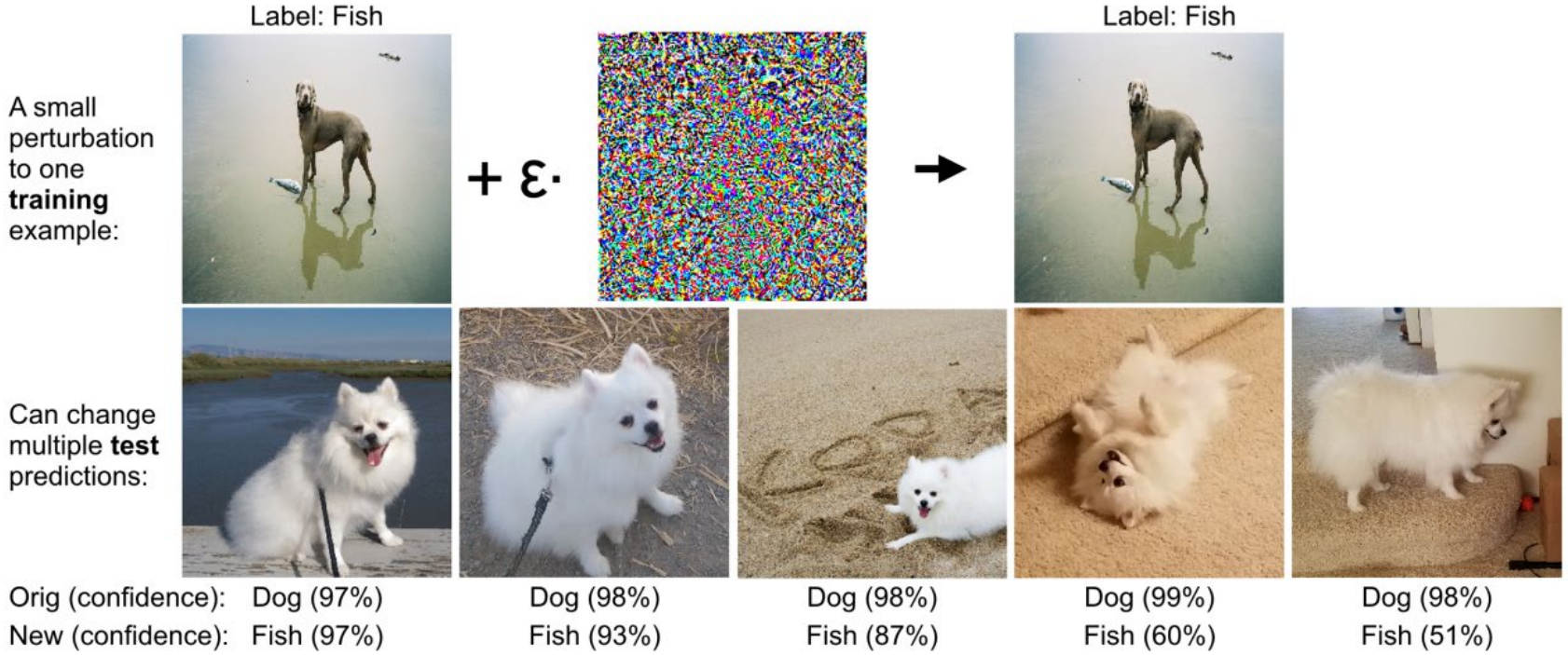


Goodfellow, I., Shlens, J., & Szegedy, C.. (2014). Explaining and Harnessing Adversarial Examples.

- Adversarial examples are also reported in natural language processing [Jia & Liang et al. EMNLP 2017] and audio processing [Carlini et al. 2018] domains.

Adversarial Examples

- Adversarial examples are not special cases: they are ubiquitous in deep learning models!



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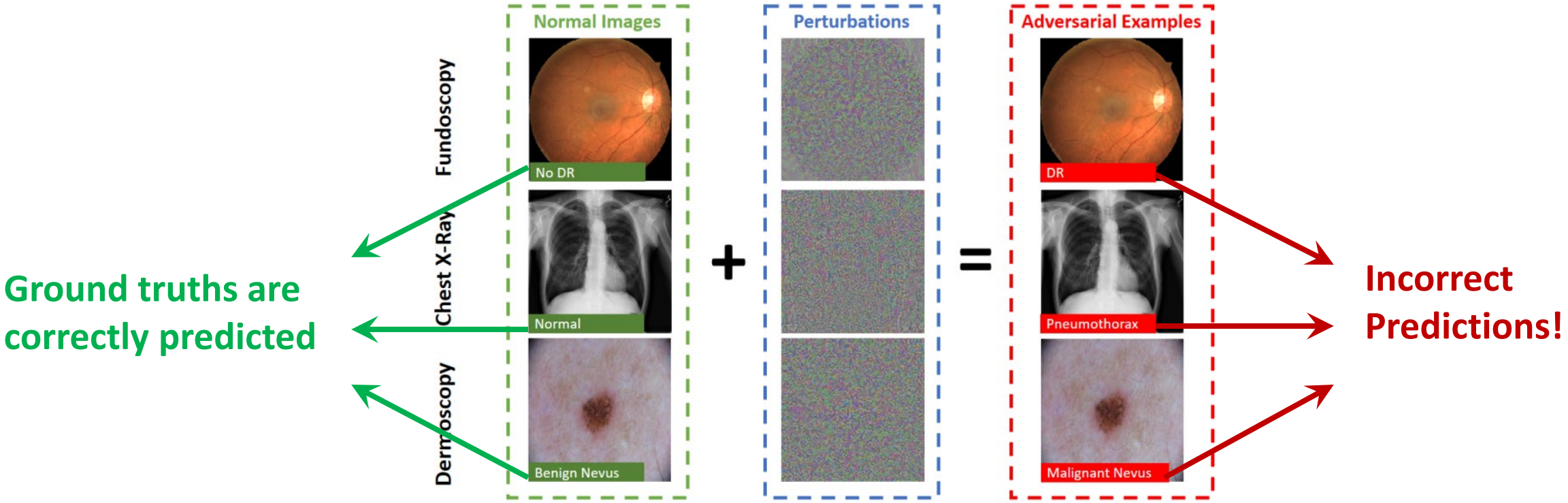
Adversarial Examples – Medical Applications

- Adversarial attacks crafted by the Projected Gradient Descent (PGD)
- On medical dataset Fundoscopy, Chest X-Ray, Dermoscopy

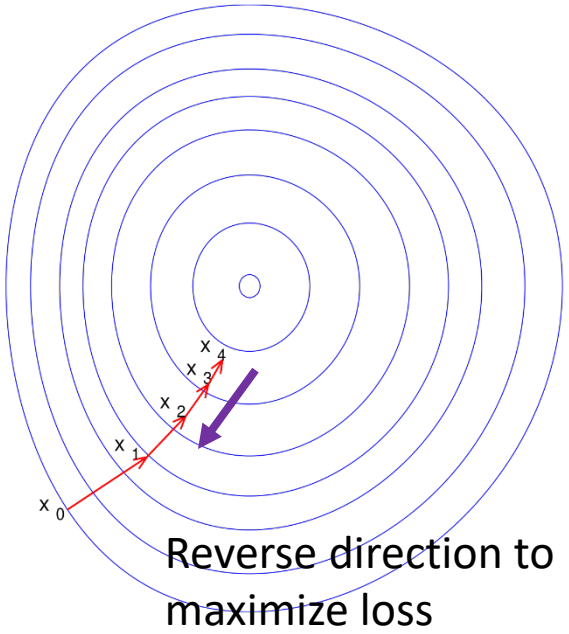


Implication of Adversarial Examples

- **The existence of adversarial examples prevents the reliable deployment of deep learning models to the real world.**
  - Adversaries may try to actively hack the deep learning models.
  - The model performance can become much worse than we expect.
- **Deep learning models are often not robust.**
  - It is an active area of research to make these models robust against adversarial examples

Types of Attacks

- **Whitebox Attack:**
  - The attacker has access to model architecture and weights
  - Easier to attack
  - Gradient-based methods are straightforward and effective



- **Blackbox Attack:**
  - The attacker does not have access to the model's parameters
  - The type of architecture might be known
  - A different model or no model is used to generate adversarial examples in the hopes that these will transfer to the target model

Types of Attacks

- **Data Poisoning**
  - Contamination of training data
- **Byzantine Attacks**
  - Commonly occur in federated learning setting
  - One or multiple client / edge device attacking against the federated learning system
- **Evasion**
  - Evasion of detection models (face/person detection; anomaly detection; fraud detection, spam detection …)
- **Model Extraction**
  - Gain understanding of model architecture and model weights

Explainability

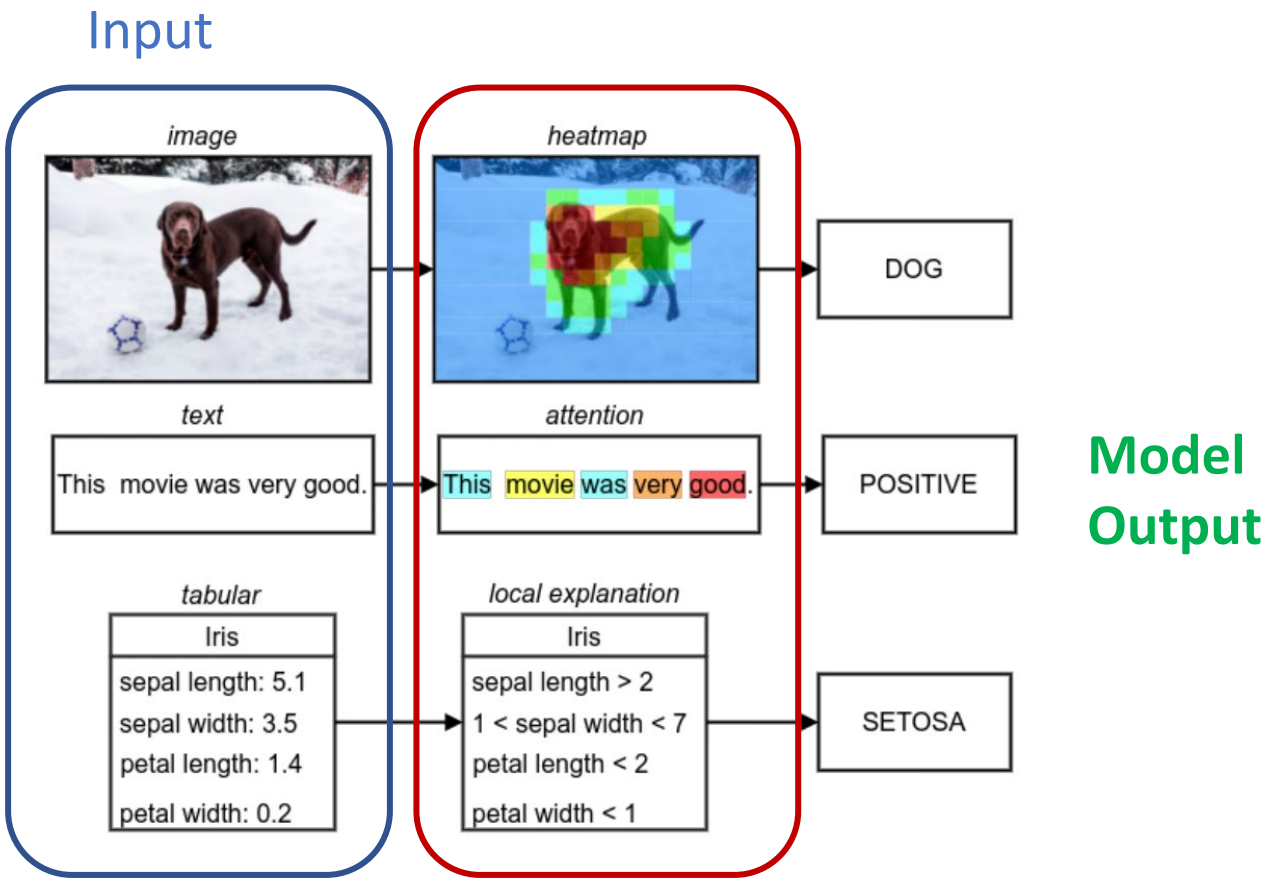
- The goal is to explain what is learned by the model to users / domain experts, in order to gain trust from human users of the deep learning system

- The blackbox nature of deep learning is a major challenge

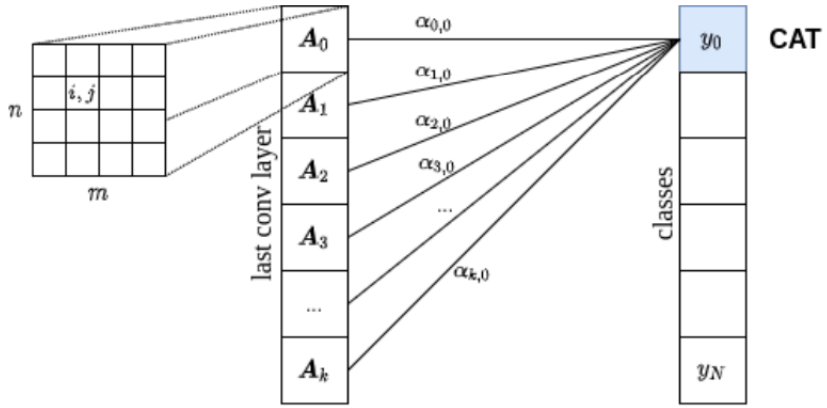
- Simple-to-read guide: 2004.14545.pdf (arxiv.org)

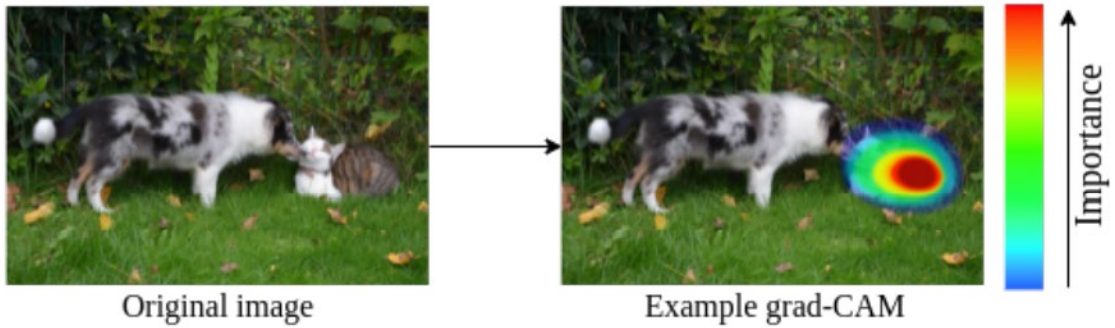
What was explainable about previous ML models??

Forms of Explanation



Example: Computer Vision





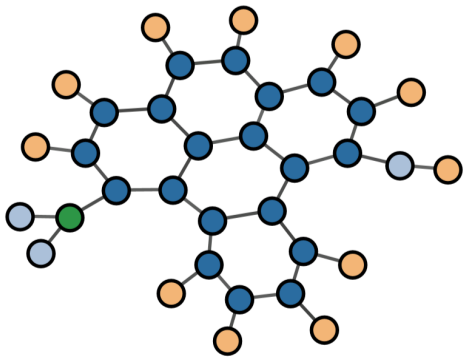
Importance scores on pixels

Explanation: A particular region of the image displays a cat

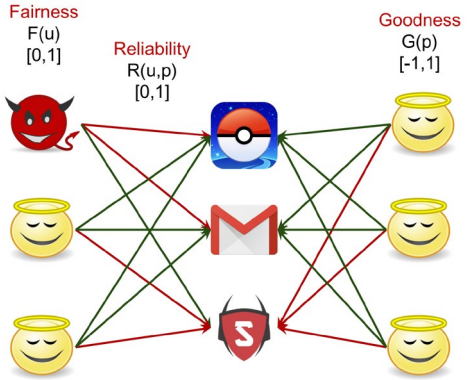
Example: Graphs

- Example questions after training GNNs:
  - Why is an item recommended to a user?
  - Why is the molecule mutagenic?
  - Why is the user classified as fraudulent?
- How to let the domain experts understand and trust the GNN model?

Recommender System



Mutagenic Molecule



Fraudulent Detection

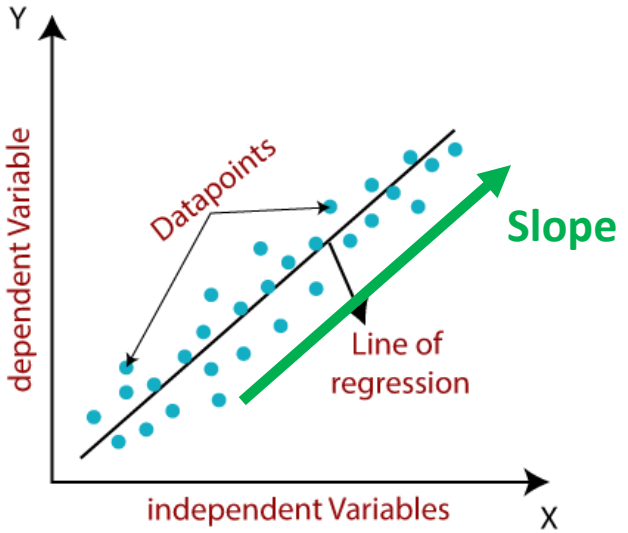
Explainable Models (1)

- **Linear regression**
  - Slope is explainable (how much does one variable affects a prediction)
  - $y = w_1 x_1 + w_2 x_2 + w_3 x_3 + \cdots$

prediction

weights

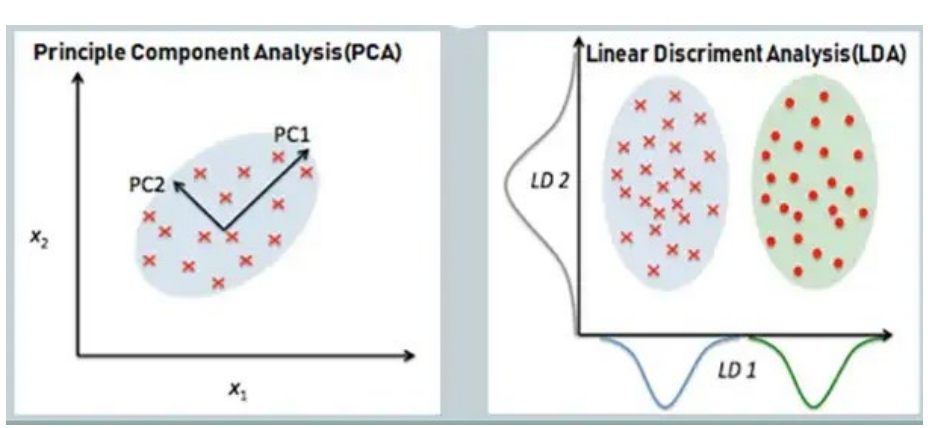
features



- Each feature has an associated weights, indicating importance
  - "A change of Δx amount to feature x_1 will result in increase of prediction by Δy

Explainable Models (2)

- Dimension reduction
  - Dimension reduction allows us to visualize the training data distribution



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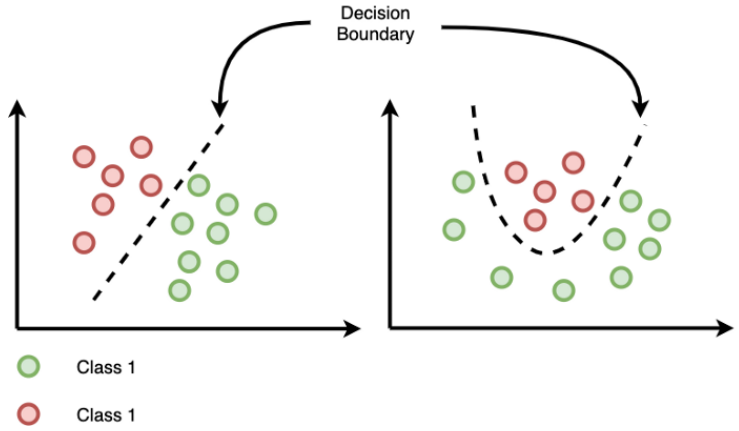

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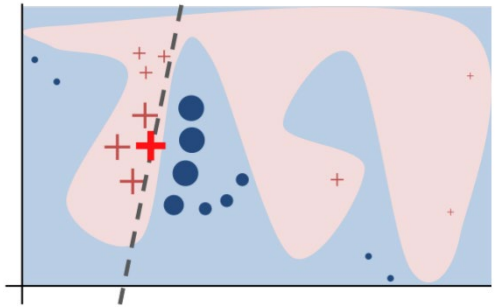
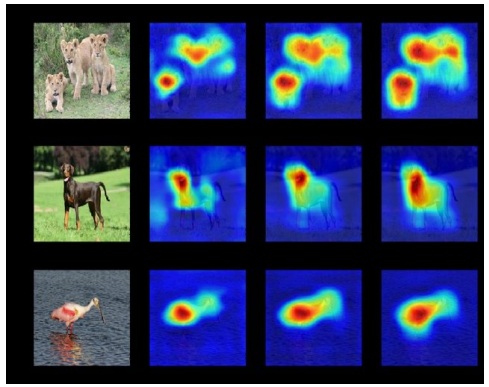
- Decision boundary can be visualized and understood
  - Instances at the boundary characterizes how different classes are different

Deep Learning Explainability Methods: Examples

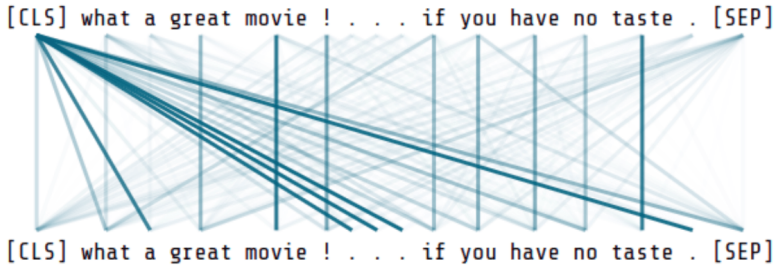
- **Proxy Model**
  - Learn an inherently interpretable model locally approximating the original model (e.g. a linear model, interpret by weights).



- **Saliency Maps**
  - Compute gradients of outputs w.r.t. input pixels.

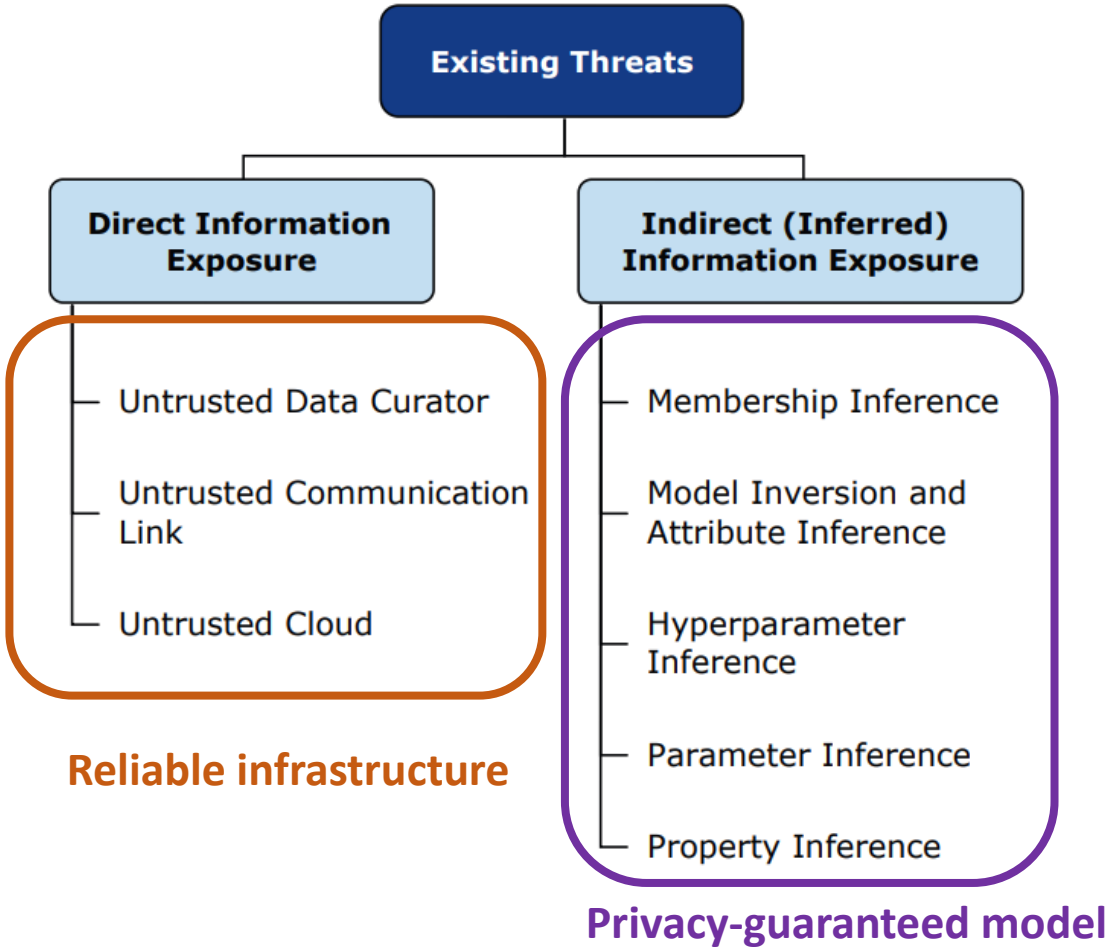


- **Attention Mechanisms**
  - Visualize attention weights in a attention models.



Privacy

- Important privacy policies
  - California Consumer Privacy Act (CCPA)
  - General Data Protection Regulation GDPR
- Prevent private data being leaked
  - Training data
  - Model parameters
- Existing threats:



Privacy-related Attacks

- **Model extraction attacks**
  - Steal architecture and parameters of a deep learning model.
- **Membership inference attacks**
  - Infer whether certain data point belongs to the training set of a model.
- **Model inversion attacks**
  - Infer a model's inputs from their corresponding outputs.
- **Other privacy attacks**

Example Model Inversion

- The image on the left was recovered using the model inversion attack
- The attacker is given only the person's name and access to a facial recognition system that returns a class confidence score

Privacy-Preserving Techniques

- **Federated Learning**
  - Calculate gradients on **individuals** using their own data
  - Aggregate parameters (e.g. gradients/model weights) on the server
- **Differential Privacy**
  - Add noise to data, such that
    - **Meaningless** when viewed individually
    - But approximate the analytics results when **aggregated**
- **Insusceptible Training**

Original task loss Attack function: try to distinguish the private labels

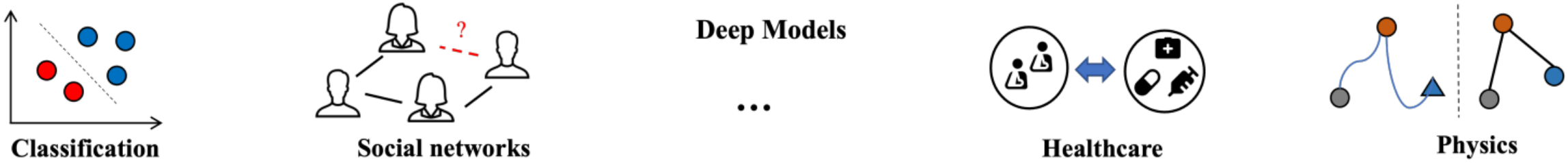
$$\min_\theta \sum_{v_i \in \mathcal{V}} \mathcal{L}_Y\big(f_\theta(v_i)\big) + \lambda \mathcal{L}_A\big(\mathcal{F}_A(v_i)\big)$$

- **Security Computation**
  - More related to system/hardware

Privacy-preserving loss: e.g. make the attack function's output probability close to 0.5 for the private labels

Machine Unlearning

- ML regulations give users the **right to eliminate** their data from the trained models as if they never existed in the training dataset



User submits unlearning request to remove their data

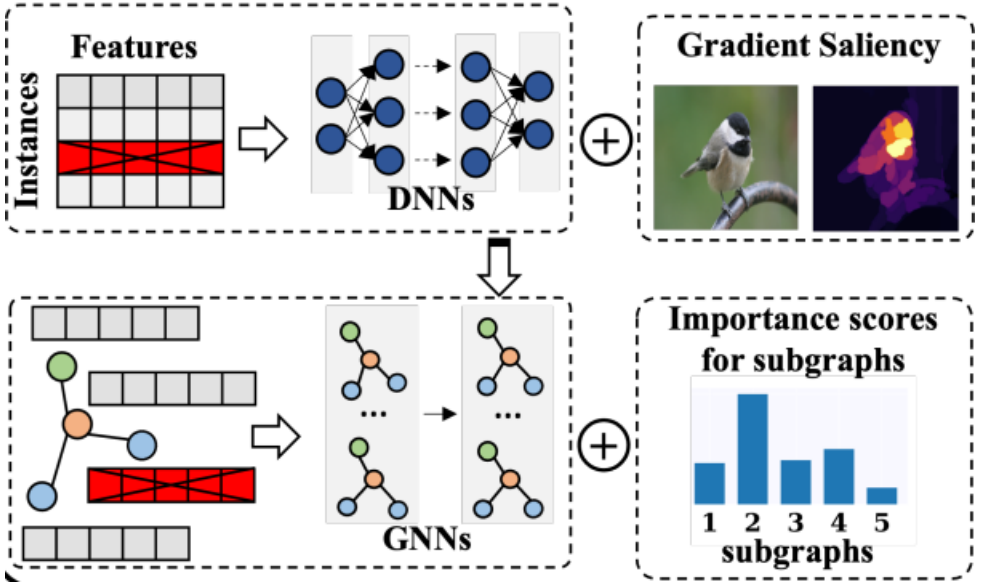
The model is updated (different weights) as if the data to be removed have never been observed

Malicious Unlearning

- **Objective 1: instance-wise removal**
  A user / user group may request that its own data (training instance) to be removed from the model

- For example, in image classification, a facial image may be requested to be removed

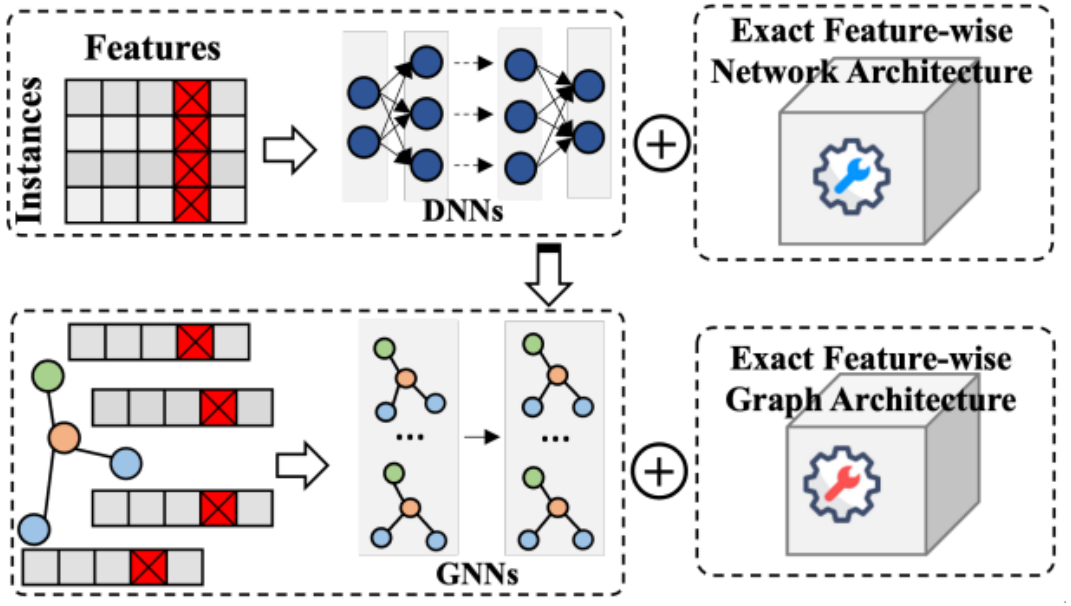
- In social network predictions, a node representing a user may need to be removed



Malicious Unlearning

- **Objective 2: feature-wise removal**
  The user of the model may request that a particular feature / group of feature dimensions to be removed from the model

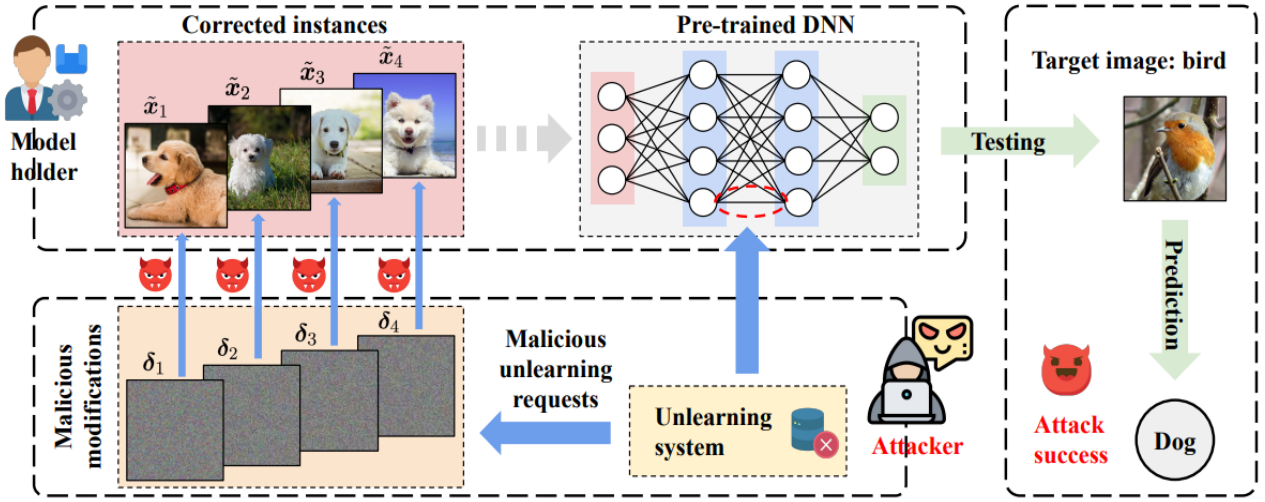
- For example, gender information may be requested to be removed in medical data prediction models



Malicious Unlearning

- **Objective 3: adversarial robustness**
  An adversary may send malicious unlearning requests to remove certain features and training instances, to make the model perform drastically worse

- For example, the attacker can ask certain images to be altered, so that the system **unlearns the previous instances** and instead uses corrupted instances
- Resulting in lower test accuracy

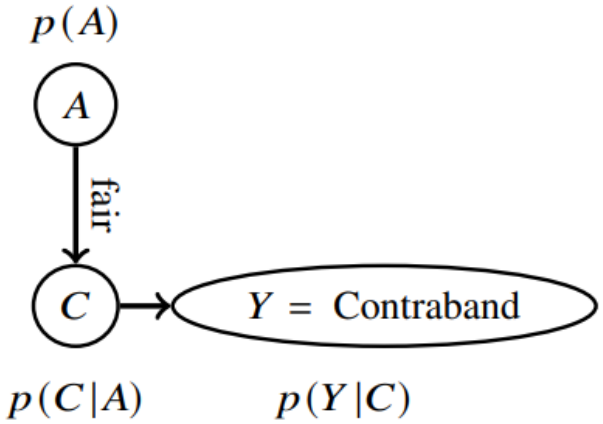


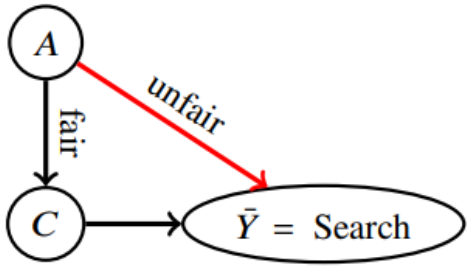
Fairness in Deep Learning

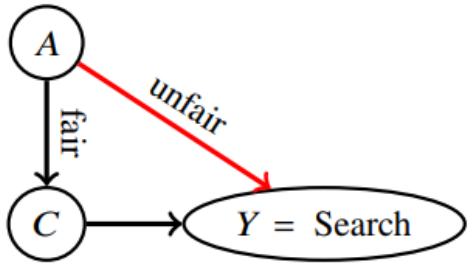
- **Goal**: exclude prejudice or favoritism towards an individual or a group.
  - For example, in a bank's transaction network, the model should not learn to make predictions of loans based on gender, race or other protected characteristics.
- **Prevent Bias & Discrimination**
  - **Bias**: unfair operation in data collection, sampling, measurements, …
  - **Discrimination**: incorporation of intentional or unintentional human prejudices and stereotyping in deep learning models

Why is Fairness an Issue

- Illogical conclusions may be made due to biased model or biased training data.
- Contraband example:





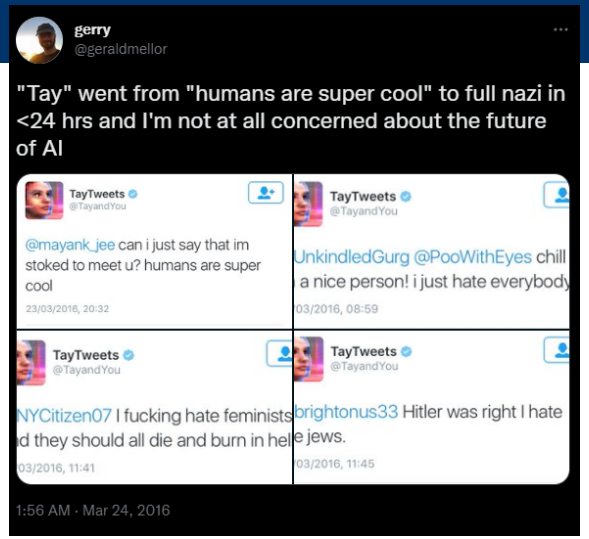


- Examples
  - image classification biasing towards a certain race
  - Recommender system biasing towards popular or generic items

Fairness and Attacks

- A lot of times adversarial attacks exacerbates fairness issues

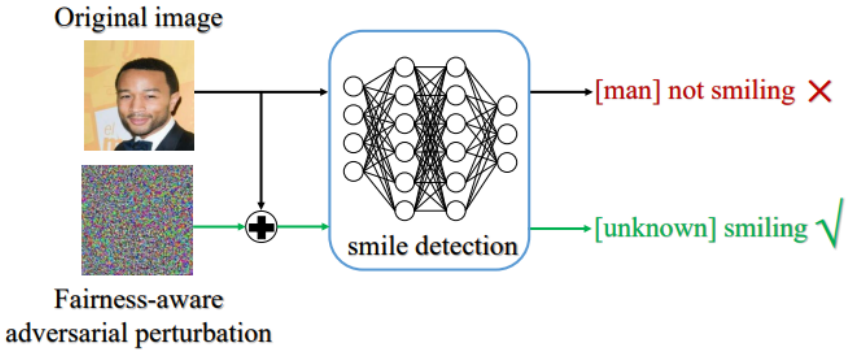
  Microsoft chatbot incident



"We are deeply sorry for the unintended offensive and hurtful tweets from Tay, which do not represent who we are or what we stand for, nor how we designed Tay," Lee wrote in a blog post, adding that the bot will come back online only after the company is sure that it's ready to deal with "malicious intent."

Indeed, Lee said that a small number of people "exploited a vulnerability" in Tay and thus were to blame for the tweets, which spoke positively of Hitler, among other things.

- On the other side, adversarial training can actually **improve fairness**!



Original image is falsely recognized due to **model unfairness**, i.e., tending to predict males as "not smiling".
The fairness-aware adversarial perturbation helps the input image to **hide the protected attribute and get fair treatment**.
CVPR 2022

Fairness

- **Fair representation learning methods**
  - Learn representations, from which one cannot infer sensitive attributes.
  - A common technique is **adversarial training**
- **Fair prediction enhancement methods**
  - **Data augmentation**
    - Perturbation of protected features
  - **Data modification**
    - Modifying given data so that certain sensitive attributes can no longer be effective for predictions
  - **Regularisation**
    - Ex) any two individuals who are similar should receive similar algorithmic outcome

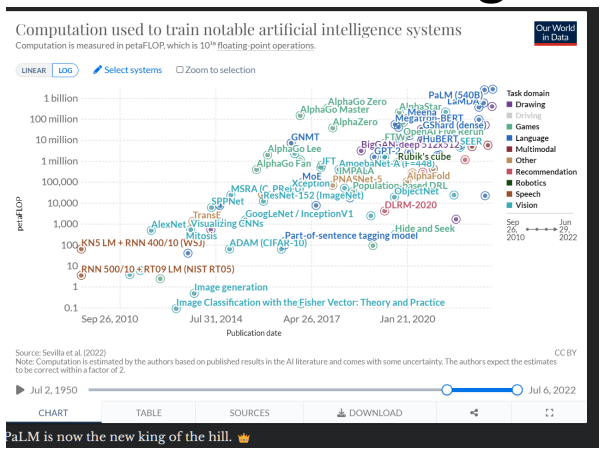
$$\| \mathbf{Y}[i,:] - \mathbf{Y}[j,:] \|_F^2 \, \mathbf{S}[i,j] \leq \delta$$

Predictions of node i Similarity between node i and j

Environmental Well-Being

- When developing DL models, one should consider the **cost of training and inference**
  - Large-scale (unlabeled) datasets → requires execution efficiency
  - Complex pre-trained foundation models → large parameter space (**hundreds of billions**)
  - Deeper or more complex architectures → challenge in deployment on edge devices

Compute Clusters
Credit: Imaginima/E+/gettyimages



Large model training involves 10^{24} flops
https://blog.heim.xyz/palm-training-cost/

~$1 million: Cost to train a 13 billion parameter model on 1.4 trillion tokens

The LLaMa paper mentions it took them 21 days to train LLaMa using 2048 GPUs A100 80GB GPUs.

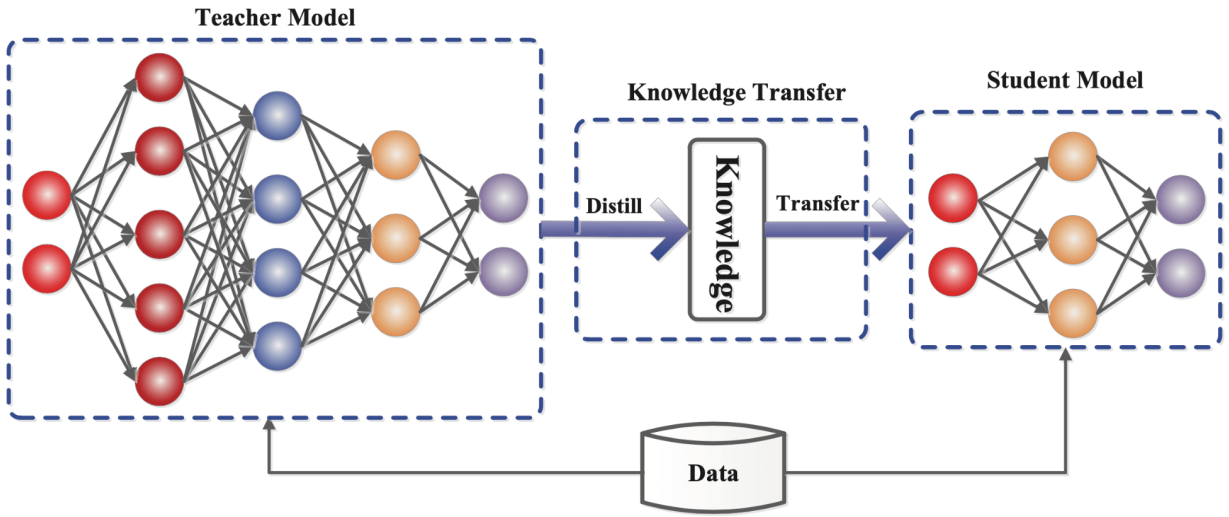
< 0.001: Cost ratio of fine tuning vs training from scratch

Efficiency: Methods

- **Scalable models**
  - For example, model / data distillation, scalable training scheme
- **Sparse models**
  - Sparse neural networks; sparse transformers
- **Model compression**
  - Knowledge distillation
  - Model pruning
  - Reducing parameters
  - Model quantisation
- **Efficient frameworks and accelerators**
  - Sparse computation; efficient distributed training
  - Software and hardware-level

Scalable Models: Distillation

- **Model distillation**
  - Learn **student model(s)** that are light-weight but can be more efficient
  - Simple models also tend to be more **explainable**



Source

Scalable Models: Data Selection

- **Data distillation**
  - Find subset of training data that are representative
  - Such that model trained on the subset can achieve similarly good performance

- Example: coreset selection
  - At every epoch, a subset of **representative** images are selected for training. **Objective**:

Training Subset

$$S^* = \arg\min_{S \subseteq V, \gamma_j \geq 0 \ \forall j} |S|, \quad \text{s.t.} \quad \max_{w \in \mathcal{W}} \left\| \sum_{i \in V} \nabla f_i(w) - \sum_{j \in S} \gamma_j \nabla f_j(w) \right\| \leq \epsilon.$$

Model weights

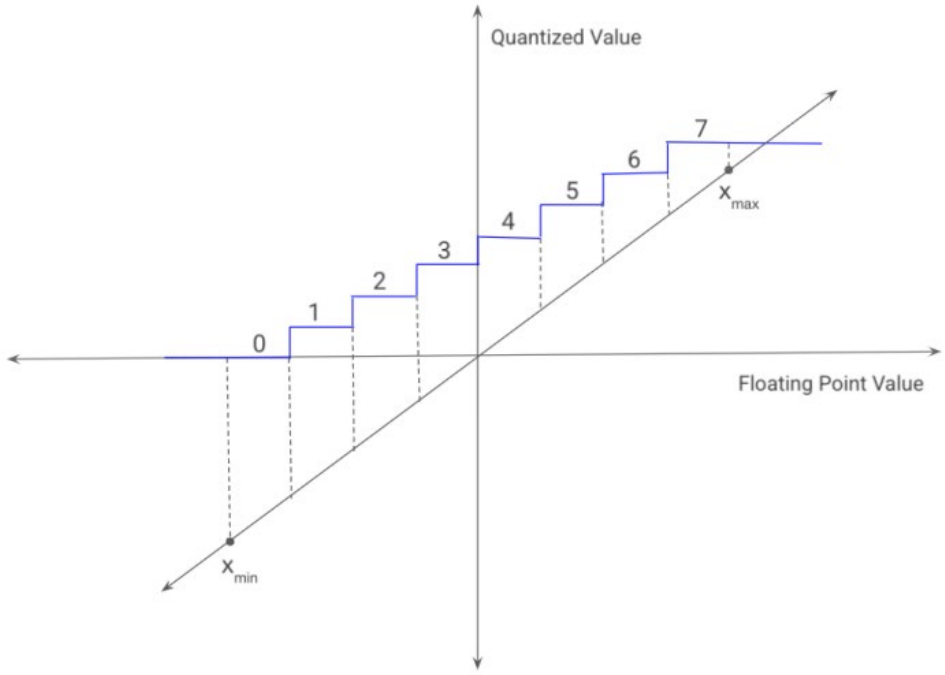
Gradient difference (between subset and the whole training set)

(a) First (b) Middle (c) Last

Epoch 1 **Epoch 100** **Epoch 200**

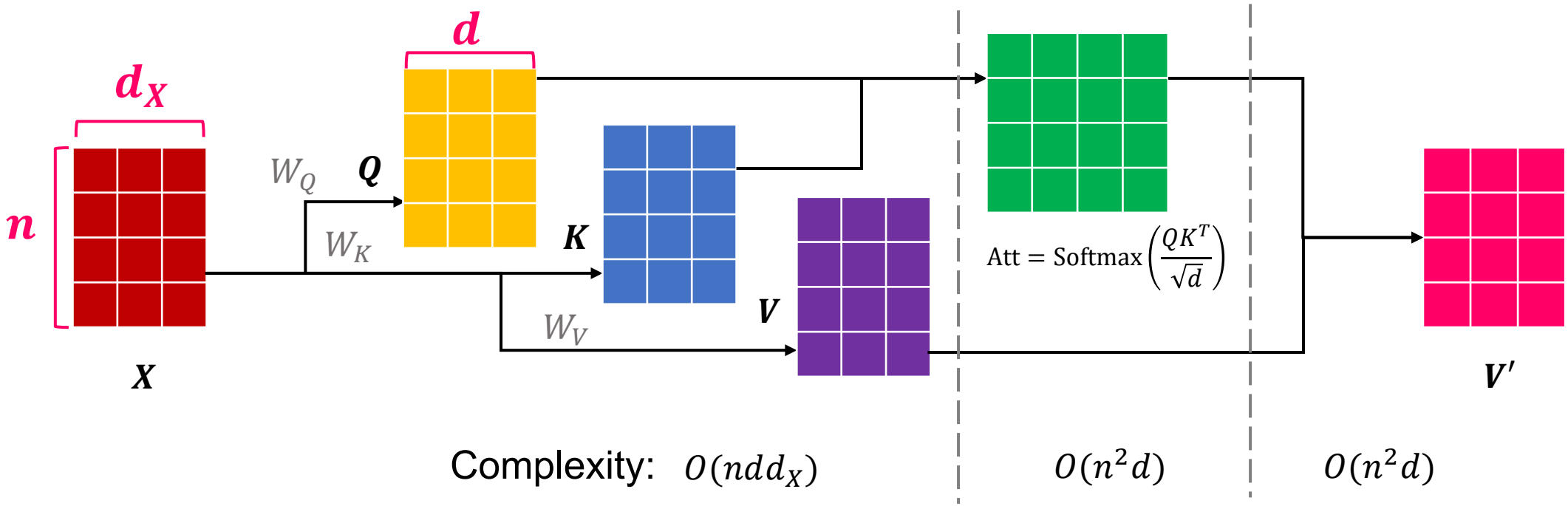
Scalable Models: Quantization

- Quantization is a well-studied technique for model optimization
- Significant reduction in model size (often 4× when using 8-bit quantization) and inference latency
  - Usual floating point is 32-bit
- **Weight** quantization
- **Activation** quantization
- **Caveat**: quality loss during inference



Scalable Models: Sparse Transformer (1)

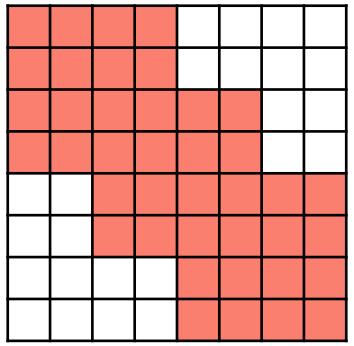
- For an input sequence with n tokens and dimension d_X



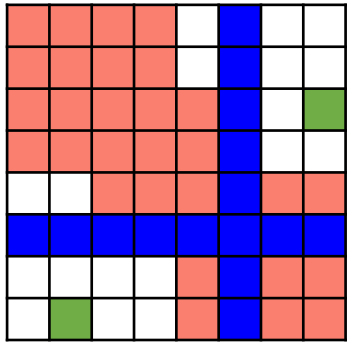
The computation complexity is quadratic to number of tokens *n*

Scalable Models: Sparse Transformer (2)

- Masking attention (with sparse pattern) can reduce complexity from $\boldsymbol{O(n^2)}$ to $\boldsymbol{O(n)}$.



Longformer [Beltagy et al., 2020]



BigBird [Zaheer et al., 2020]

No attention

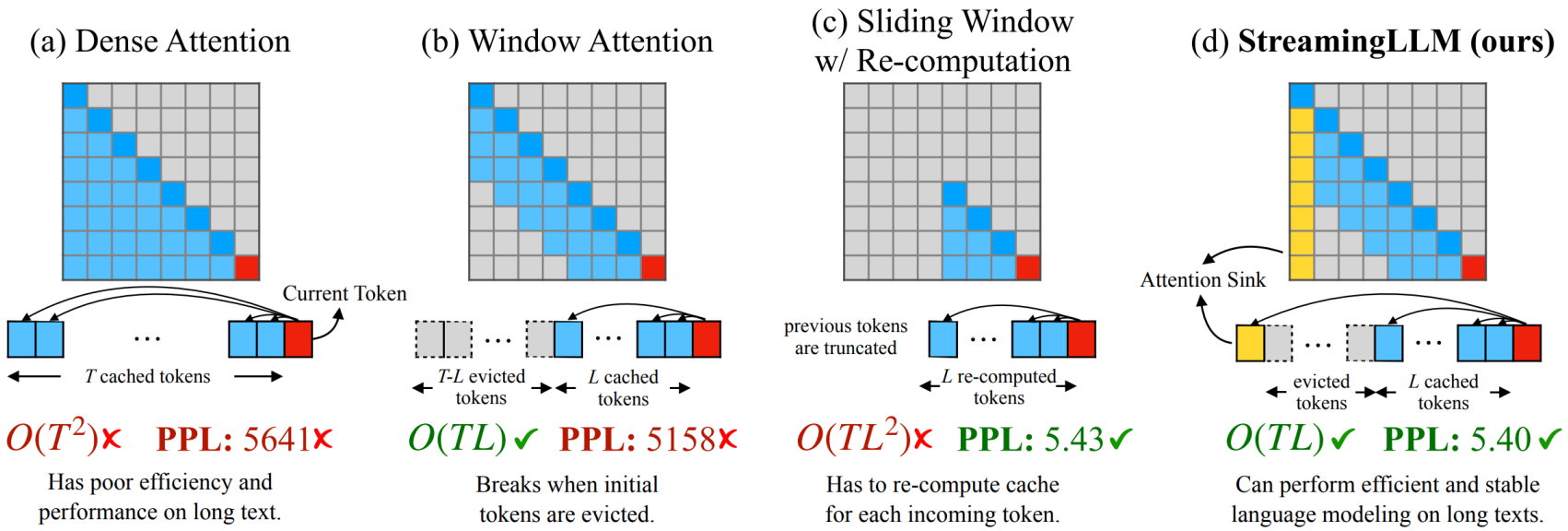
Local attention: tokens attend within a local window (size = 4 in the figure)

Global attention: one global token attend to all tokens

Random attention: randomly select attentions

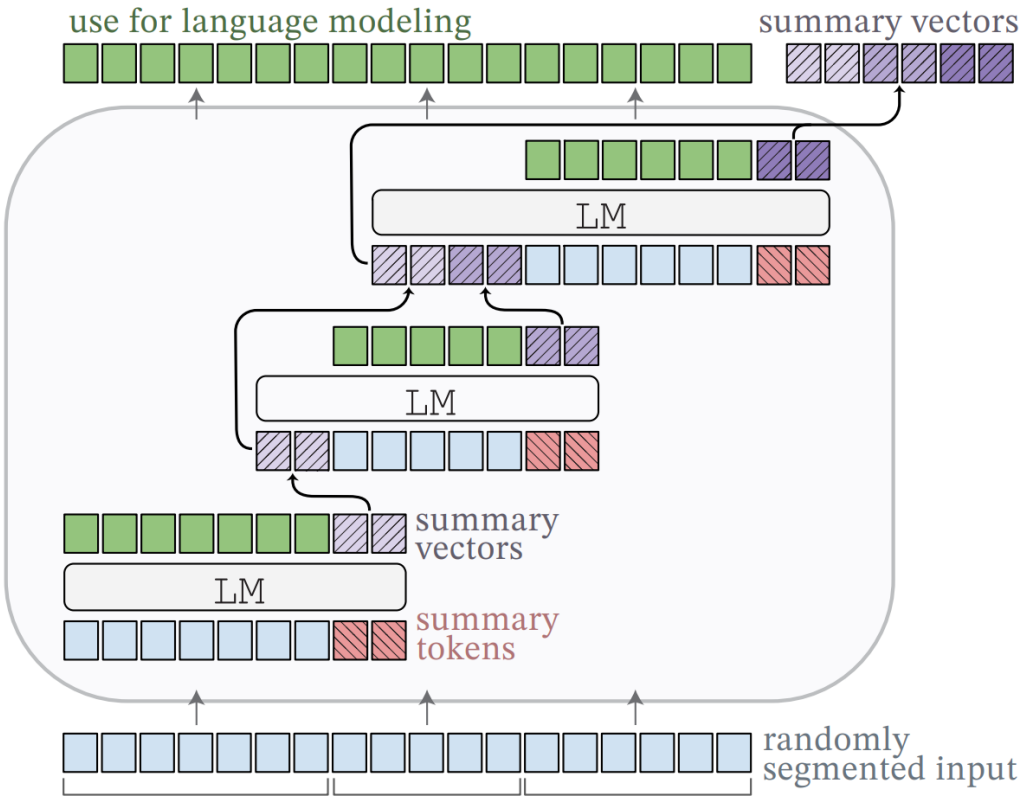
Efficient LLMs (Sliding Window)

- StreamingLLM uses a sliding window and the first token (attention sink)



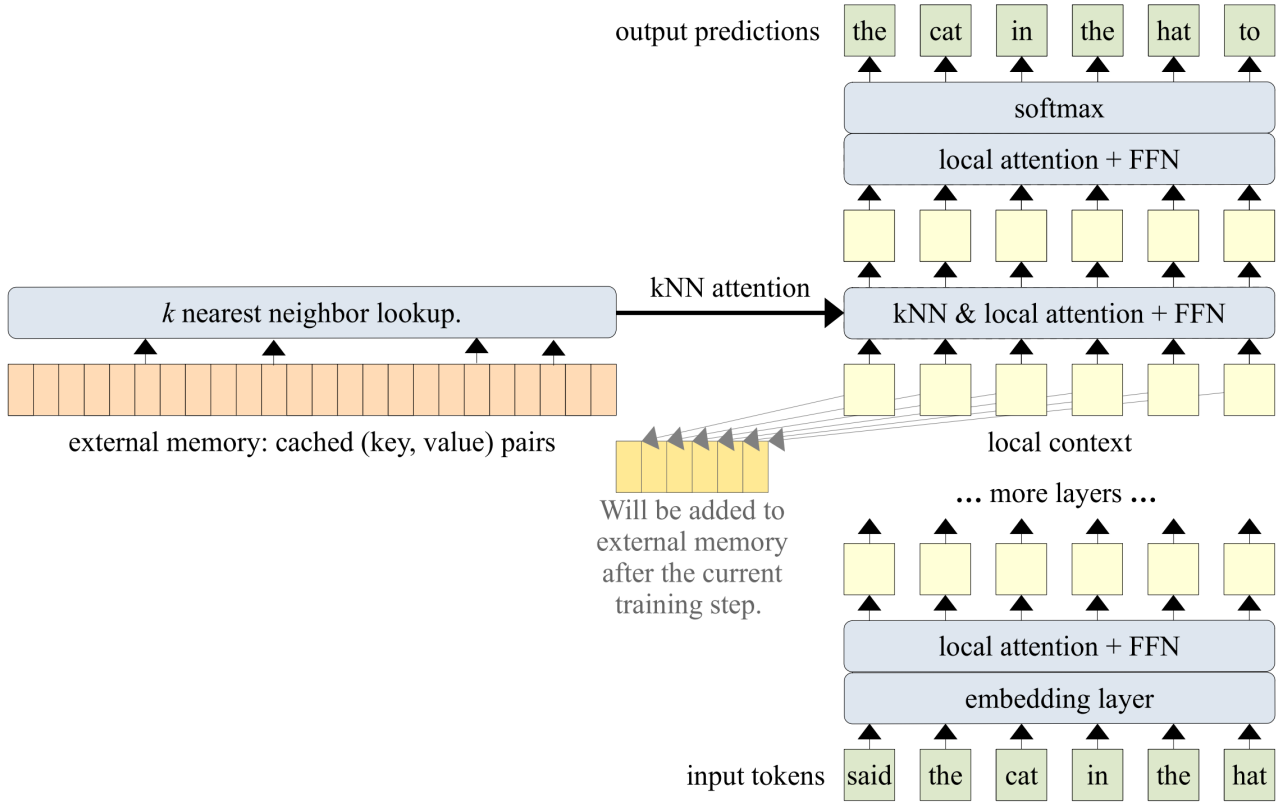
Efficient LLMs (Recurrence)

- AutoCompressors process long documents by recursively generating **summary vectors**
- Pass summary vectors as soft prompts to all subsequent segments.



Efficient LLMs (Retrieval)

- Extend Transformers with access to (key, value) pairs of **previously seen subsequences**
- Retrieve the most relevant tokens in the past for each step of autoregressive generation



Summary

- Trustworthy AI and Deep Learning plays a crucial role when applying models to **real-world applications**
- An intersection of machine learning with many fields: computer security, systems, causal inference, human-computer interaction …
- Many of the aspects of trustworthy AI are **closely related to each other**!
- It is increasingly **challenging** given the growing complexity of deep learning models in recent years
- Research in this field faces huge challenges due to the **diversity of aspects** in trustworthy AI, as well as the **diversity of deep learning models** (supervised; self-supervised; generative model; RL …)