Machine Learning and related Verification Problems

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Adapted from Slides by Prof. Huan Zhang from Spring 2025

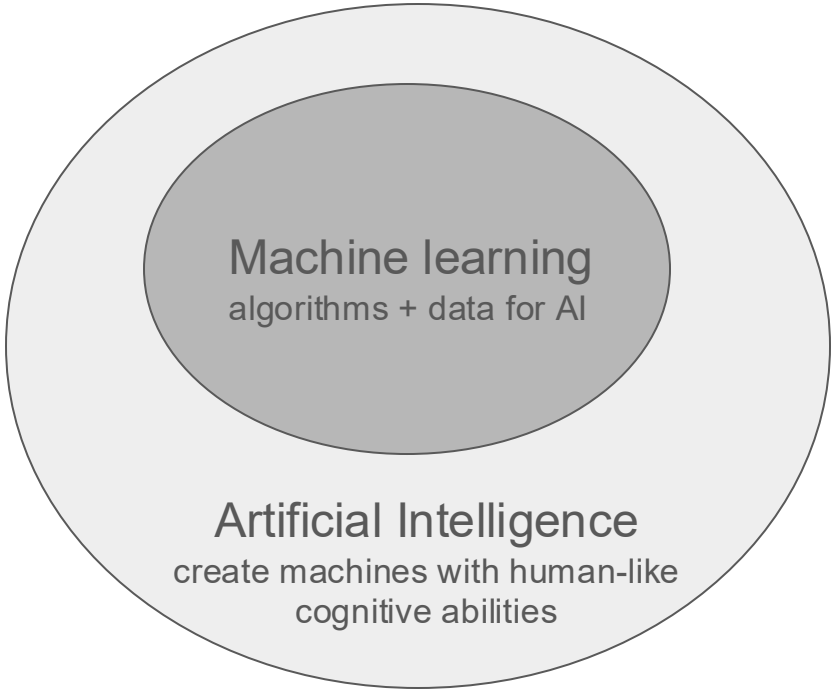
What is machine learning?

"the capacity of computers to **learn** and adapt **without following explicit instructions**, by using **algorithms** and **statistical** models to analyse and infer from patterns in **data**"

-- Oxford English Dictionary

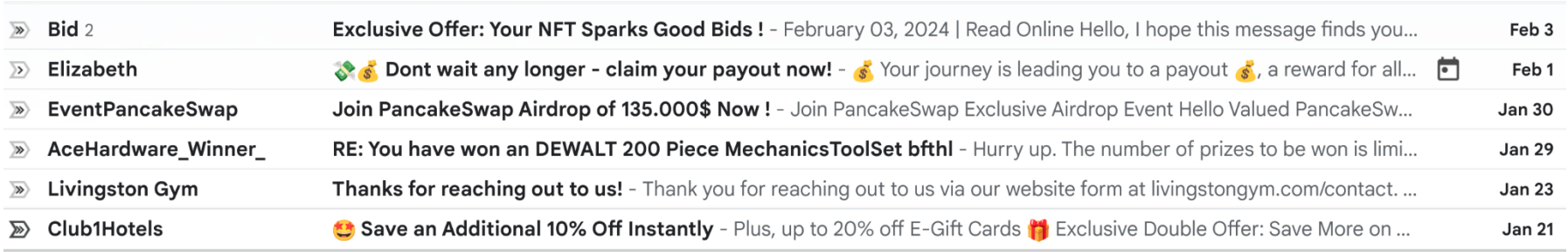
"a field of study in artificial intelligence concerned with the development and study of **statistical algorithms** that can **learn** from **data** and generalize to unseen data, and thus perform tasks **without explicit instructions**."

--Wikipedia



Example: spam email classification

These are what show up in my Gmail “spam” folder:



Bid 2	**Exclusive Offer: Your NFT Sparks Good Bids !** - February 03, 2024 | Read Online Hello, I hope this message finds you...	Feb 3
Elizabeth	💸💰 **Dont wait any longer - claim your payout now!** - 💰 Your journey is leading you to a payout 💰, a reward for all...	Feb 1
EventPancakeSwap	**Join PancakeSwap Airdrop of 135.000$ Now !** - Join PancakeSwap Exclusive Airdrop Event Hello Valued PancakeSw...	Jan 30
AceHardware_Winner_	**RE: You have won an DEWALT 200 Piece MechanicsToolSet bfthl** - Hurry up. The number of prizes to be won is limi...	Jan 29
Livingston Gym	**Thanks for reaching out to us!** - Thank you for reaching out to us via our website form at livingstongym.com/contact. ...	Jan 23
Club1Hotels	🤩 **Save an Additional 10% Off Instantly** - Plus, up to 20% off E-Gift Cards 🎁 Exclusive Double Offer: Save More on ...	Jan 21

TODO: write a program to classify whether an email is a spam email?

Step 1: collect data

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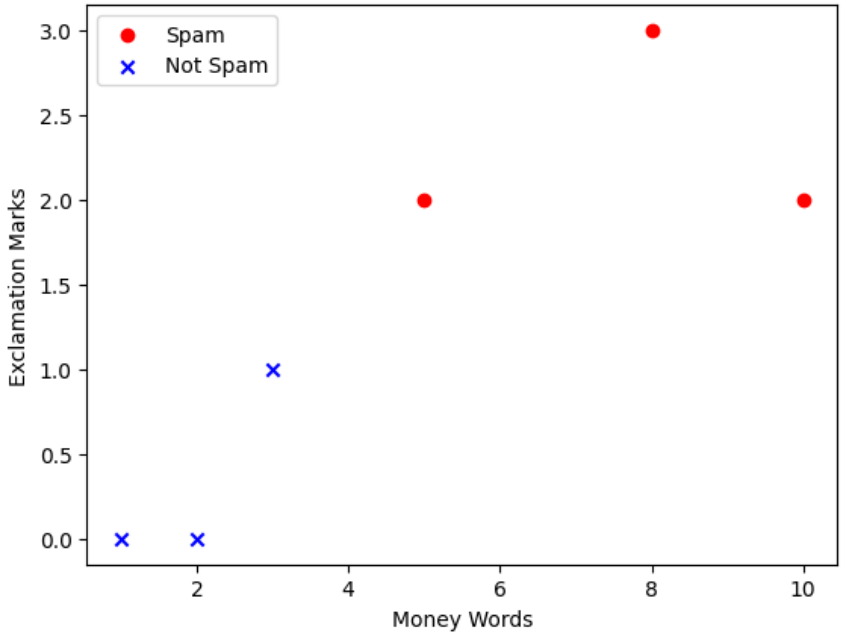
Define some “Features”:
Count of “money words” (“payout”, “$”, “dollar”, “prizes”, “NFT”, …)
Count of exclamation marks

Step 1: collect data

Money Words (x_1)	Exclamation Marks (x_2)	Spam (y)
10	2	1
2	0	0
5	2	1
3	1	0
8	3	1
1	0	0



Non-machine-learning approach: write a program explicitly

Define some "Features":
Count of "money words" ("payout", "$", "dollar", "prizes", "NFT", …)
Count of exclamation marks

```
def is_spam(count_money_word, count_exclamation_mark):
    if a * count_money_word + b *count_exclamation_mark >= threshold:
        return True
    else:
        return False
```

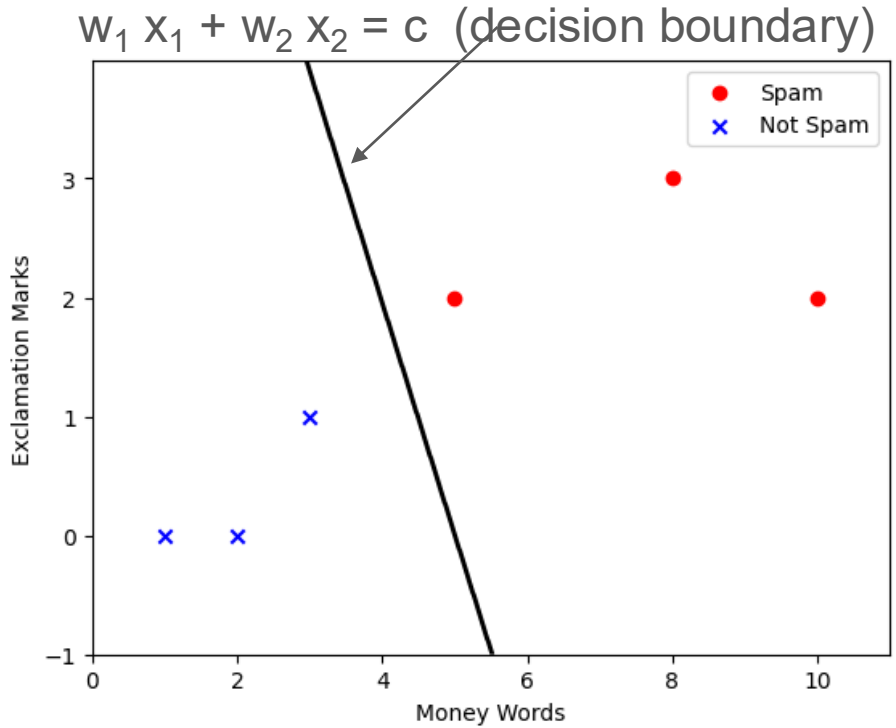
A human programmer chooses `a`, `b`, `threshold`

Step 2: learning from data (model training)

Instead of choosing these parameters, we learn these from data

Algorithms to find this classifier (not discussed in this class):

- Logistic regression
- Support vector machines



Step 3: prediction

Given **model weights** $w \in R^N$

Given **features** of an input $x \in R^N$

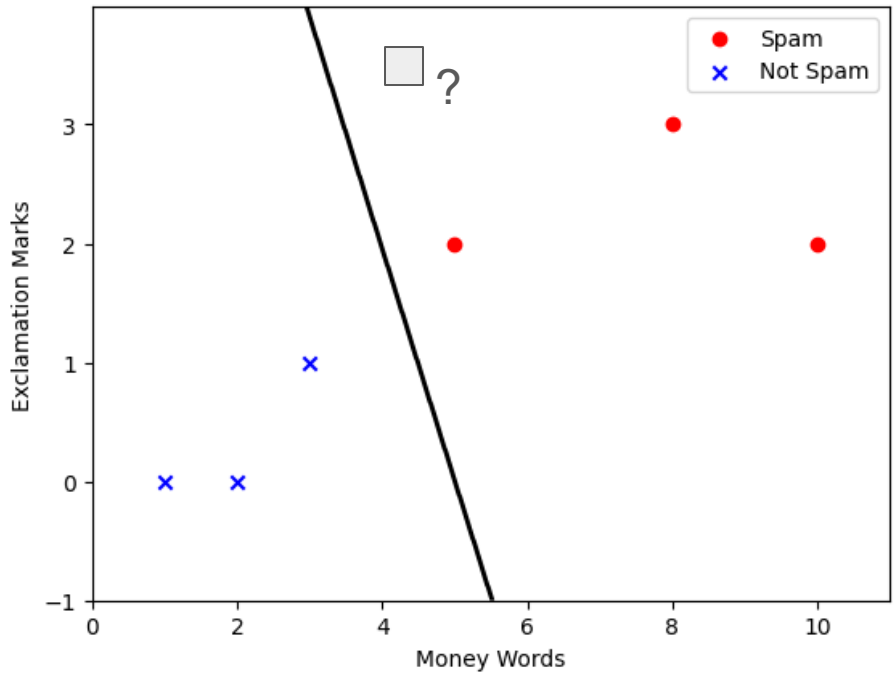
If $w^T x > c$: predict positive class (e.g., spam)

If $w^T x < c$: negative class (e.g., not spam)

Note that by simple transformations on w and x, we just need to check $w'^T x' > 0$ or $w'^T x' < 0$:

$w' = [w_1, \ldots, w_N, -c]$

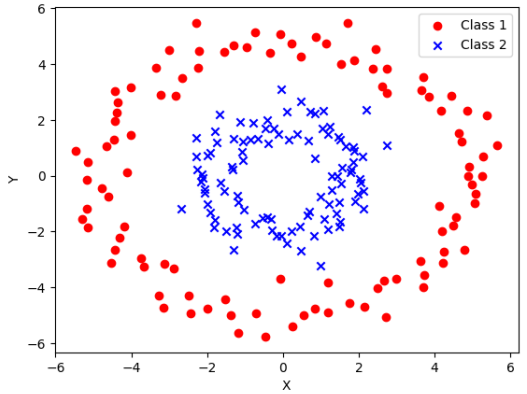
$x' = [x_1, \ldots, x_N, 1]$



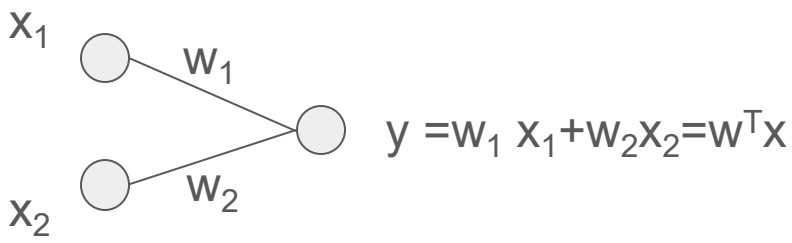
When linear function does not work well

To solve most practical classification problems, non-linear classifiers are needed. Many different approaches:

- Kernel method
- **Neural networks**
- Tree ensembles
- …



Neural Networks: let's just stack linear functions multiple times?



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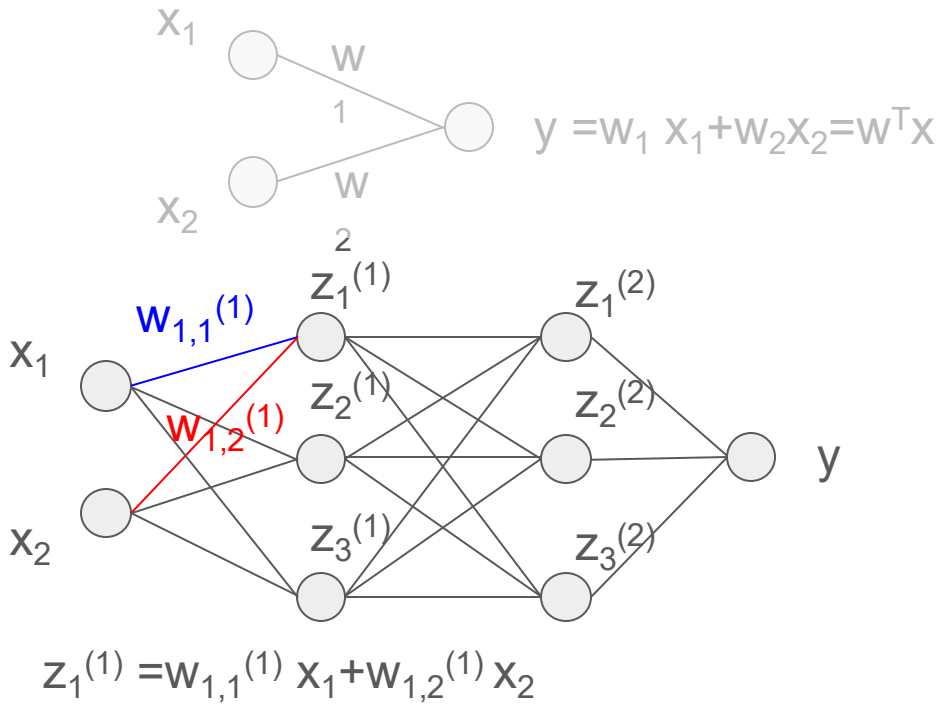
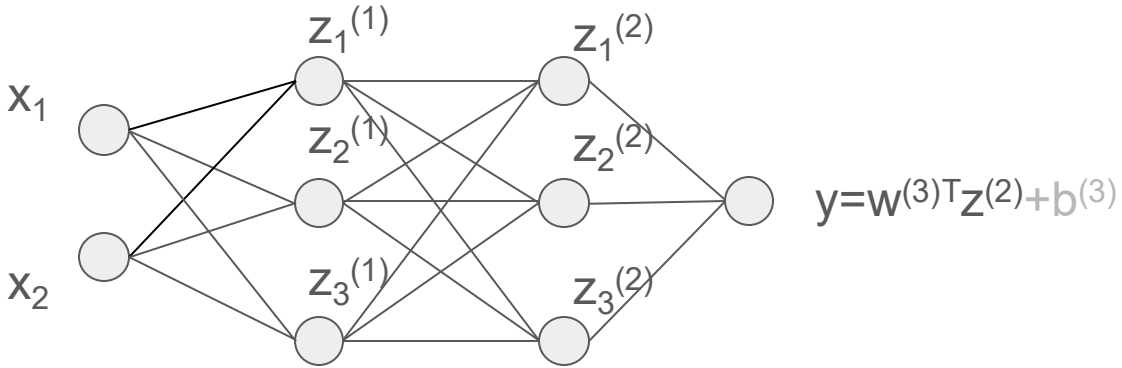


In general we write in matrix form: $z^{(1)}=W^{(1)}x$, $W^{(1)}$ is a 3x2 matrix above

Neural Networks: let's just stack linear functions multiple times?

$z^{(1)}=W^{(1)}x+b^{(1)}$ $z^{(2)}=W^{(2)}z^{(1)}+b^{(2)}$ A bias term can be added

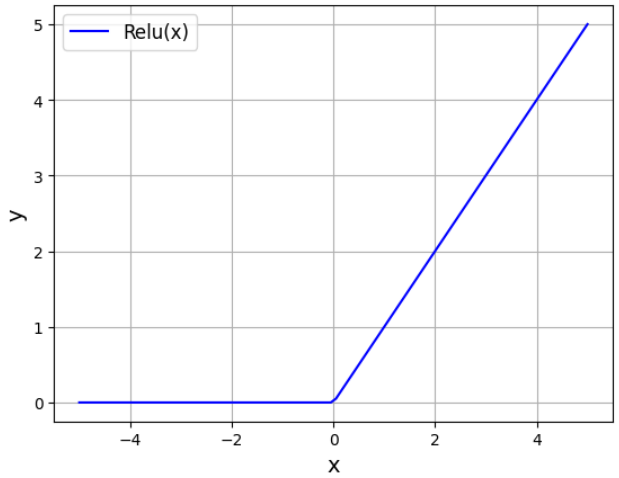


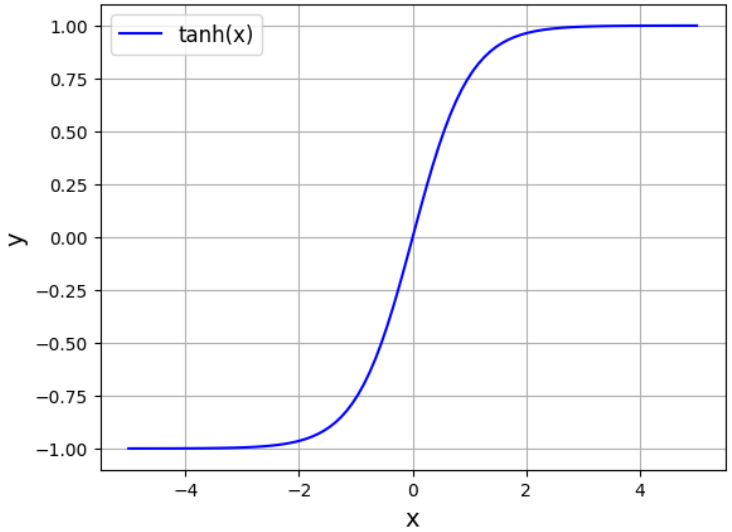
$y=w^{(3)T}z^{(2)}=w^{(3)T}W^{(2)}z^{(1)}=w^{(3)T}W^{(2)}W^{(1)}x$ still a linear function of x!

Must introduce nonlinear functions (“activation” functions)

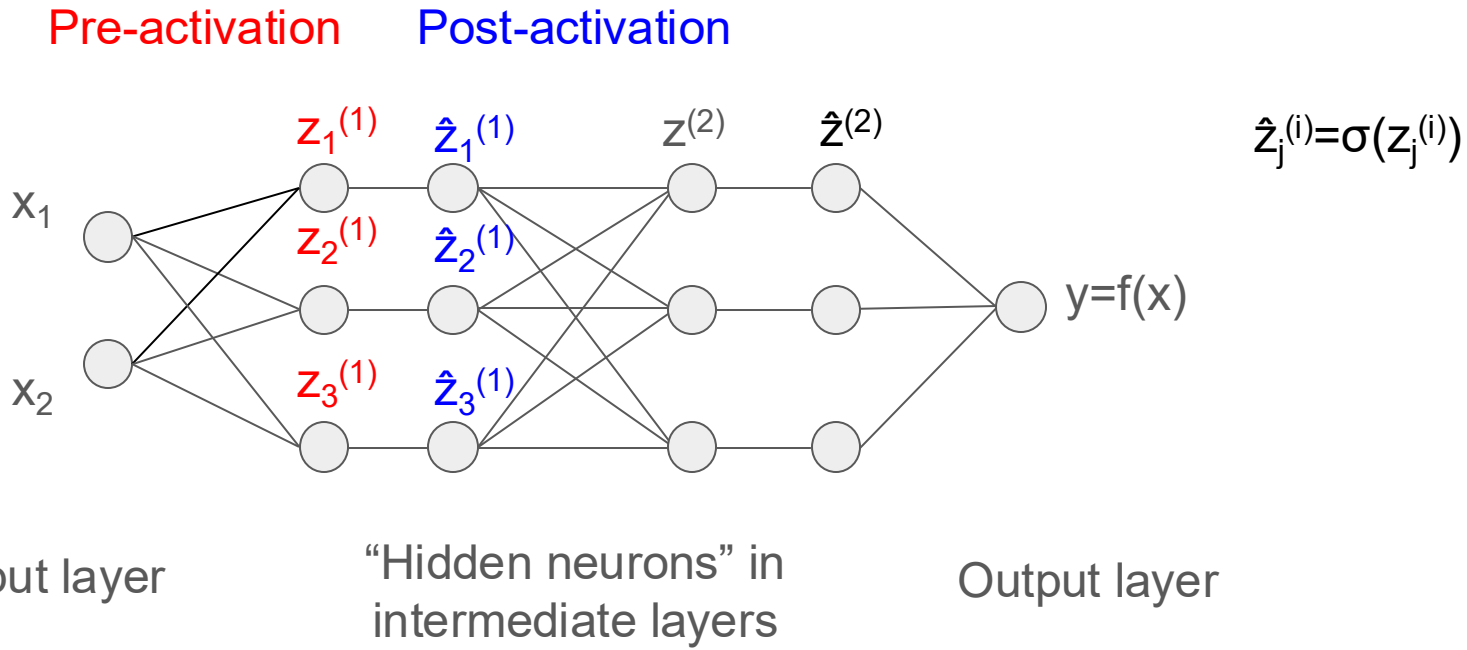
ReLU: rectified linear unit

ReLU(x) := max(0, x)



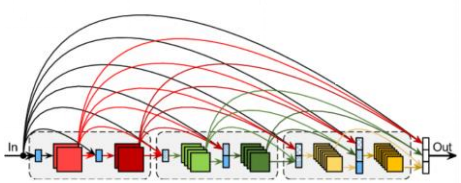


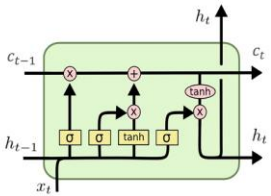
Neural Networks: linear + non-linear layers (multi-layer perceptron)

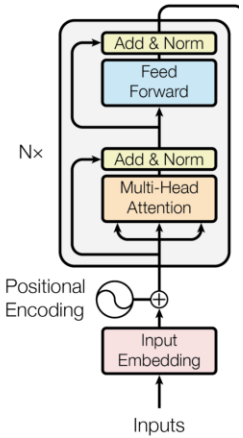


Neural networks are "**Universal approximators**"

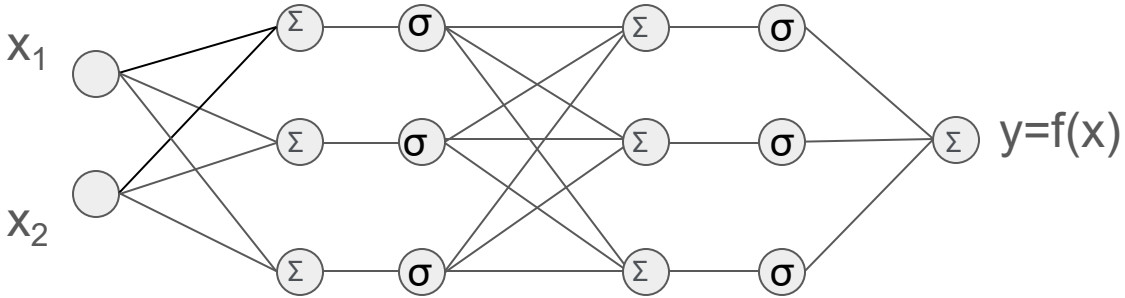
Many other neural network architectures available





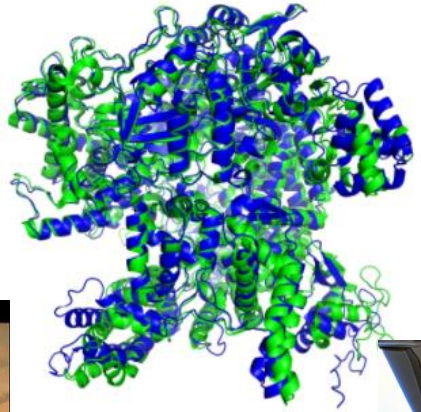


In general, neural networks can be presented as a “computation graph”



Many other neural network architectures available

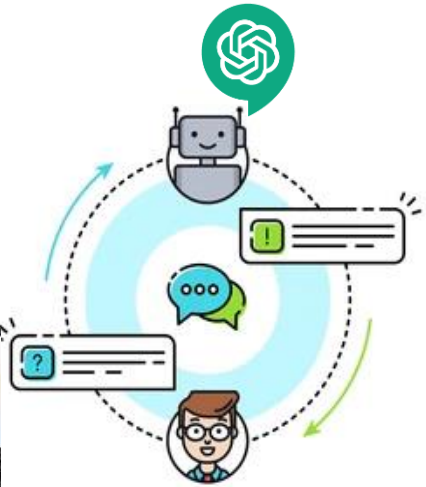
AlphaGo (2020)



AlphaFold (2021)

"A robot manipulating an aircraft"

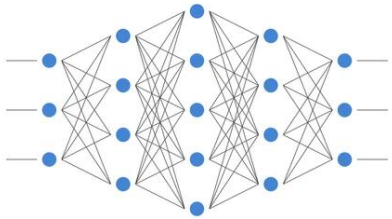
Stable Diffusion (2022)



ChatGPT, LLMs (2023+)

Neural networks have fragile decision boundaries (adversarial inputs)

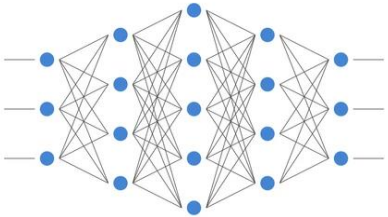
Eykholt et al. 2018



Deep Neural Networks

“Speed limit 45”

Sharif et al. 2018



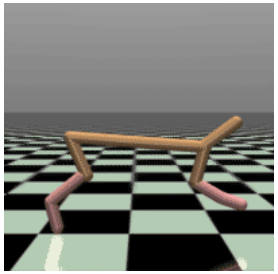
“Brad Pitt”

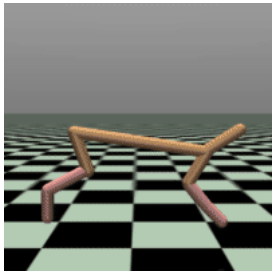
“Adversarial examples”

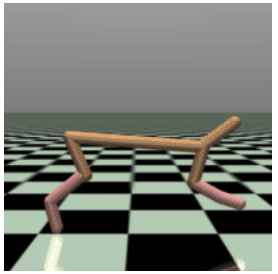
Neural networks are not safe enough for mission-critical tasks

Neural network controlled robots (simulated) + adversarial sensor noise

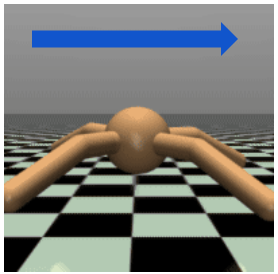
HalfCheetah

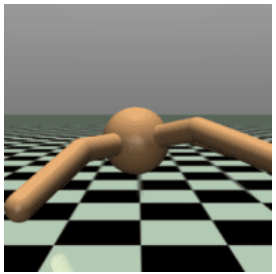


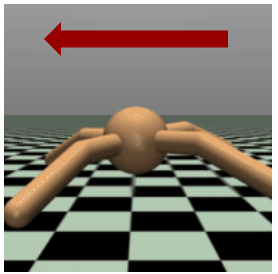




Ant







No attack

MAD attack

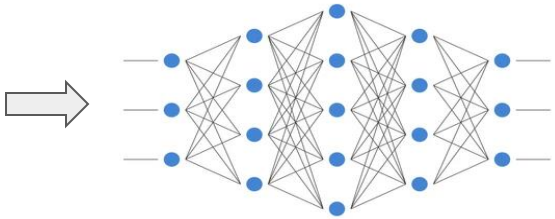
Optimal attack

[Z*C*XLLBH **NeurIPS 2020**]

[Z*CBH **ICLR 2021**]

Formal verification of neural networks: robustness verification

Eykholt et al. 2018



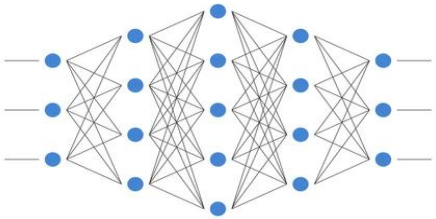
STOP 😀

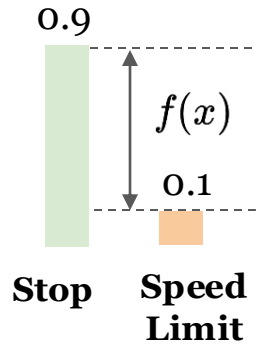
Speed limit 😈

Goal: **prove** adversarial examples do *not* exist!

Formal verification of neural networks: robustness verification

Attacker may put *anything* here



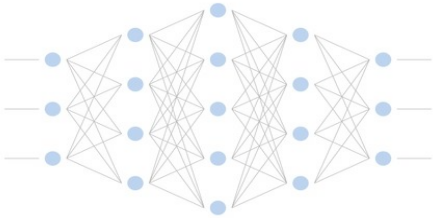


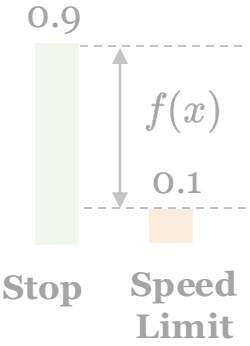
Score for each label

$$f(x) > 0 \Rightarrow \text{No adversarial examples}$$

Formal verification of neural networks: robustness verification

Attacker may put *anything* here





Score for each label

Just an **example** of how $f(x)$ can be defined

Just an **example** of verification problem

$$\text{Prove:} \quad \forall x \in \mathcal{S},\ f(x) > 0$$

$\mathcal{S}$ = all possible pixel perturbations

$x_1 \in \mathcal{S}$

$x_2 \in \mathcal{S}$

$x_3 \in \mathcal{S}$

...

For multi-class cases, we can define multiple $f_i(x)$, one for each class

Verification example: ACAS Xu system

3MB DNN represents a large (2GB) lookup table for collision avoidance of unmanned aircraft

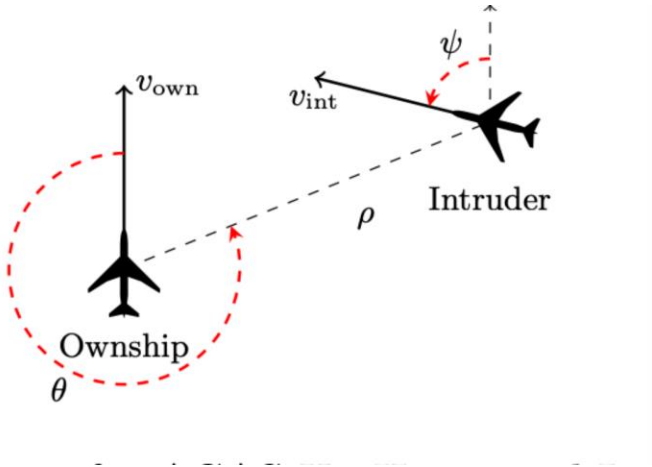
Input: $x \in \mathbb{R}^5$, x = (d, θ, ψ, v_own, v_in)
d: Distance; θ: relative angle; ψ: relative heading; v_{own}, v_{in}: speeds

Output $y \in \mathbb{R}^5$: Clear of Conflict (COC), or advisory weak/strong left/right. Five scores for these actions:

y_0: COC, y_1: weak left at 1.5 deg/s

y_2: strong left at 3.0 deg/s

y_3: weak right y_4: strong right



"Neural Network Verification Methods for Closed-Loop ACAS Xu Properties", Bak et. al.

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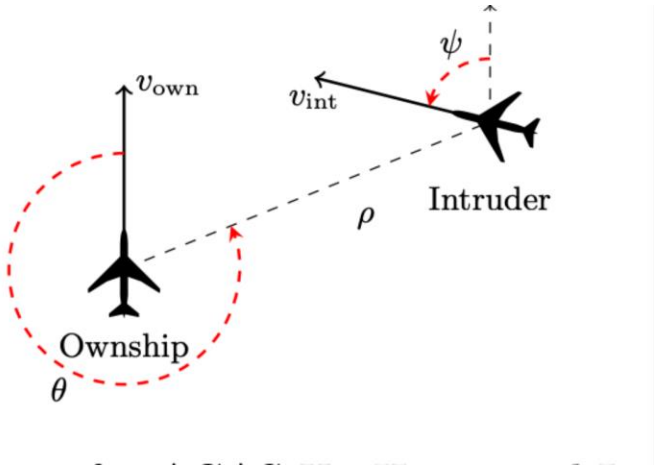
d: Distance; θ: relative angle; ψ: relative heading; v_{own}, v_{in}: speeds

Output $y \in \mathbb{R}^5$: Clear of Conflict (COC), or advisory weak/strong left/right.

Requirement: E.g. If the intruder is far then the score for COC should be above some threshold

$\forall x \in \mathbb{R}^5$, $d \geq 55947$, $v_{own} \geq 1145$, $v_{in} \leq 60$
Prove: $y_0 > 1500$



"Neural Network Verification Methods for Closed-Loop ACAS Xu Properties", Bak et. al.

Verification example: Neural Network Controlled Systems

Controller input x: angle θ, angular velocity $\dot{\theta}$

Controller output: torque u applied to pendulum

Requirement: the controller can stabilize the pendulum ($\theta = \dot{\theta} = 0$) eventually

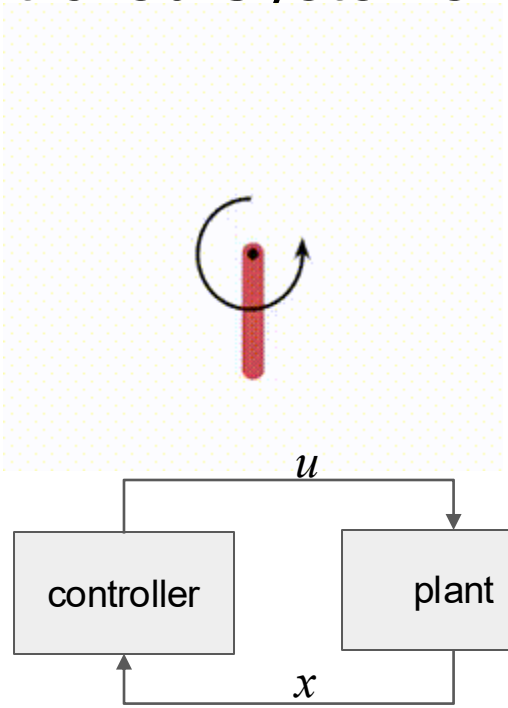
Need to use Lyapunov theory to verify that the "energy" of the system keeps decreasing over time.

$$V(x_{t+1}) - V(x_t) \leq 0, \quad \text{for all} \quad x_t \in \mathcal{S}$$
$$x_{t+1} = f(x_t, \pi(x_t))$$

Physical system dynamics

Controller NN

"Region of attraction"



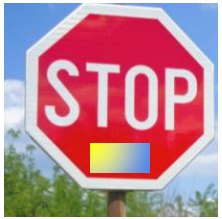
"Lyapunov-stable Neural Control for State and Output Feedback: A Novel Formulation", Yang et. al.

"Neural lyapunov control", Chang et al.

Verification of neural networks

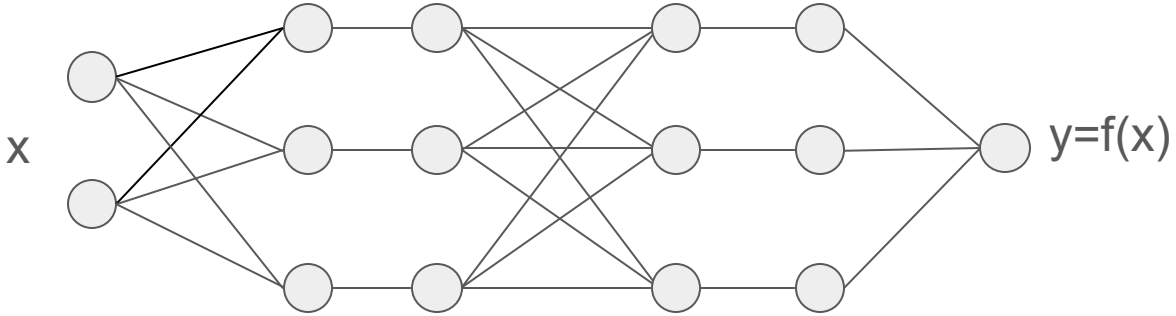
For all desired input x (image, text, sensor readings, etc), f(x) meets some conditions

Satisfiability problem: does there *exist* x, such that f(x) does not meet these conditions?



$$x \in S \ \wedge \ y \leq 0 \ \wedge \ y = f(x)$$

Can also be multiple conditions, like in some ACAS Xu requirements and robustness verification of multi-class classification



Verification of neural networks

Does there *exist* x, such that:

$$x \in S \ \wedge \ y \leq 0 \ \wedge \ y = f(x)$$

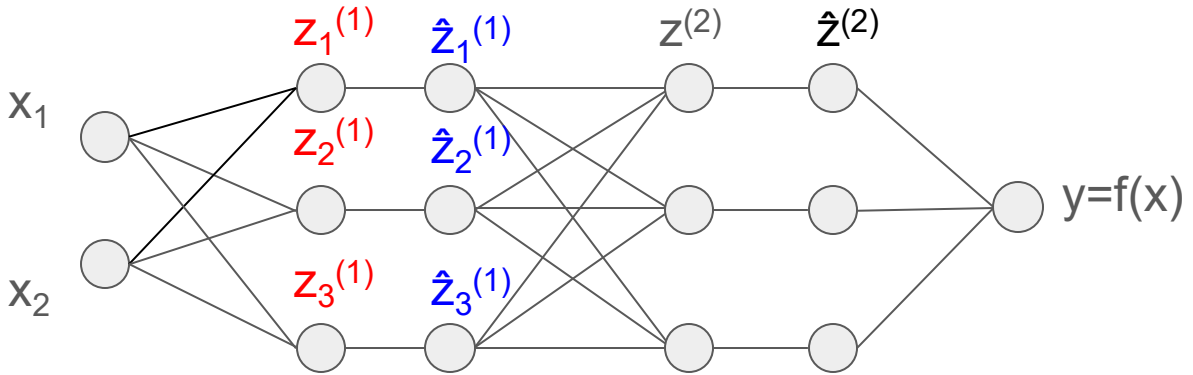
$x \in S$ condition is easy to handle for box constraints:

$$x_i \leq u_i \ \wedge x_i \geq l_i$$

How to handle $y = f(x)$?

Verification of neural networks

How to handle the constraint y = f(x)?

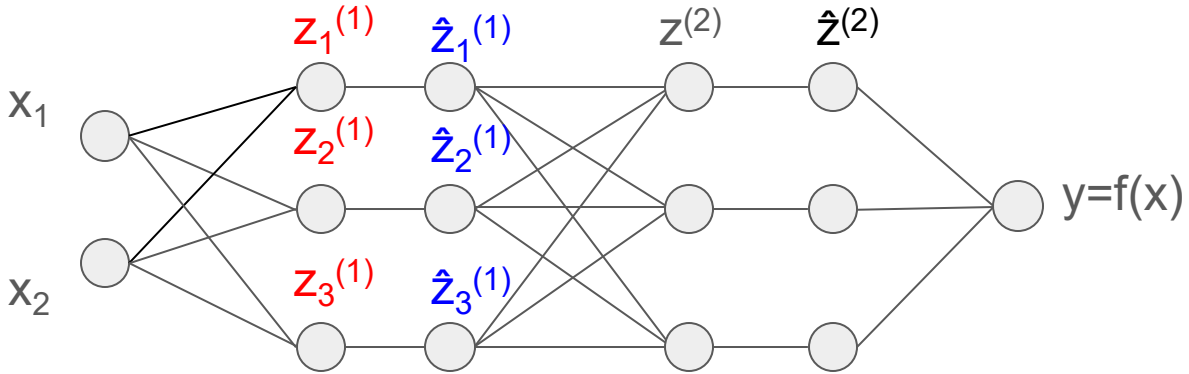


$\hat{z}_j^{(i)}=\sigma(z_j^{(i)})$

Linear layers: $z^{(1)} = W^{(1)} x$ $z^{(2)} = W^{(2)} \hat{z}^{(1)}$ $y = w^{(3)T} \hat{z}^{(2)}$

Verification of neural networks

How to handle the constraint y = f(x)?

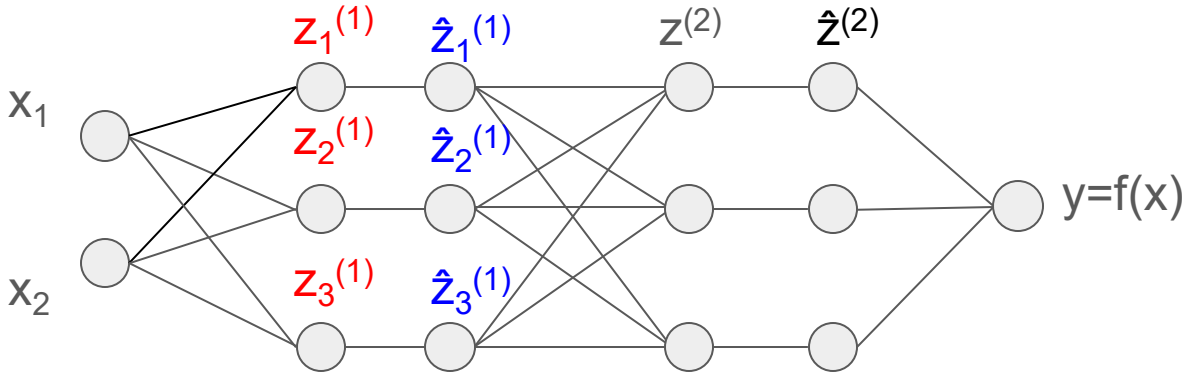


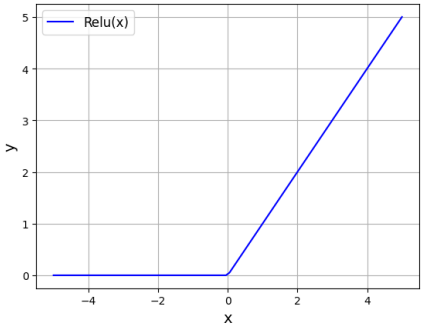
Linear layers: $z^{(1)} = W^{(1)} x$ $z^{(2)} = W^{(2)} \hat{z}^{(1)}$ $y = w^{(3)T} \hat{z}^{(2)}$

Directly copy all the linear equality constraints to the SMT formulation.

Verification of neural networks

How to handle the constraint y = f(x)?





$\hat{z}_j^{(i)}=\text{ReLU}(z_j^{(i)}) \Rightarrow (z_j^{(i)} \geq 0 \wedge \hat{z}_j^{(i)}= z_j^{(i)}) \vee (z_j^{(i)} < 0 \wedge \hat{z}_j^{(i)}= 0)$

Verification of neural networks

Satisfiability problem: $\exists\ x \in S\ \wedge\ y \leq 0\ \wedge\ y = f(x)$

$x_i \leq u_i\ \wedge x_i \geq l_i$ for each dimension of x

$((z_j^{(i)} \geq 0 \wedge \hat{z}_j^{(i)} = z_j^{(i)})\ \vee\ (z_j^{(i)} < 0 \wedge \hat{z}_j^{(i)} = 0))$ for each ReLU neuron

$z_1 = W^{(1)} x \quad \wedge \quad z^{(2)} = W^{(2)} \hat{z}^{(1)} \quad \wedge \quad y = w^{(3)T} \hat{z}^{(2)} \quad \wedge \quad y \leq 0$

Add all clauses to the formula and solve using DPLL(T) with **Linear Real Arithmetic**.

In general this is very slow!

Summary

- Machine learning models such as neural networks are becoming important components in CPS for perception and control
- Neural networks are easy to train from data using gradient methods and they make it unnecessary to write rules by hand
- On the other hand, so trained NNs have fragile decision boundaries.
- **NN verification question** asks whether there are any (small) perturbations of an input x that change the output f_NN(x) of the NN? If such perturbations exist they show fragility, a.k.a., adversarial examples
- NN verification problem can be cast as an SMT problem, but this will be slow because of many branches induced by ReLU type functions
- Checkout **verification of neural networks competitions** (VNN-COMP) for more examples of verification problems https://sites.google.com/view/vnn2023
- **Reading**:
  - https://arxiv.org/pdf/1711.07356.pdf
  - https://arxiv.org/pdf/1711.00851.pdf