



# Deep Learning Limitations and New Frontiers

Ava Soleimany

MIT 6.S191

January 26, 2022



# T-shirts! Today!



# Lecture Schedule



## Intro to Deep Learning

### Lecture 1

Jan. 24, 2022

[Slides] [Video] coming soon!



## Deep Sequence Modeling

### Lecture 2

Jan. 24, 2022

[Slides] [Video] coming soon!



## Deep Computer Vision

### Lecture 3

Jan. 25, 2022

[Slides] [Video] coming soon!



## Deep Generative Modeling

### Lecture 4

Jan. 25, 2022

[Slides] [Video] coming soon!



## Limitations and New Frontiers

### Lecture 5

Jan. 26, 2022

[Slides] [Video] coming soon!



## Uncertainty in Deep Learning

### Lecture 6

Jan. 26, 2022

[Info] [Slides] [Video] coming soon!



## Speech Recognition

### Lecture 7

Jan. 27, 2022

[Info] [Slides] [Video] coming soon!



## Guest Lecture

### Lecture 8

Jan. 27, 2022

[Info] [Slides] [Video] coming soon!



## Autonomous Driving with LiDAR

### Lecture 9

Jan. 28, 2022

[Info] [Slides] [Video] coming soon!



## Intro to TensorFlow; Music Generation

### Software Lab 1

[Code] coming soon!



## De-biasing Facial Recognition Systems

### Software Lab 2

[Paper] [Code] coming soon!



## Learning End-to-End Self-Driving Control

### Software Lab 3

[Code] coming soon!



## Final Project

### Work on final projects



## Project Competition

### Project pitches and final awards!



- Lab submission: 1/27/22
- Paper review: 1/28/22
- Final projects: 1/28/22

# Labs and Prizes

Lab 1: Music Generation



Beats Headphones

Lab 2: Computer Vision



24" HD Display Monitor

Lab 3: Reinforcement Learning



Quadcopter Drone



+ Deploy your model on  
a real self-driving car



Lab submission: 1/27/22

# Final Class Project

## Option I: Proposal Presentation

- At least 1 registered student to be prize eligible
- Present a novel deep learning research idea or application
- 3 minutes (strict)
- Presentations on Friday, Jan 28
- Submit groups by Wed 1/26 11:59pm ET to be eligible
- Submit slides by Thu 1/27 11:59pm ET to be eligible
- Instructions: [bit.ly/3qOQEug](https://bit.ly/3qOQEug)

- Judged by a panel of judges
- Top winners are awarded:



NVIDIA 3080 GPU



4x Smartwatches



3x Display Monitors

# Final Class Project

## Option 1: Proposal Presentation

- At least 1 registered student to be prize eligible
- Present a novel deep learning research idea or application
- 3 minutes (strict)
- Presentations on Friday, Jan 29
- Submit groups by Wednesday 11:59pm ET to be eligible
- Submit slides by Thursday 11:59pm ET to be eligible
- Instructions:

## Option 2: Write a 1-page review of a deep learning paper

- Grade is based on clarity of writing and technical communication of main ideas
- Due **Fri Jan 28 3:59pm ET**

# Up Next: Guest Lectures



Omer Keilaf

Amir Day

Innoviz



Jasper Snoek

Google



Anima Anandkumar

NVIDIA  
Caltech



NVIDIA.®



Miguel Jette

Jenny Drexler

RevAI



So far in 6.S191...

## 'Deep Voice' Software Can Clone Anyone's Voice With Just 3.7 Seconds of Audio

Using snippets of voices, Baidu's 'Deep Voice' can generate new speech, accents, and tones.



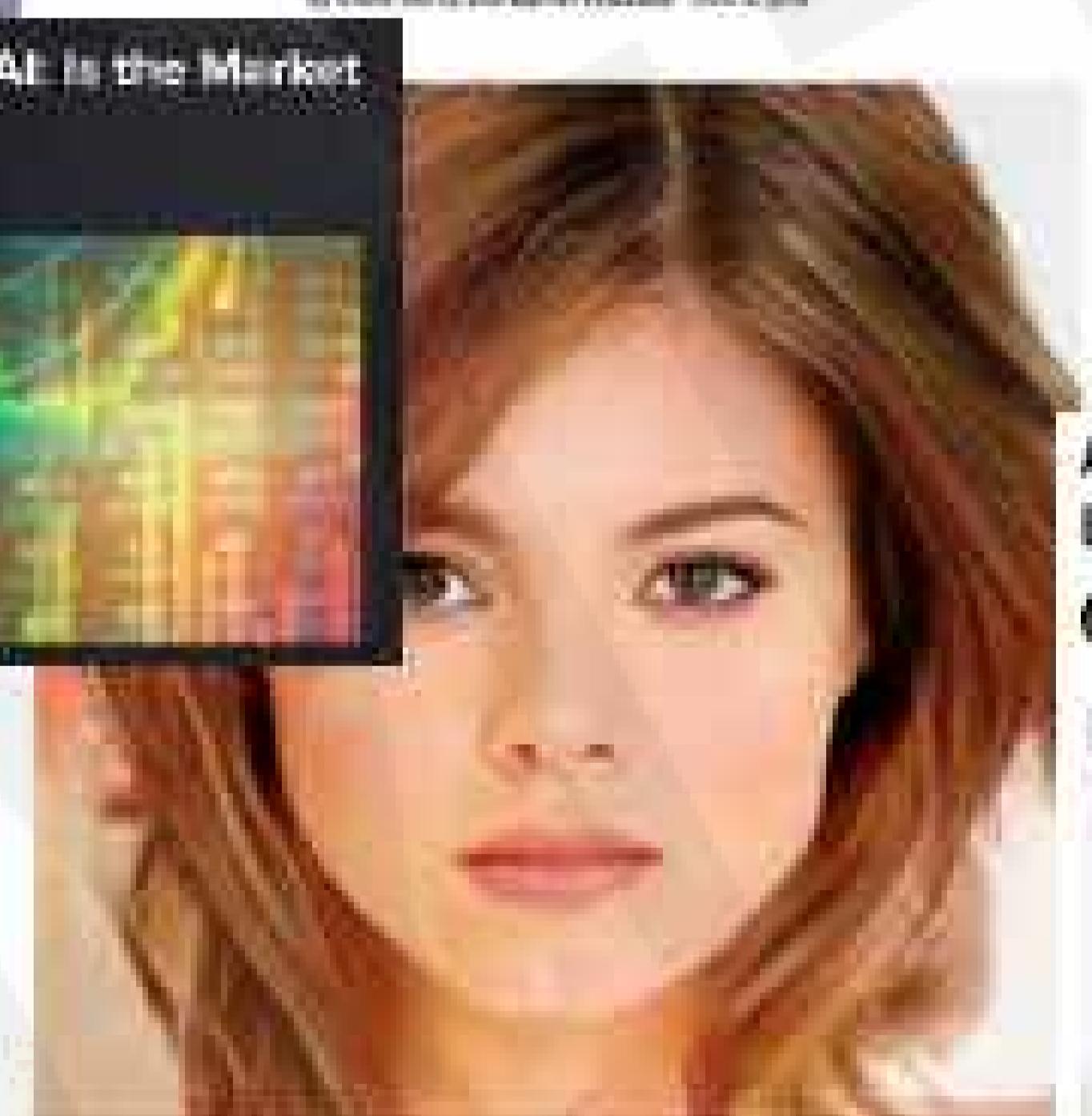
## 'Creative' AlphaZero leads way for chess computers and, maybe, science

Former chess world champion Gary Kasparov likes what he sees of computer that could be used to find cures for diseases



## How an A.I. 'Cat-and-Mouse Game' Generates Believable Fake Photos

By LISA MELLOWS | Jan 26, 2017 | 11:00 AM ET



## Google's DeepMind aces protein folding

By Robert E. Service | Dec. 6, 2016 | 11:00 PM

# The Rise of Deep Learning

Let There Be Sight: How Deep Learning Is Helping the Blind 'See'



## With DEEPMIND'S STARCRAFT TRIUMPH FOR AI



## Neural networks everywhere

New chip reduces neural networks' power consumption by up to 95 percent, making them practical for battery-powered devices.

By KENYON MILLER | Digital News | MIT News Office



## Automation And Algorithms: De-Risking Manufacturing With Artificial Intelligence

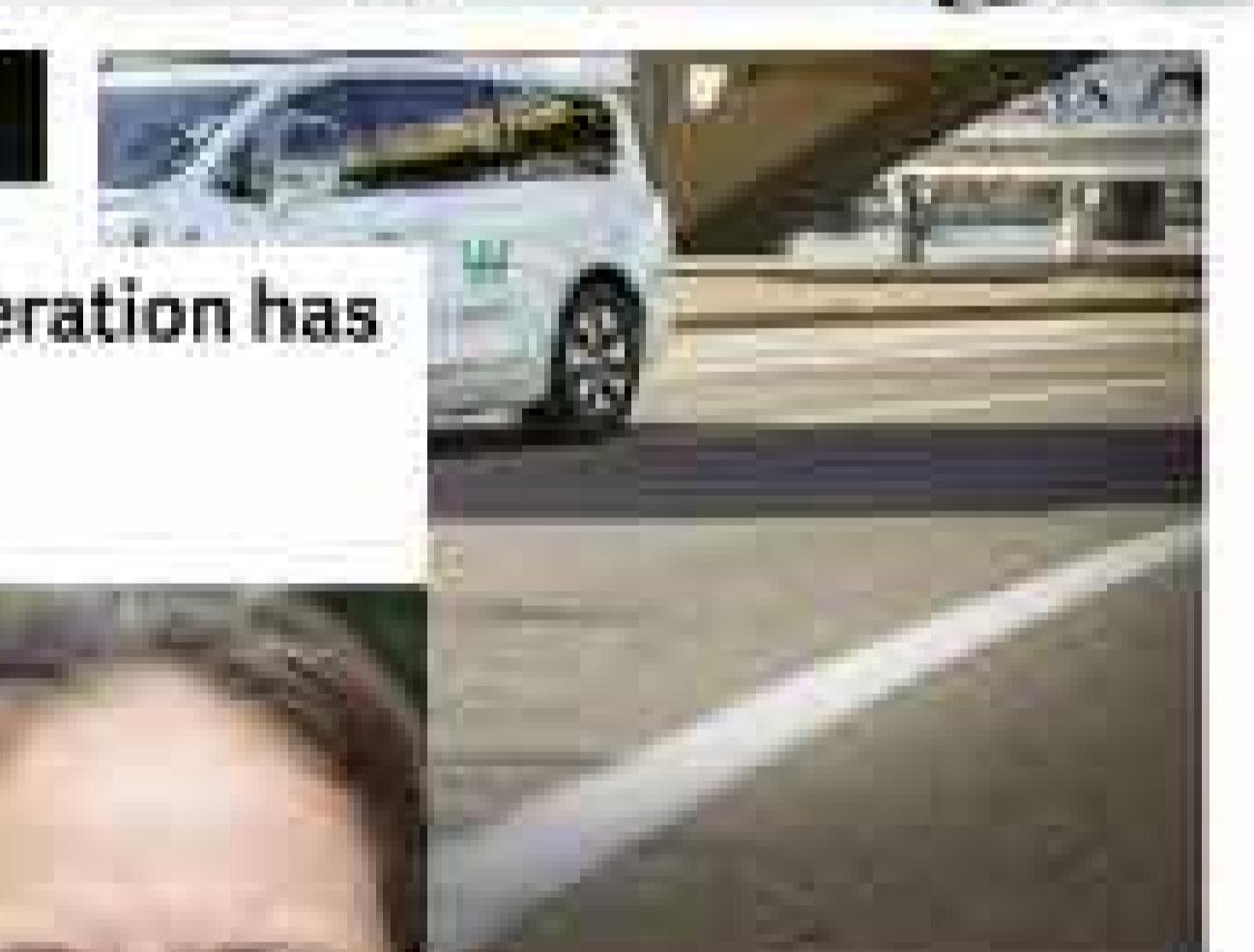


AI Can Help In Predicting Cryptocurrency Value



## Technology Outpacing Security Measures

By David Lohman | Jan 26, 2017 | 11:00 AM ET

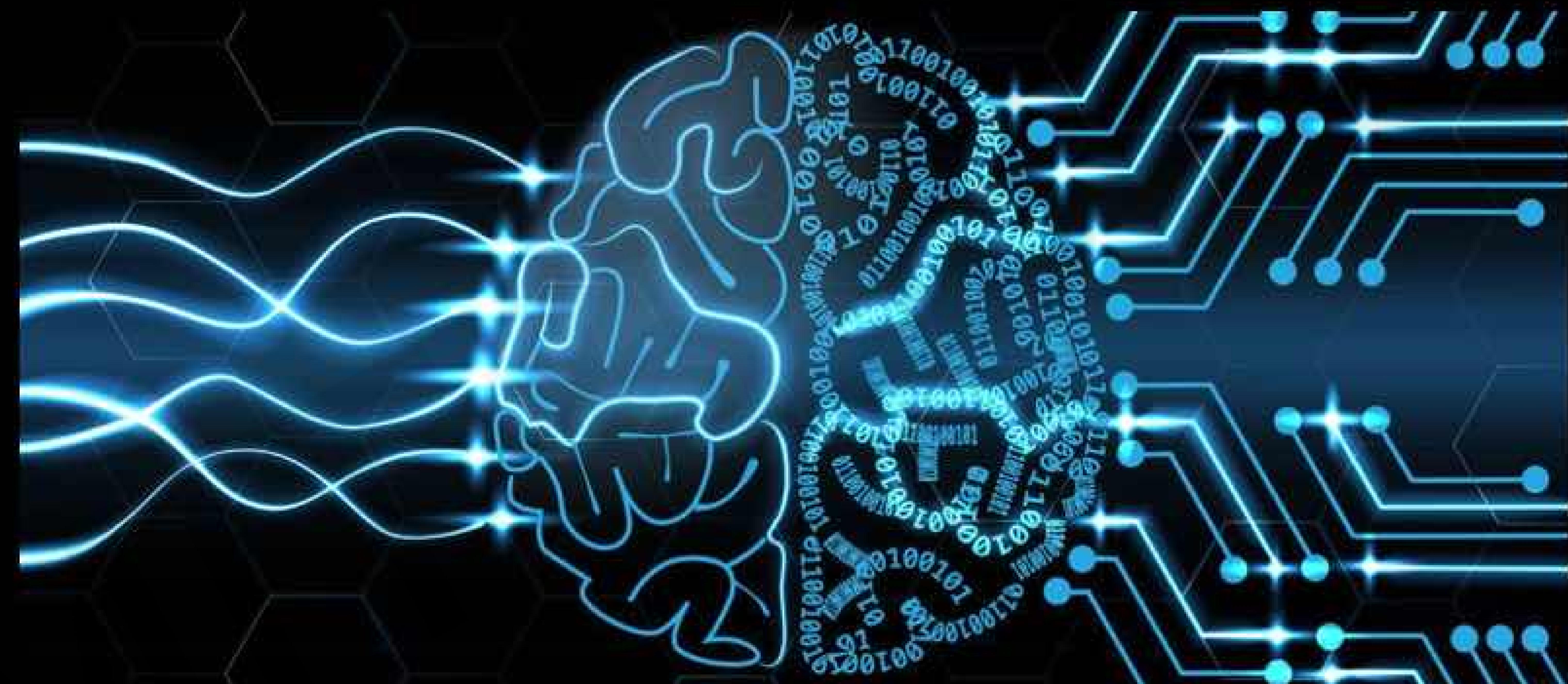


# So far in 6.S191 ...

**Data**

- Signals
- Images
- Sensors

...



**Decision**

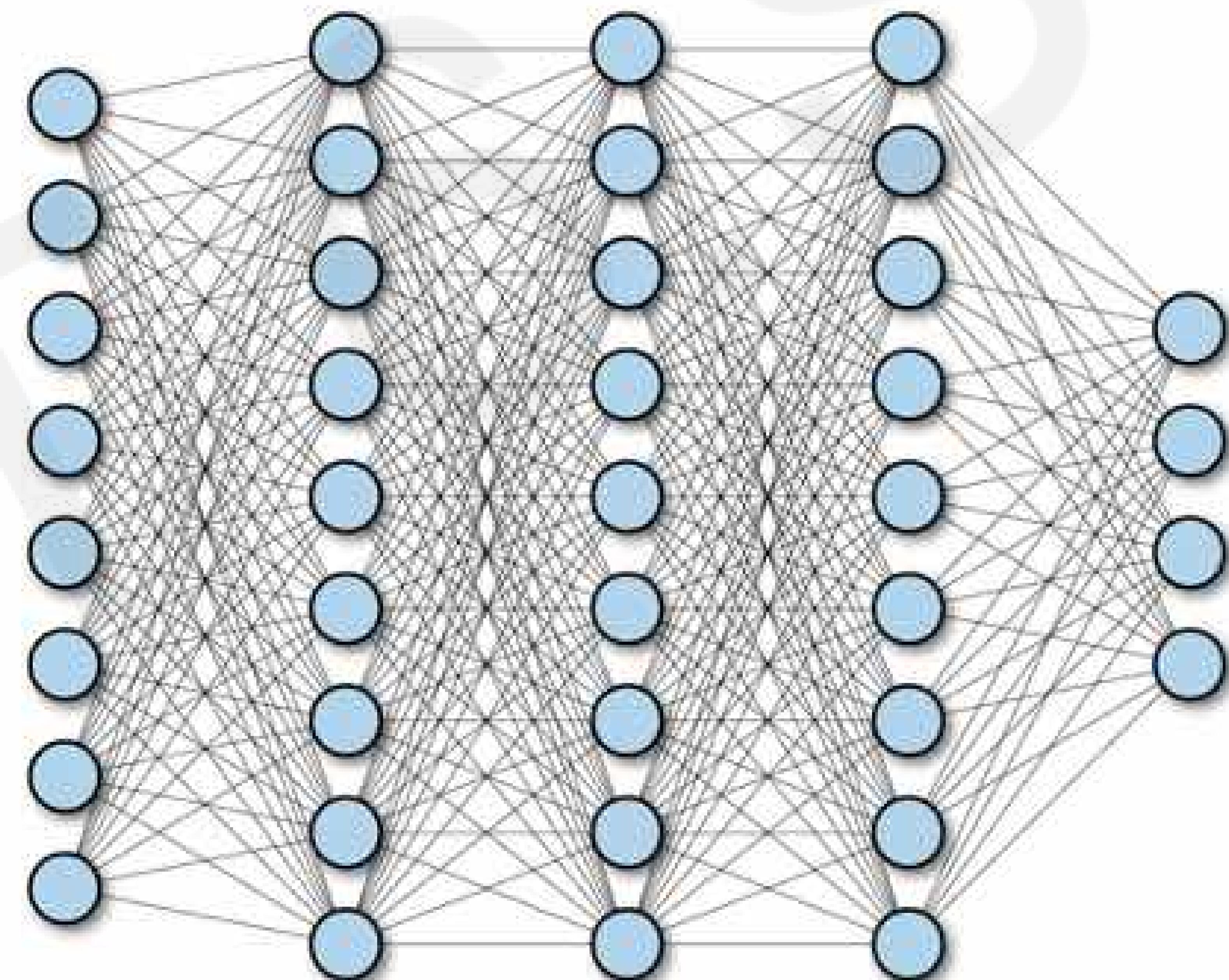
- Prediction
- Detection
- Action

...

# Power of Neural Nets

## Universal Approximation Theorem

A feedforward network with a single layer is sufficient to approximate, to an arbitrary precision, any continuous function.



# Power of Neural Nets

## Universal Approximation Theorem

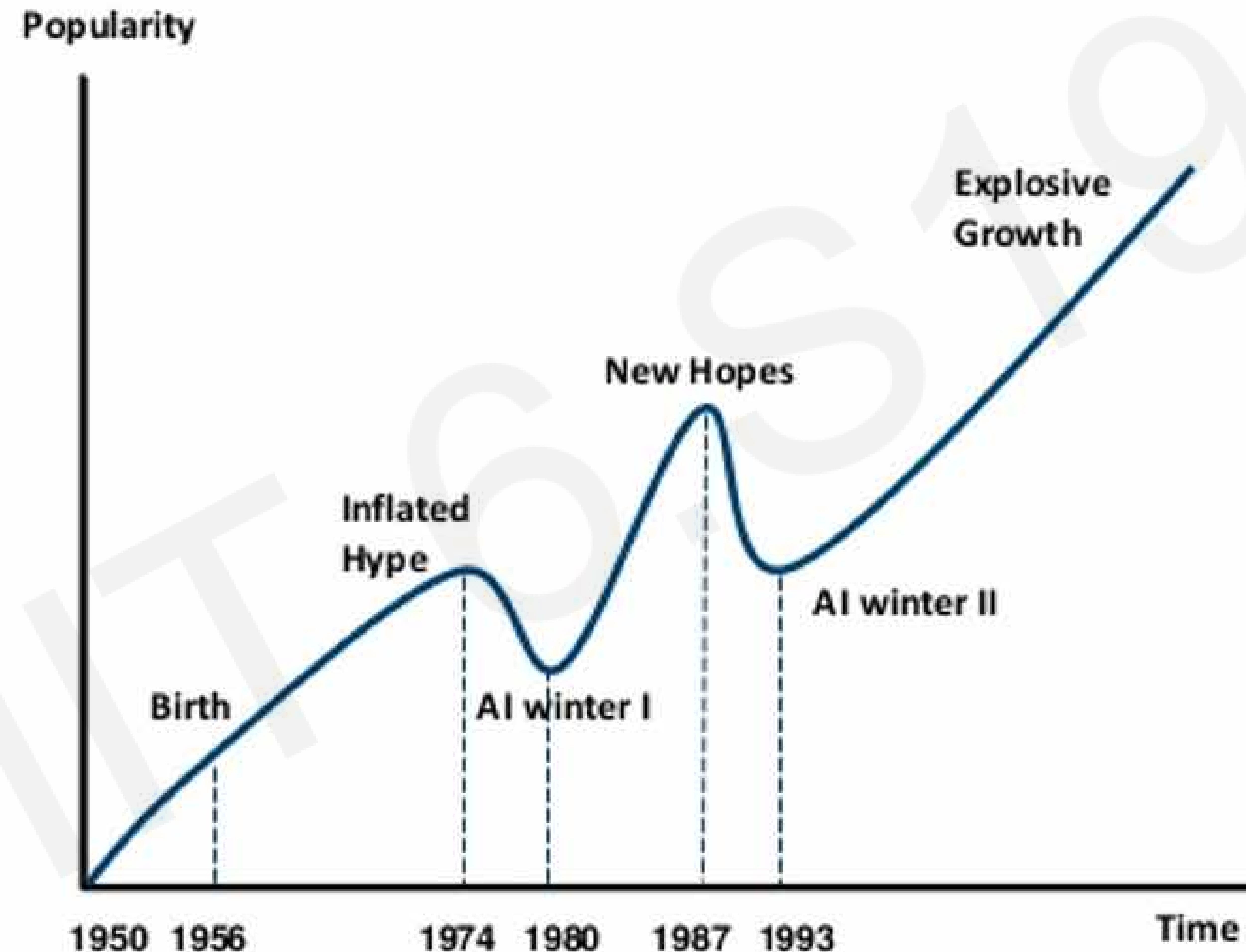
A feedforward network with a single layer is sufficient to approximate, to an arbitrary precision, any continuous function.

### Caveats:

The number of hidden units may be infeasibly large

The resulting model may not generalize

# Artificial Intelligence “Hype”: Historical Perspective



# Limitations

191

# Rethinking Generalization

"Understanding Deep Neural Networks Requires Rethinking Generalization"



dog



banana



dog



tree

# Rethinking Generalization

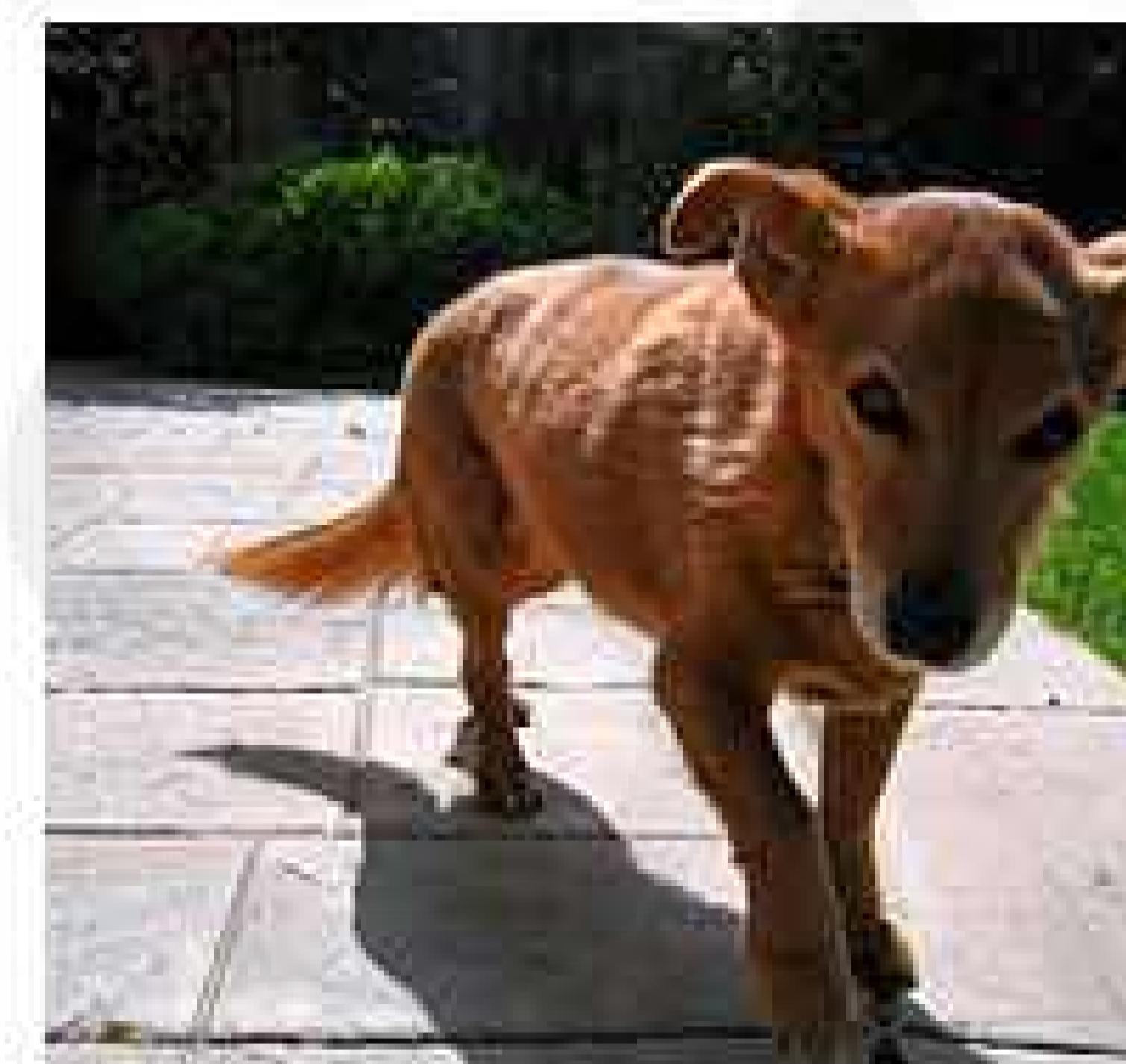
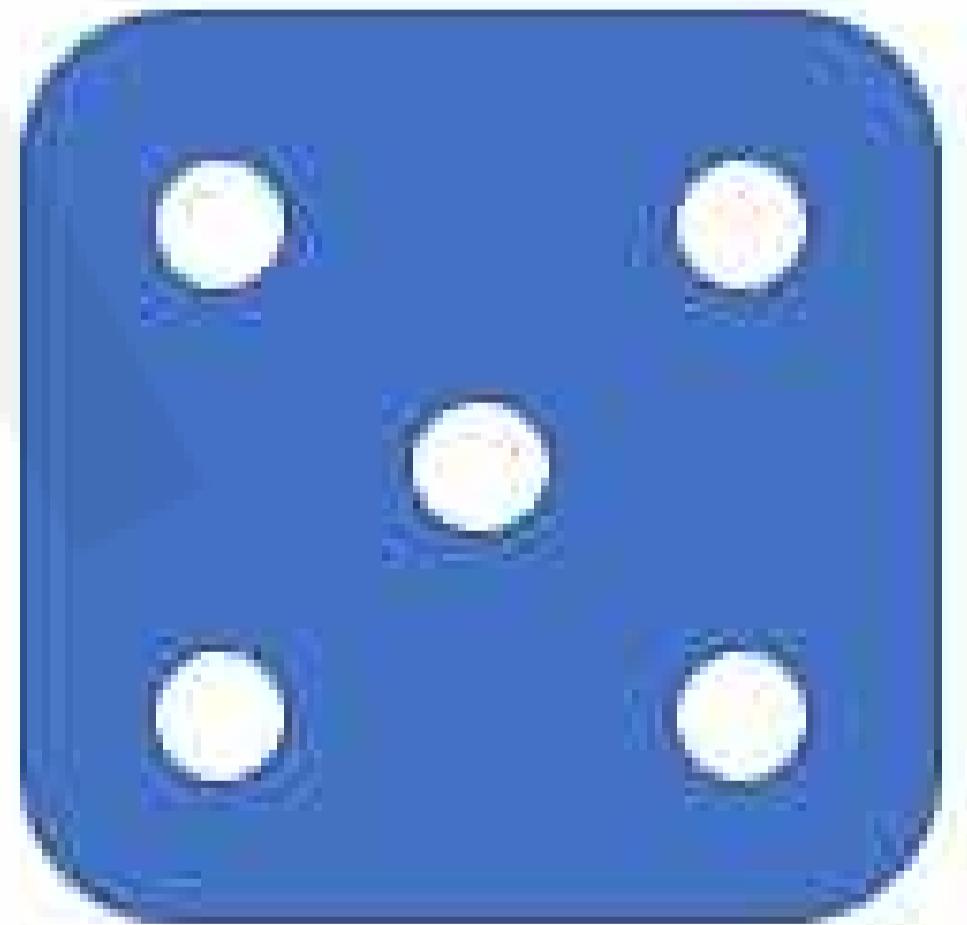
"Understanding Deep Neural Networks Requires Rethinking Generalization"



dog



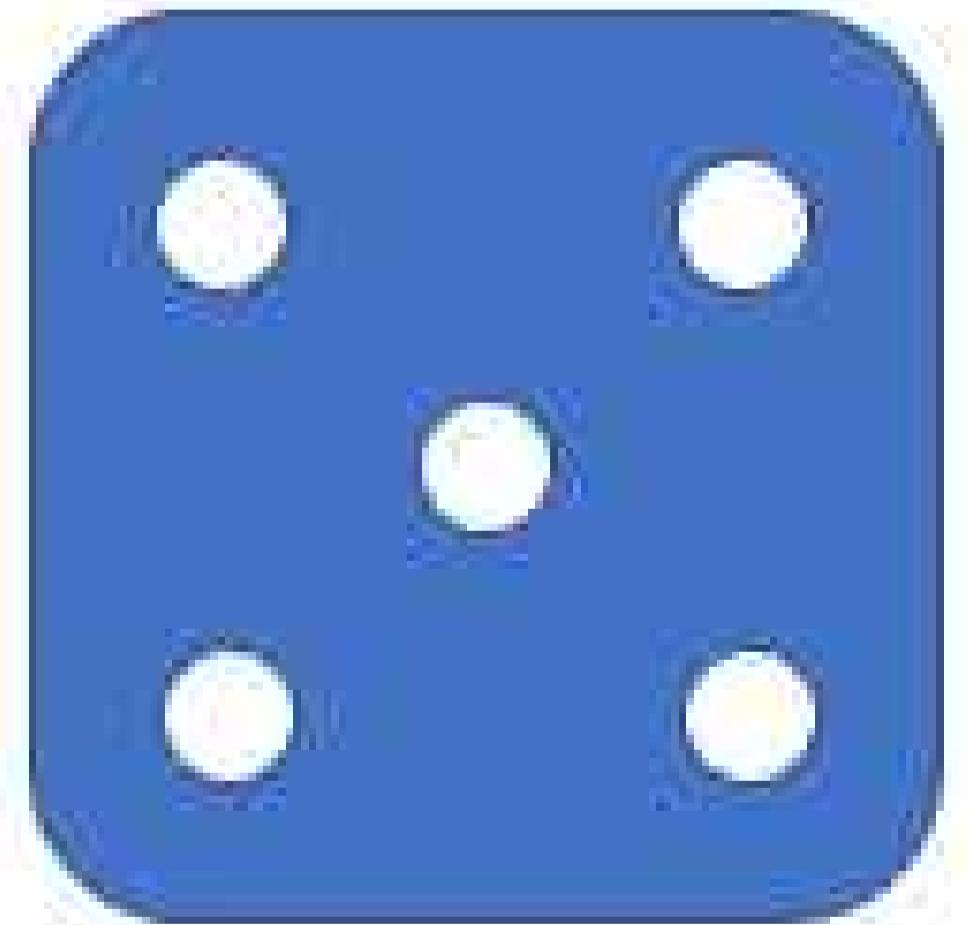
banana



dog



tree



# Rethinking Generalization

"Understanding Deep Neural Networks Requires Rethinking Generalization"



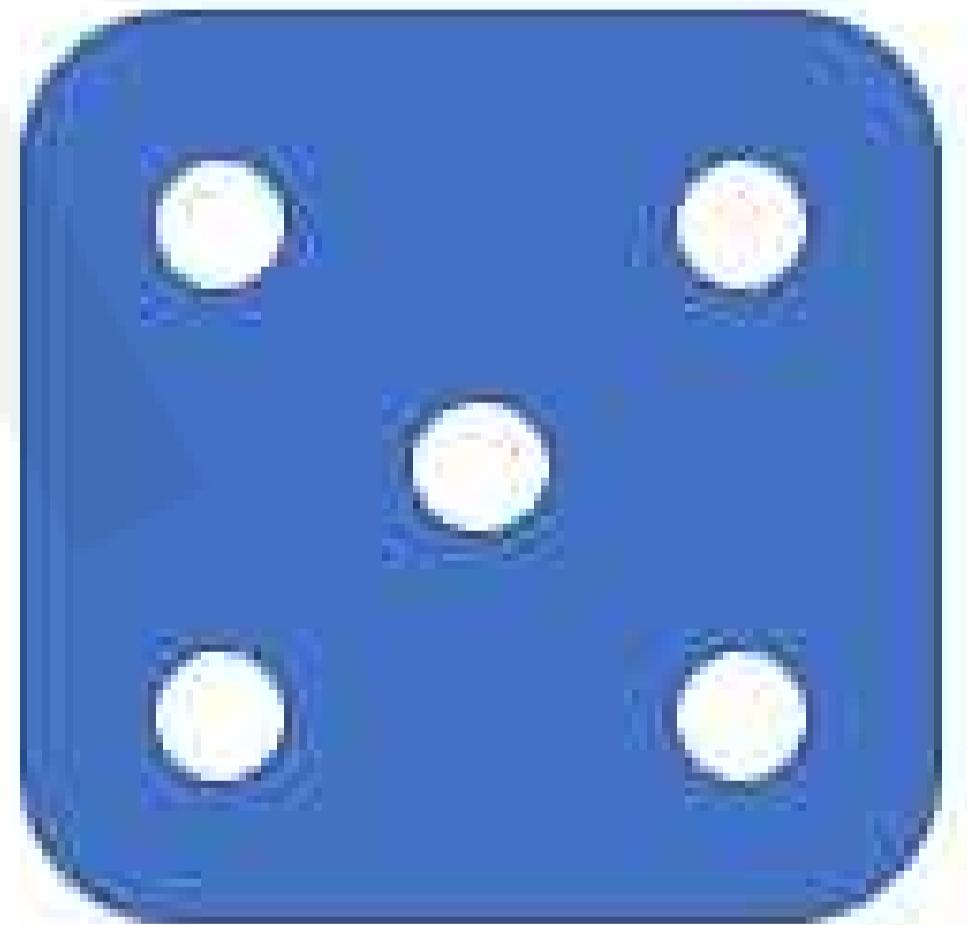
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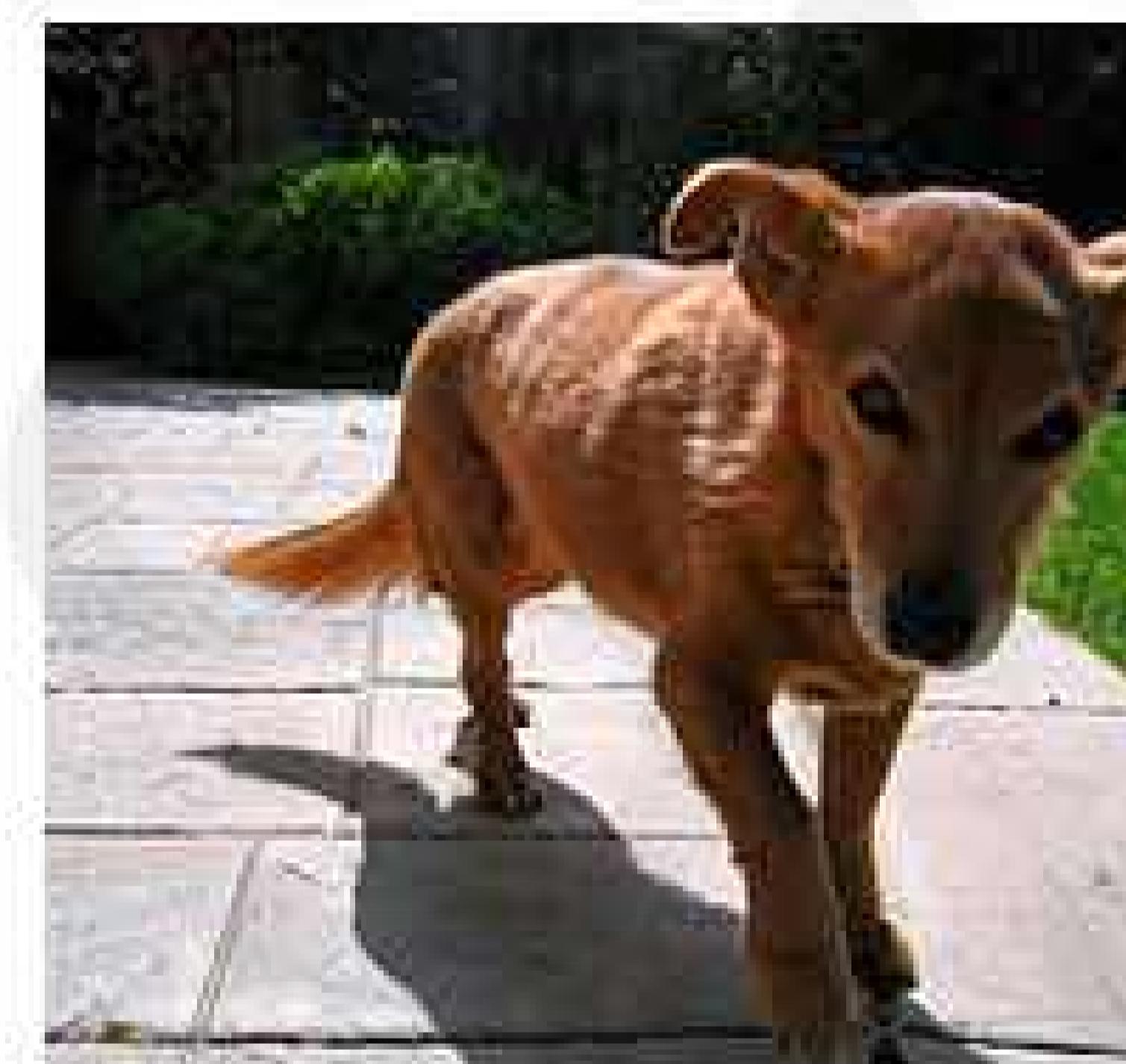
banana



banana



dog



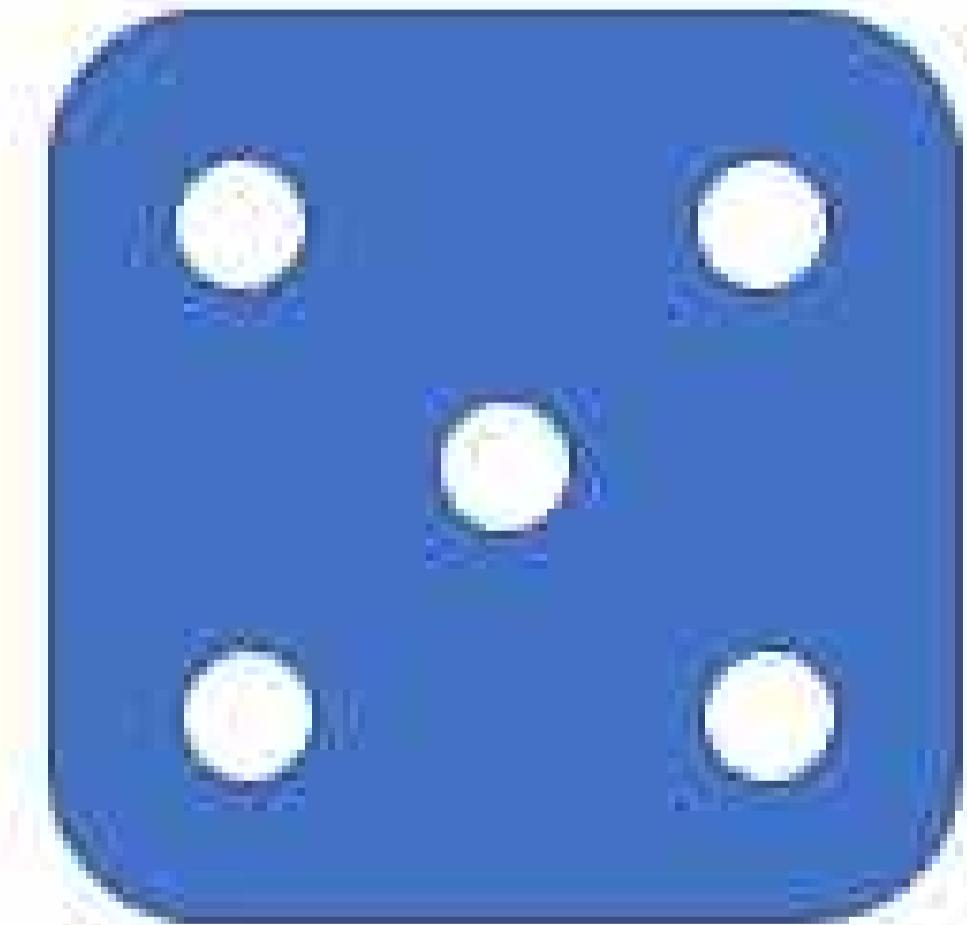
dog



tree



tree



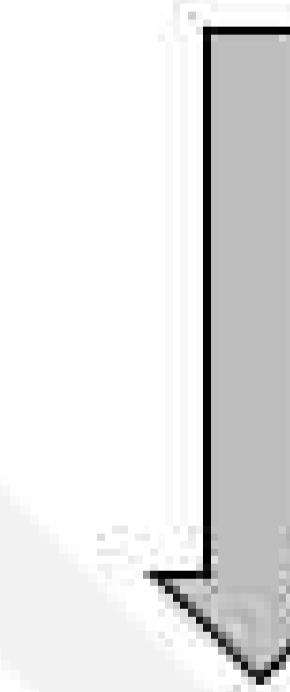
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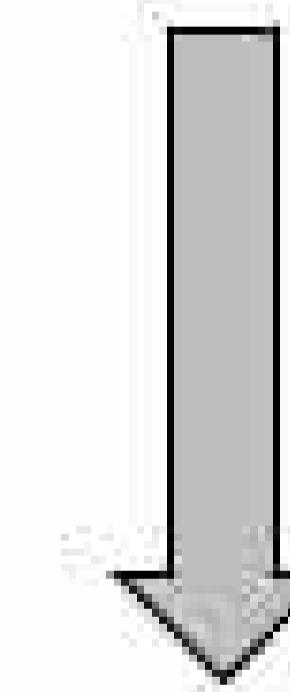


~~dog~~



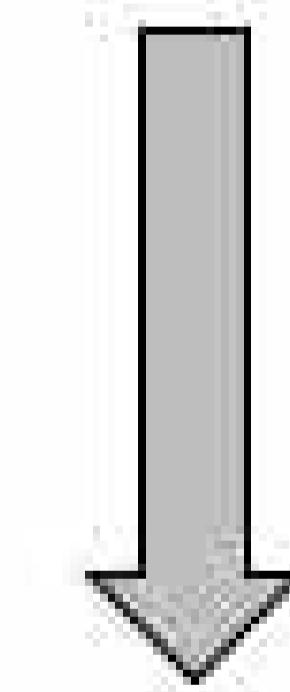
banana

~~banana~~



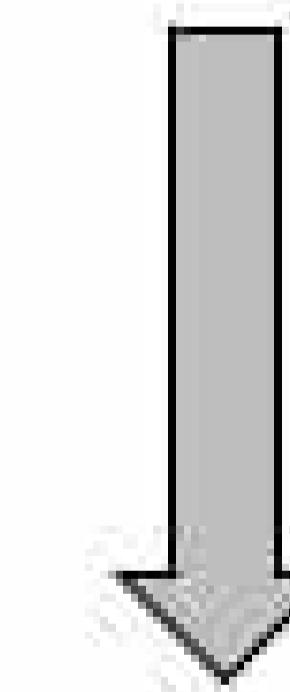
dog

~~dog~~



tree

~~tree~~



dog

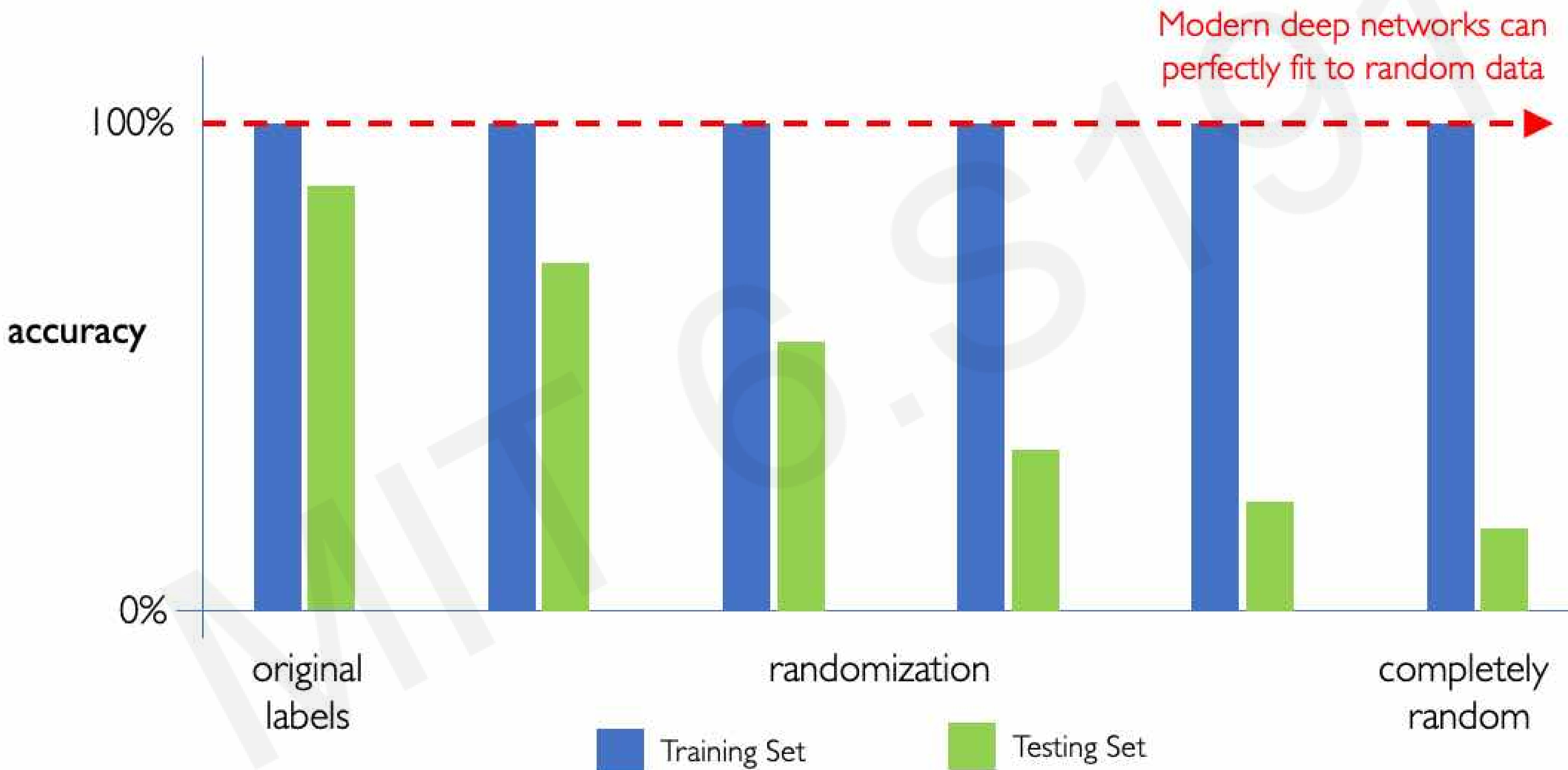
# Capacity of Deep Neural Networks



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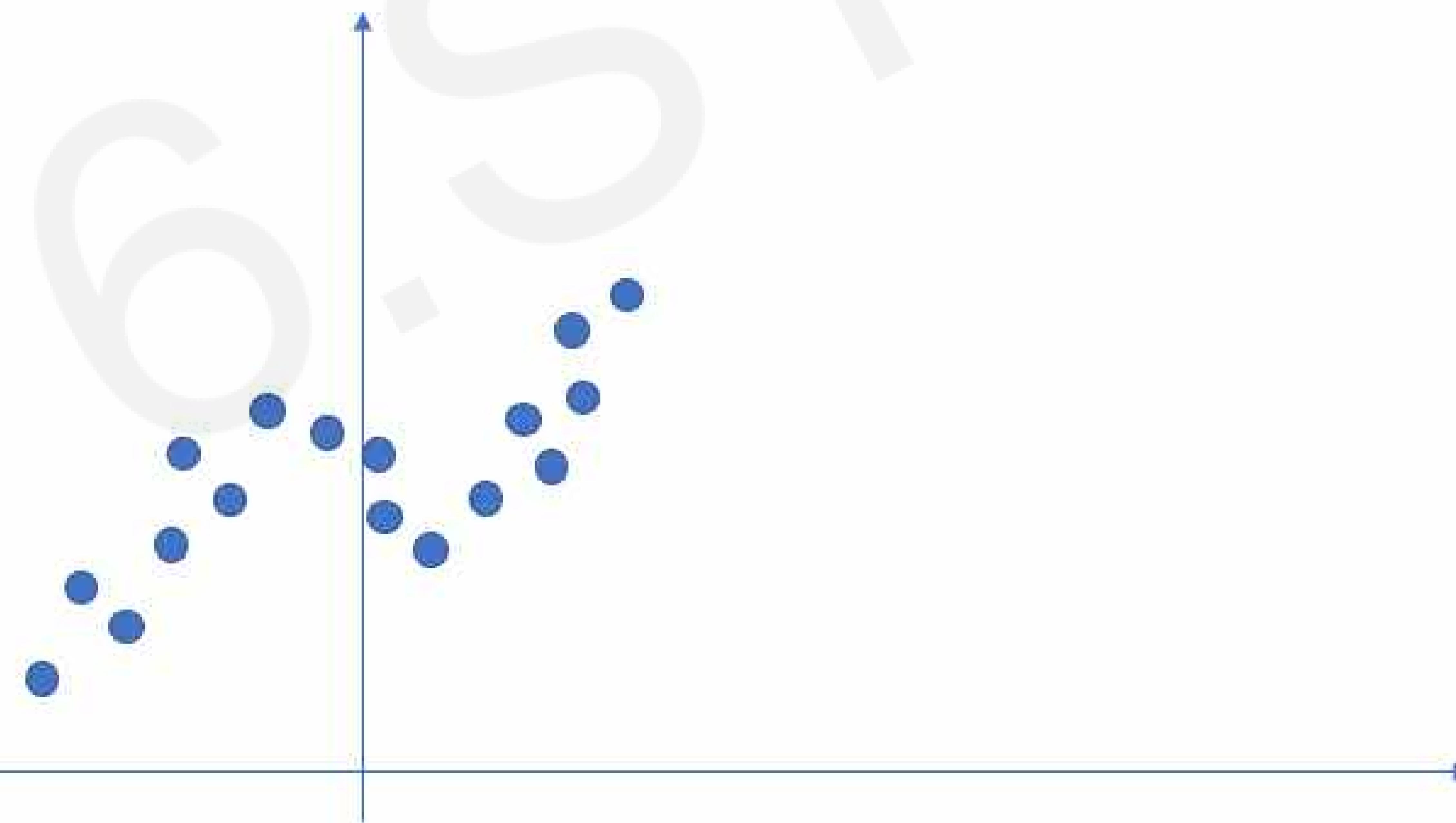


# Capacity of Deep Neural Networks



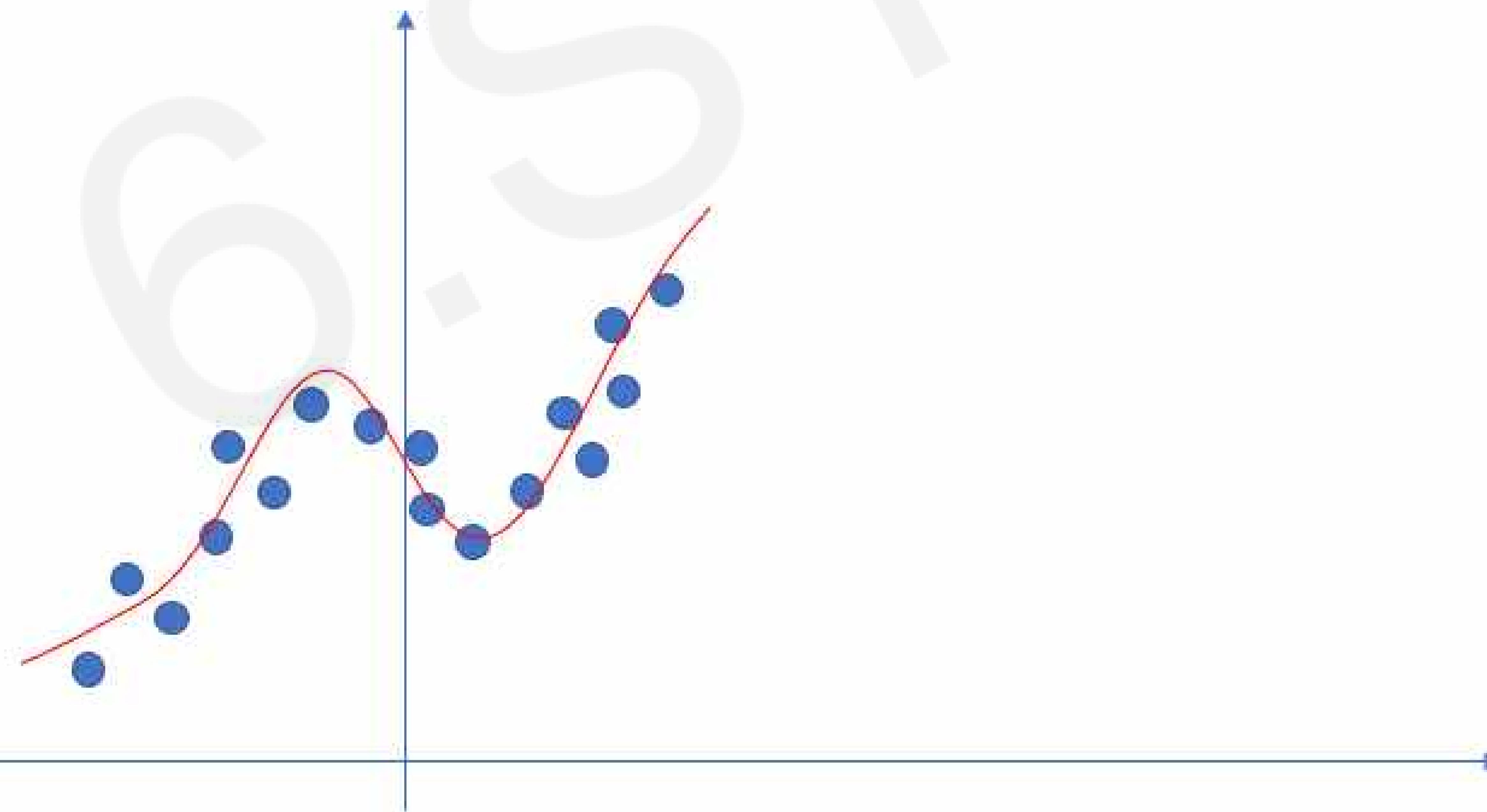
# Neural Networks as Function Approximators

Neural networks are excellent function approximators



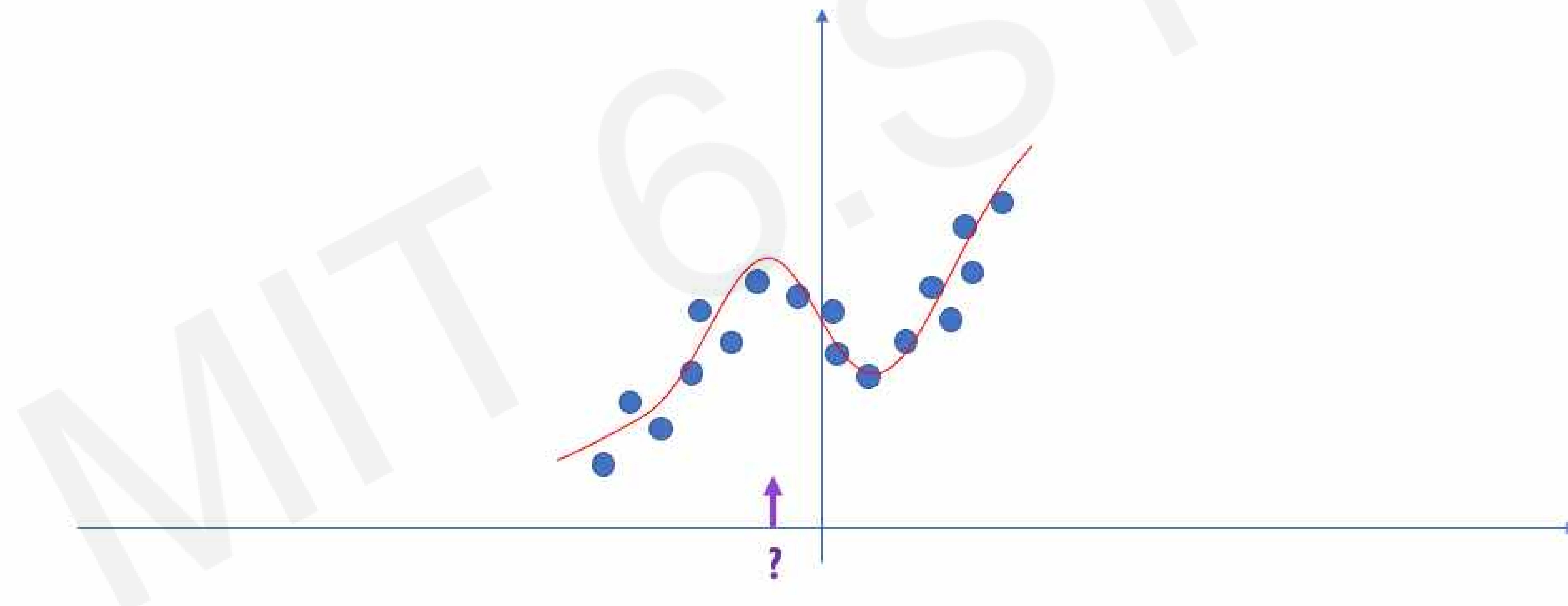
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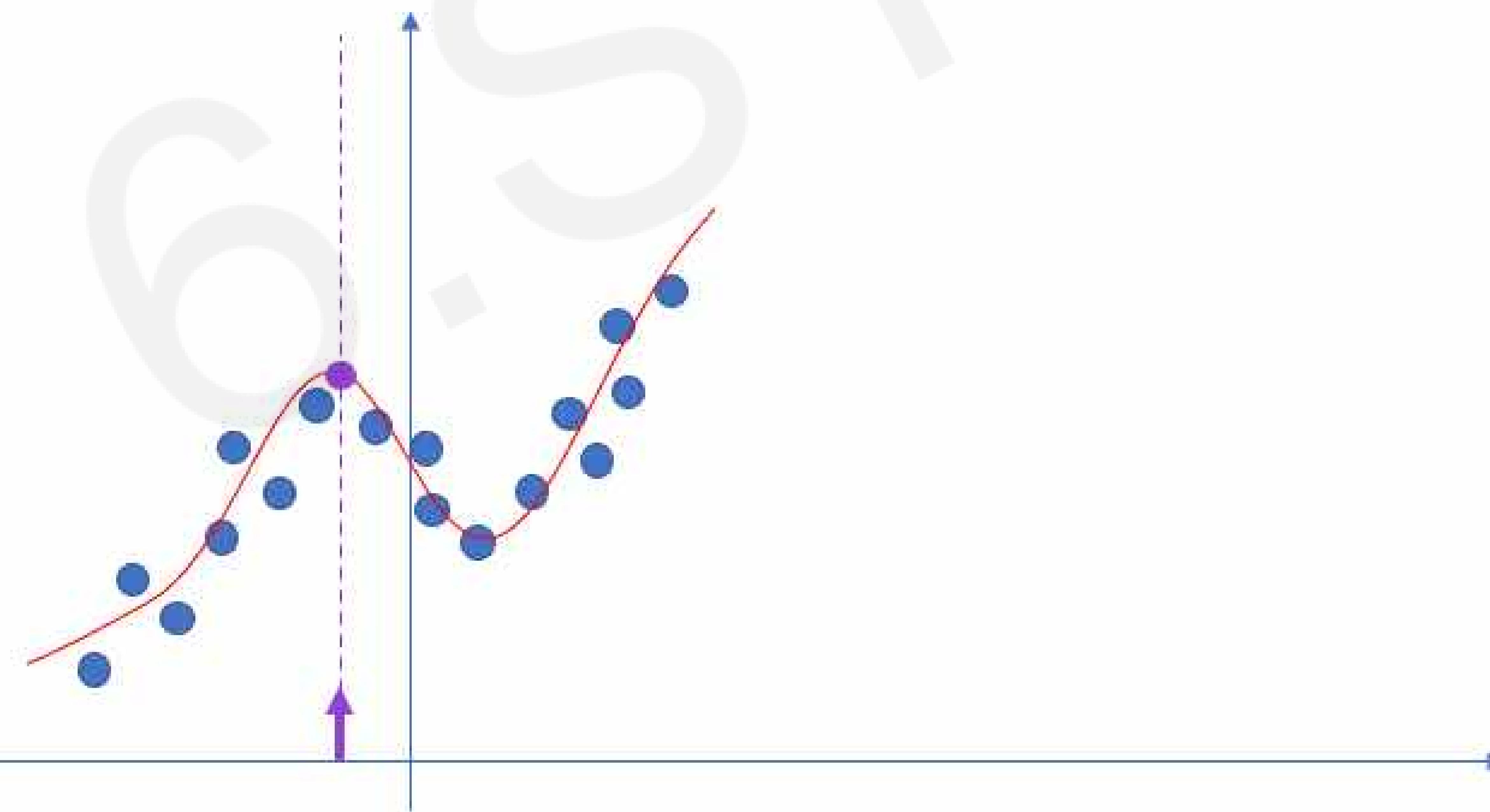
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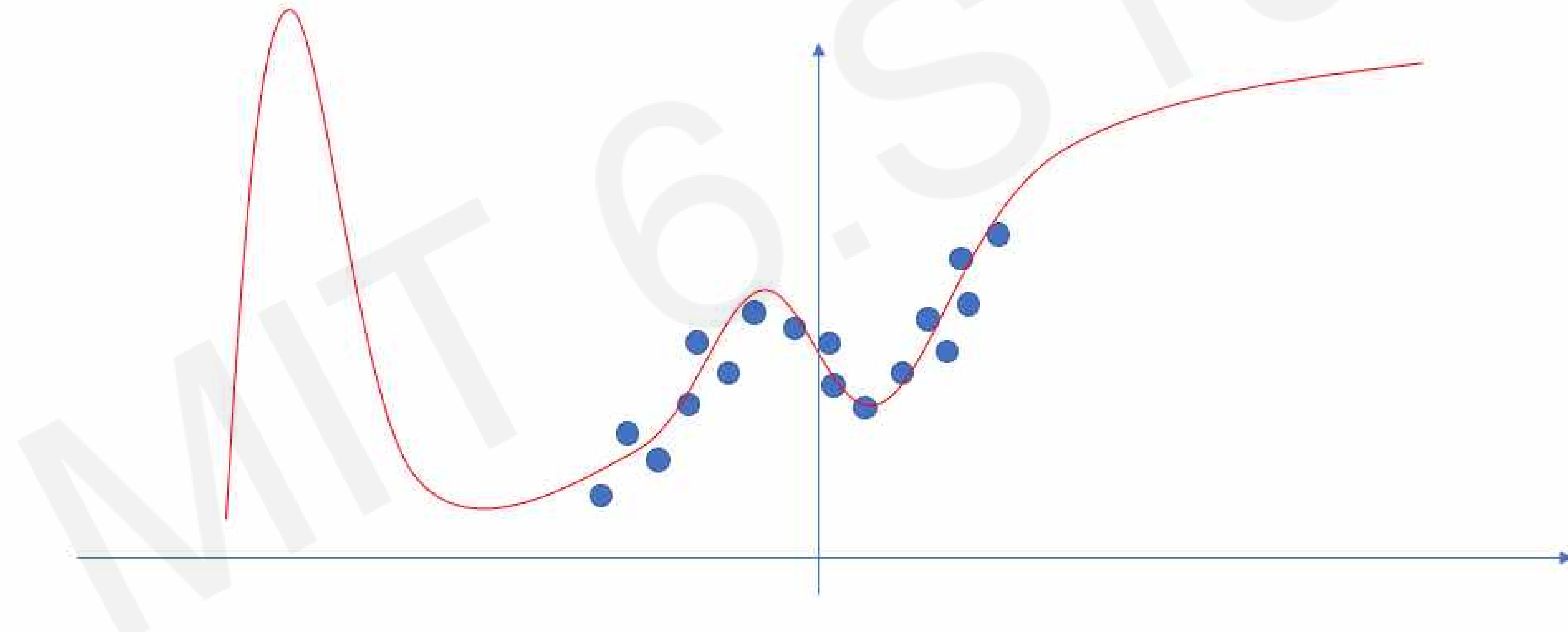
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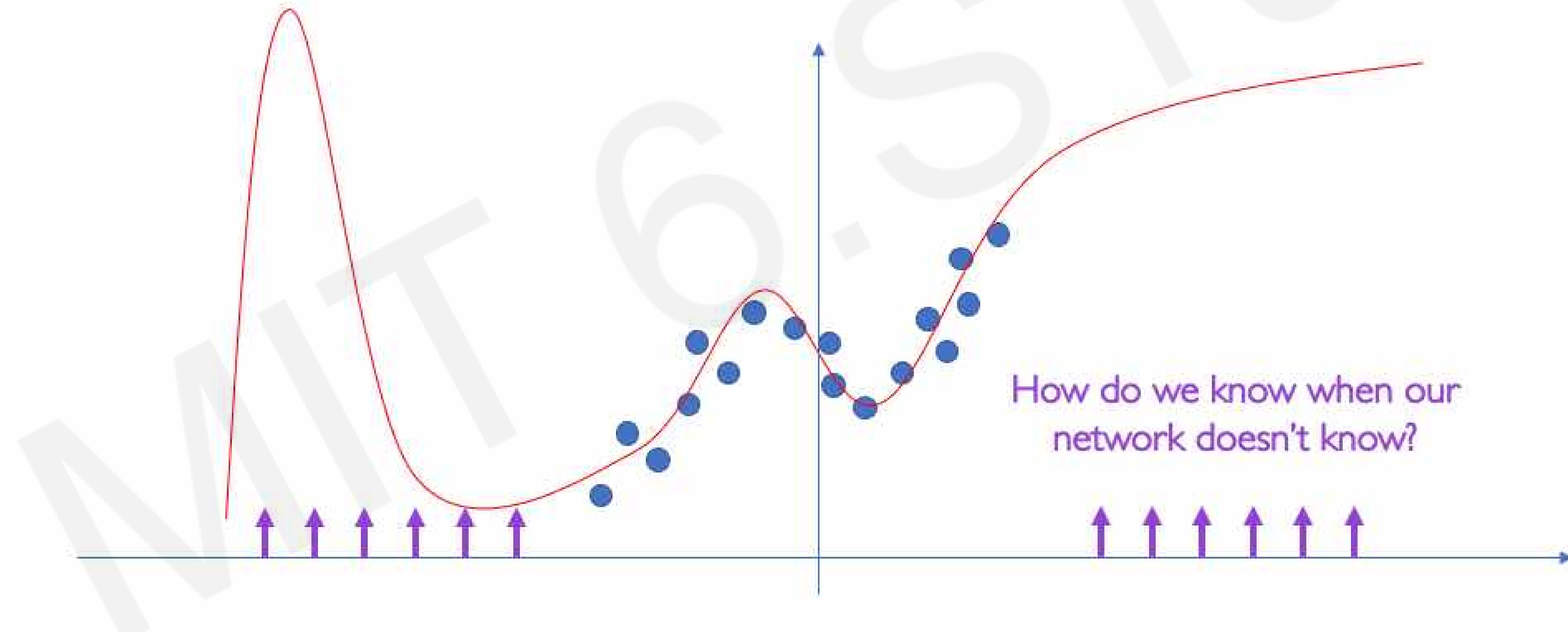
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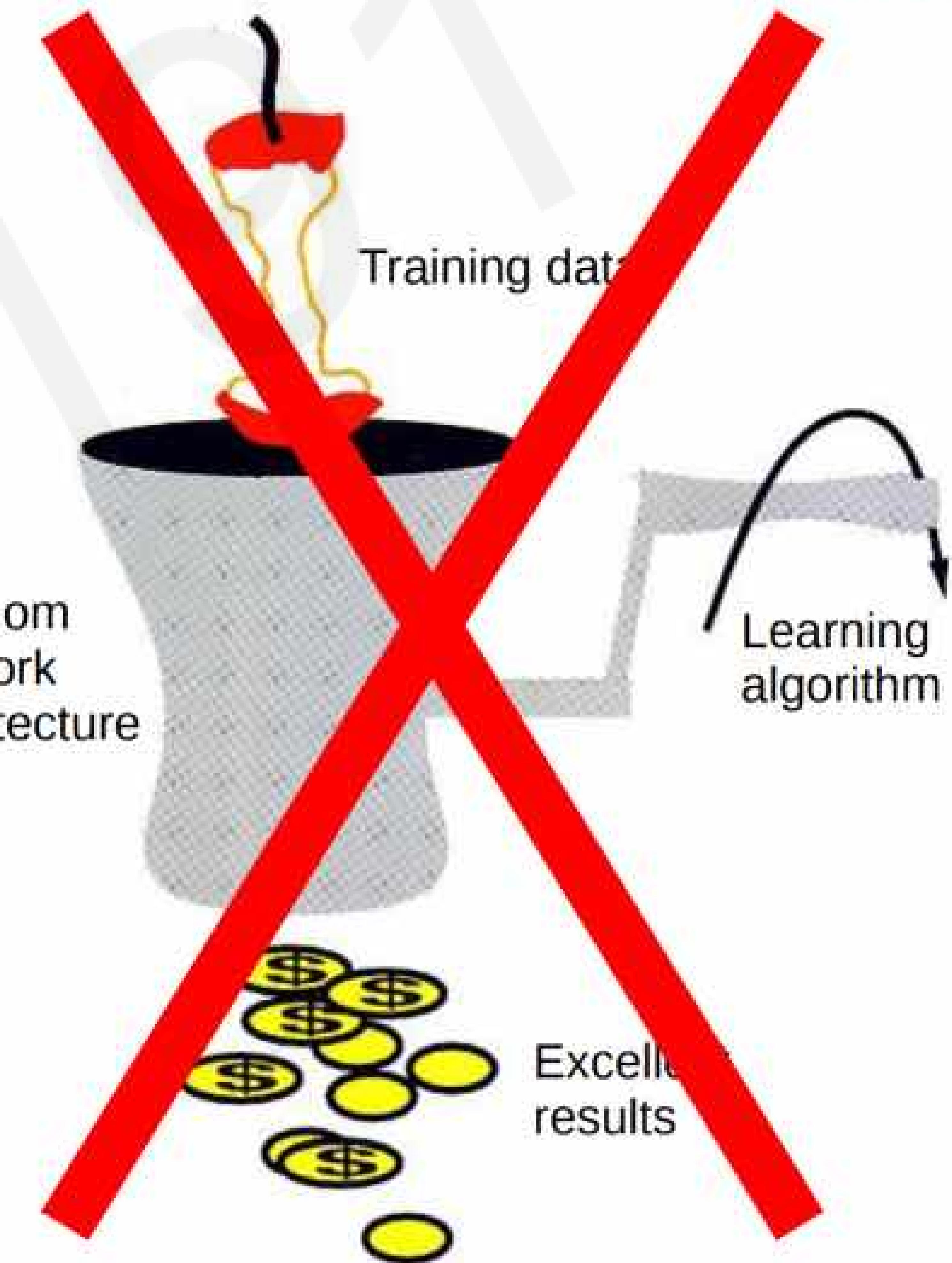
# Neural Networks as Function Approximators

Neural networks are excellent function approximators  
...when they have training data

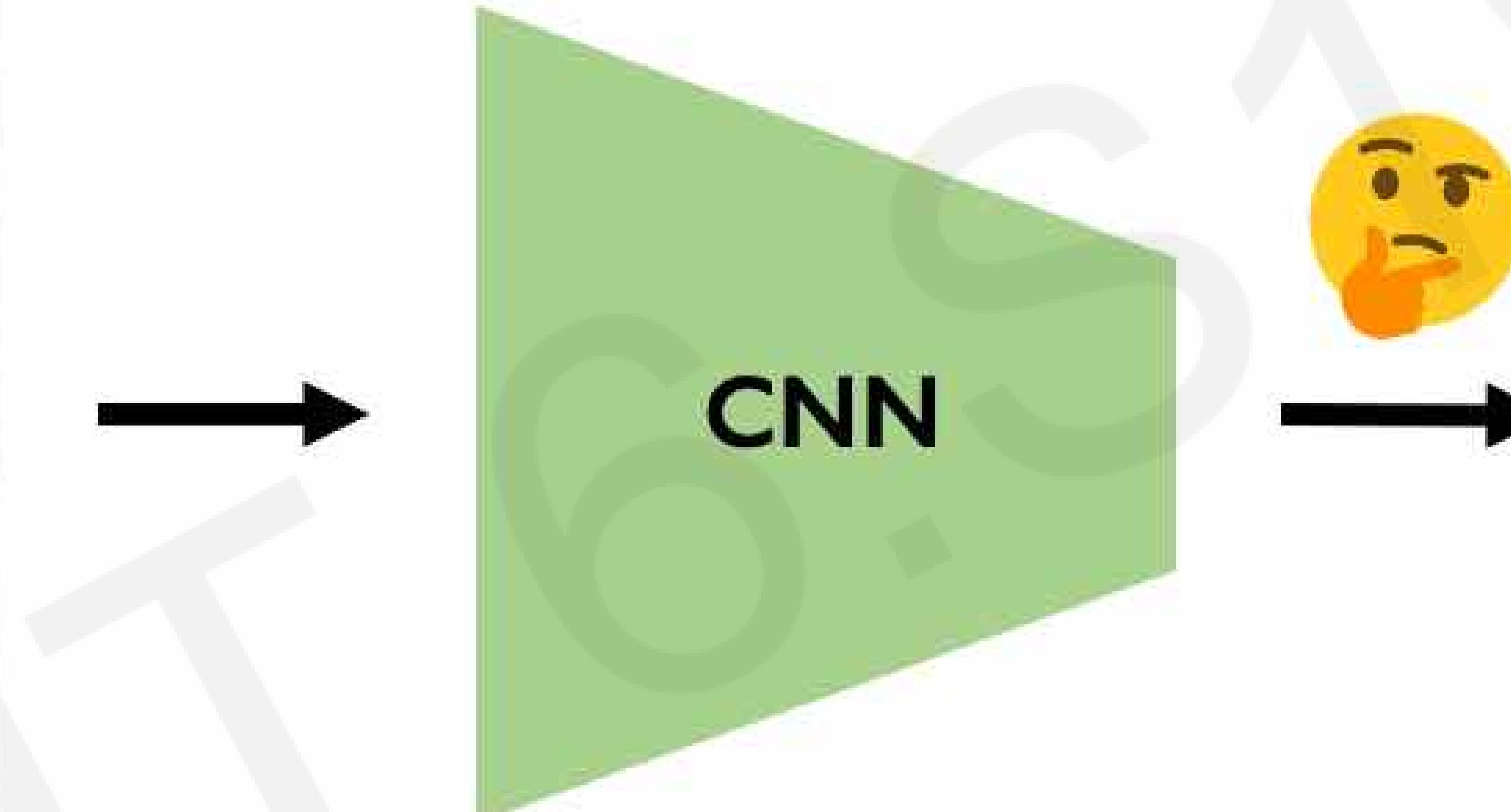


# Deep Learning = Alchemy?

NO!



# Neural Network Failure Modes, Part I



Train network to  
colorize BW images.



**Why could this be the case?**

# What Happens During Training...



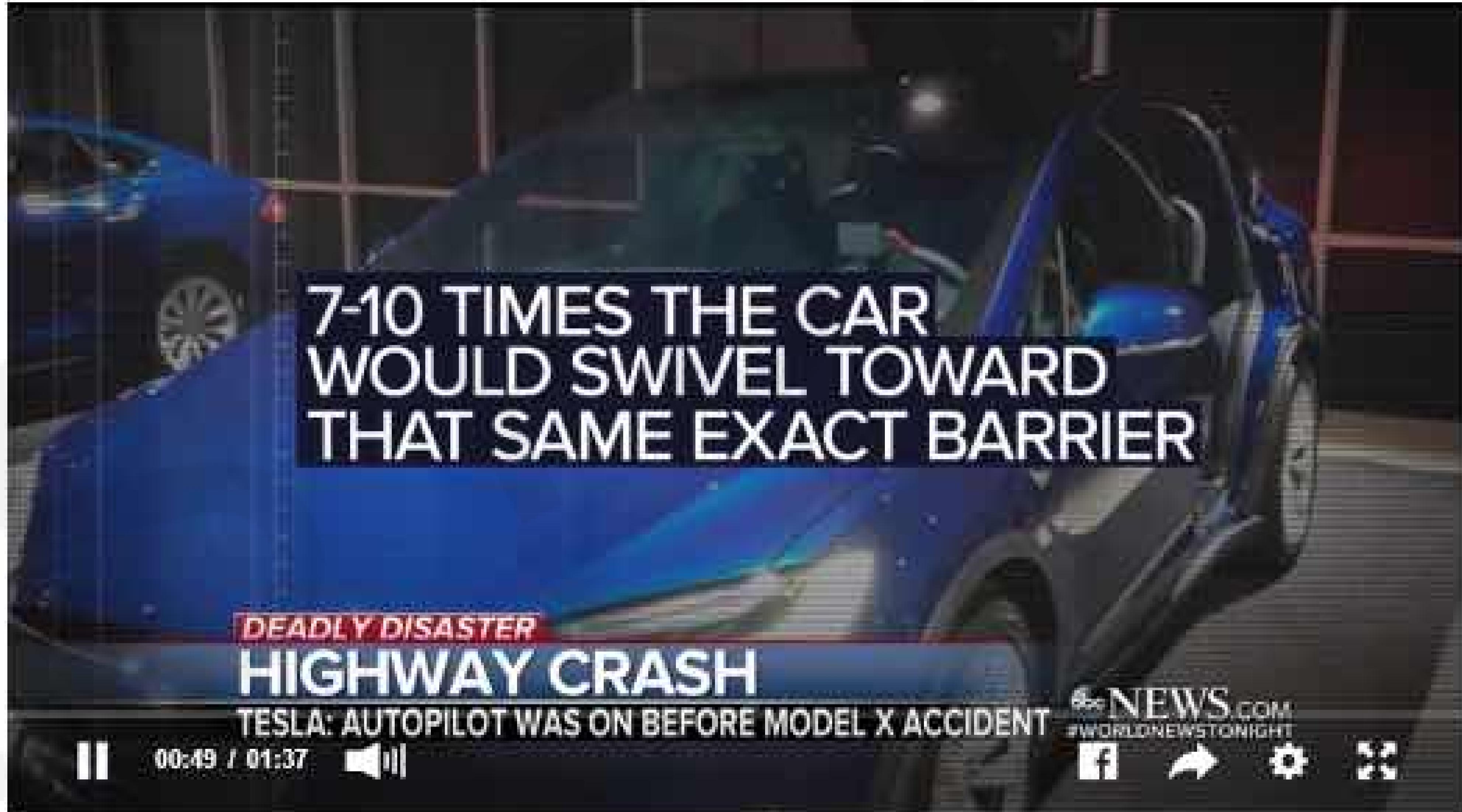
# Neural Network Failure Modes, Part II

Tesla car was on autopilot prior to fatal crash in California, company says

*The crash near Mountain View, California, last week killed the driver.*

By Mark Osborne

March 31, 2018, 1:57 AM • 5 min read



# Uncertainty in Deep Learning

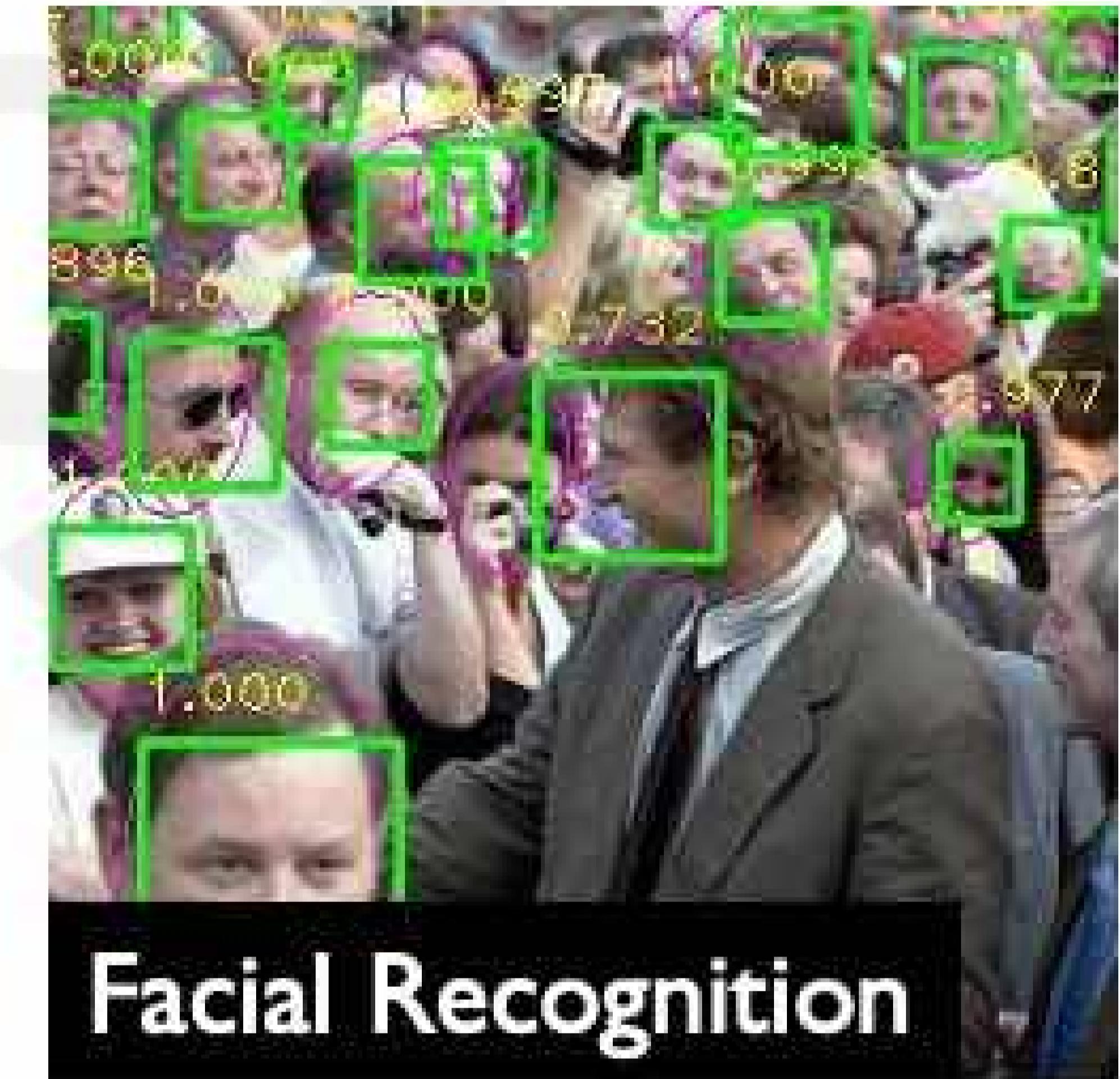
**Safety-critical  
applications**



Autonomous Vehicles

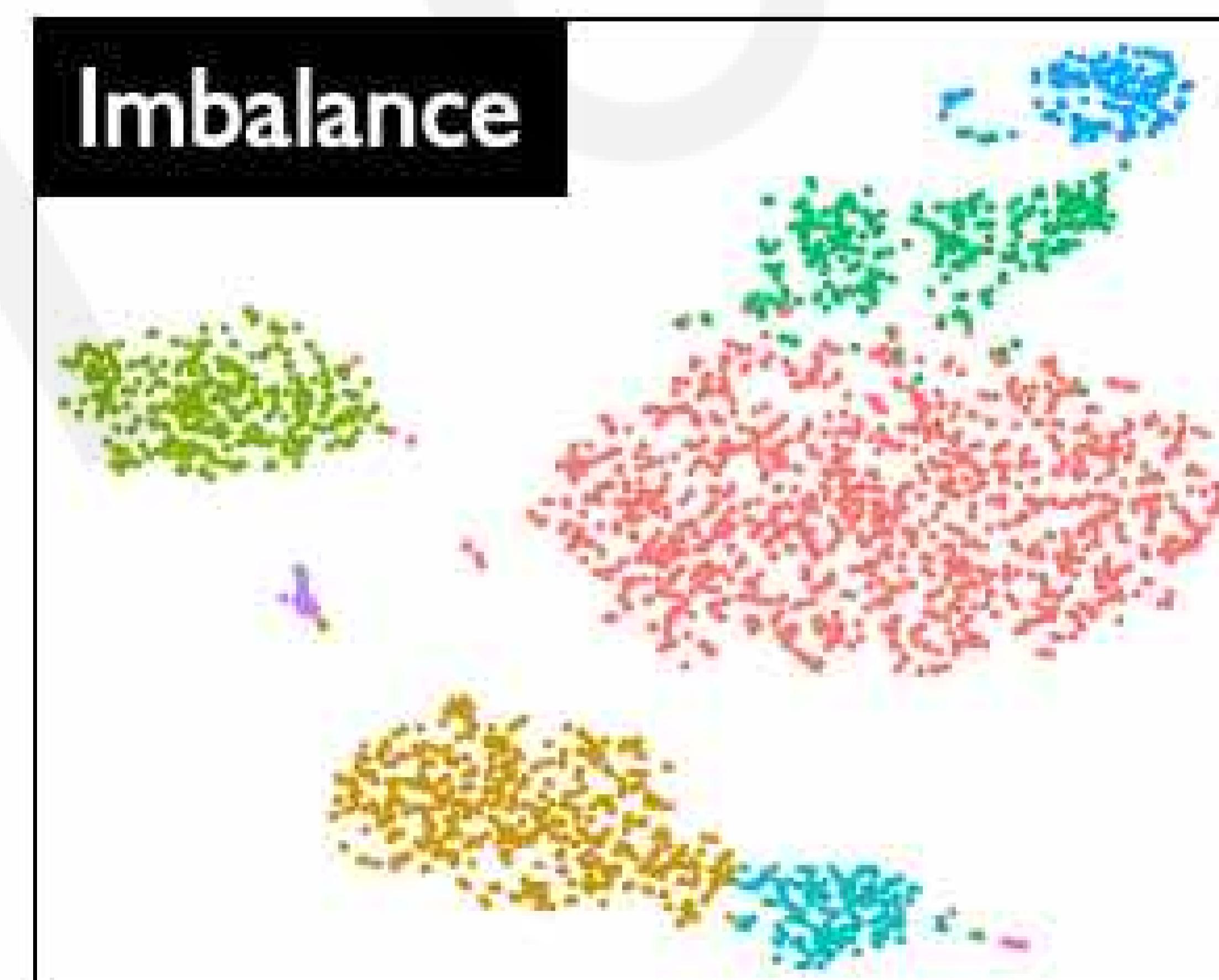


Medicine



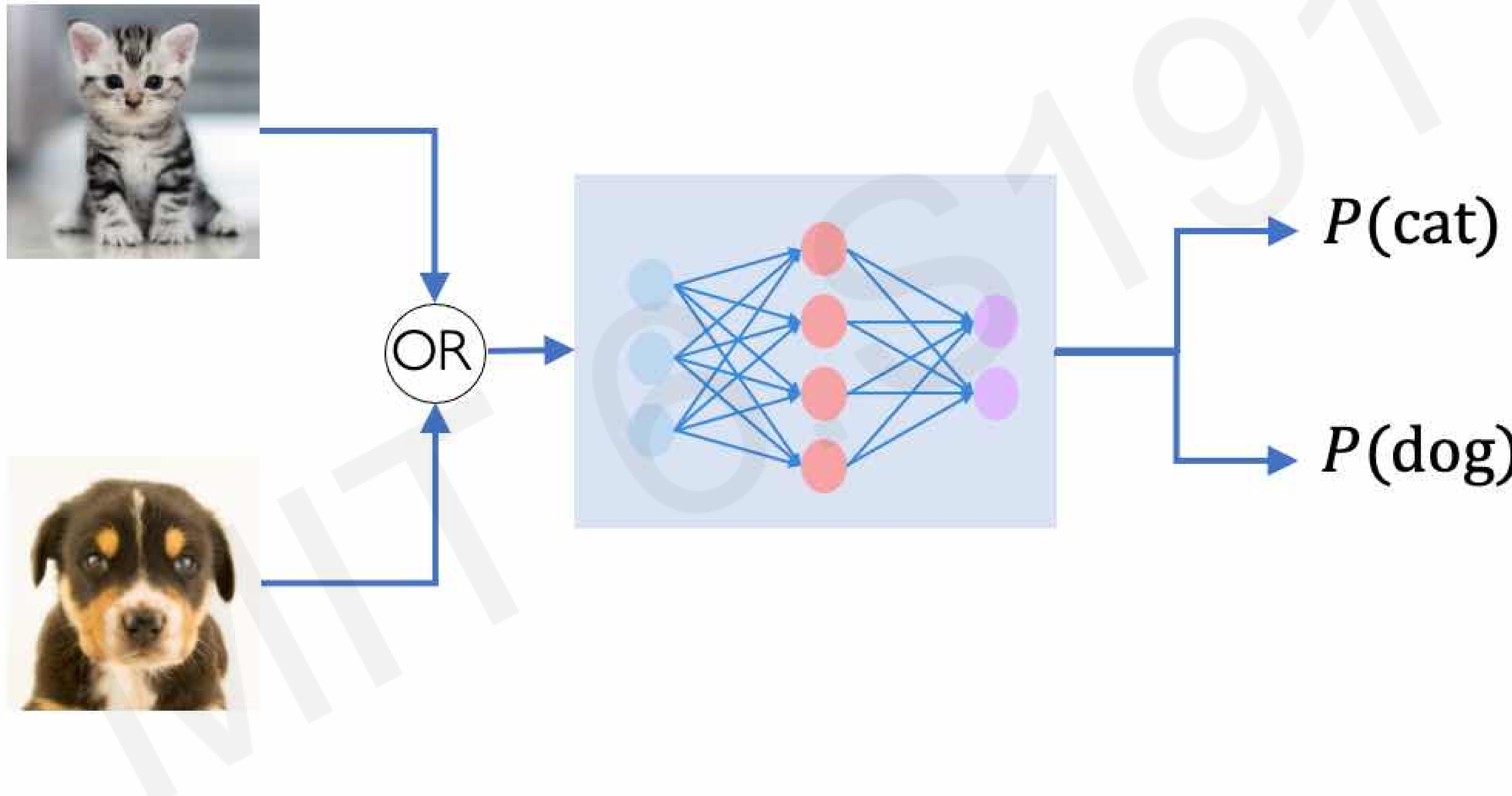
Facial Recognition

**Sparse and/or  
noisy datasets**



6.S191  
Guest  
Lecture

# What uncertainties do we need?

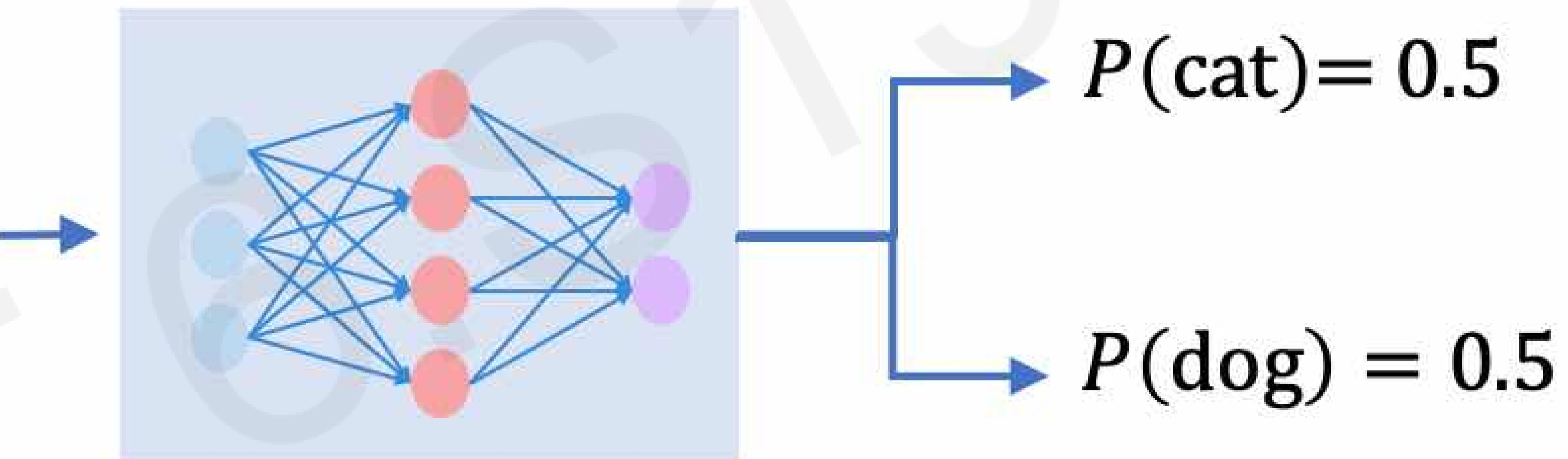


6.S191 Lecture

# What uncertainties do we need?

We need uncertainty metrics to assess the noise inherent to the data.

## aleatoric uncertainty



Remember:  $P(\text{cat}) + P(\text{dog}) = 1$

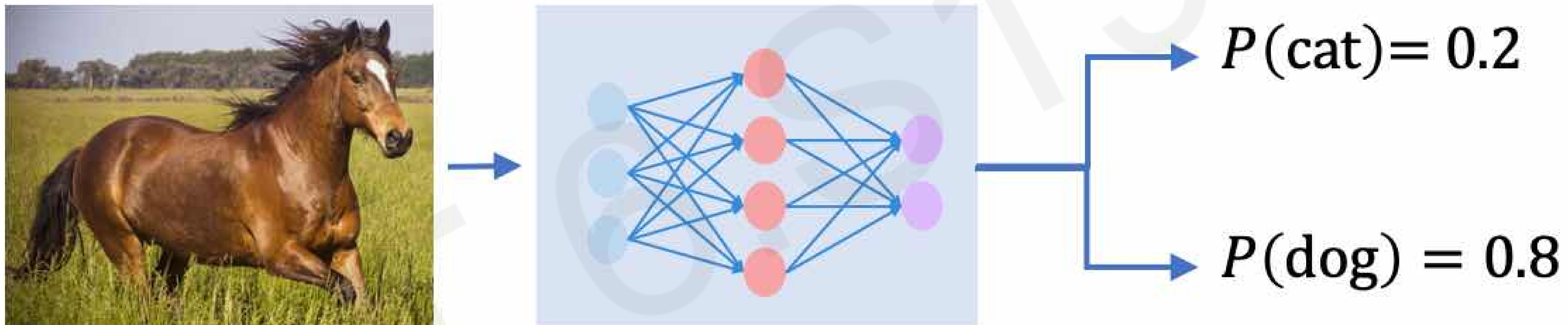


6.S191 Lecture

# What uncertainties do we need?

We need uncertainty metrics to assess the network's confidence in its predictions.

## epistemic uncertainty

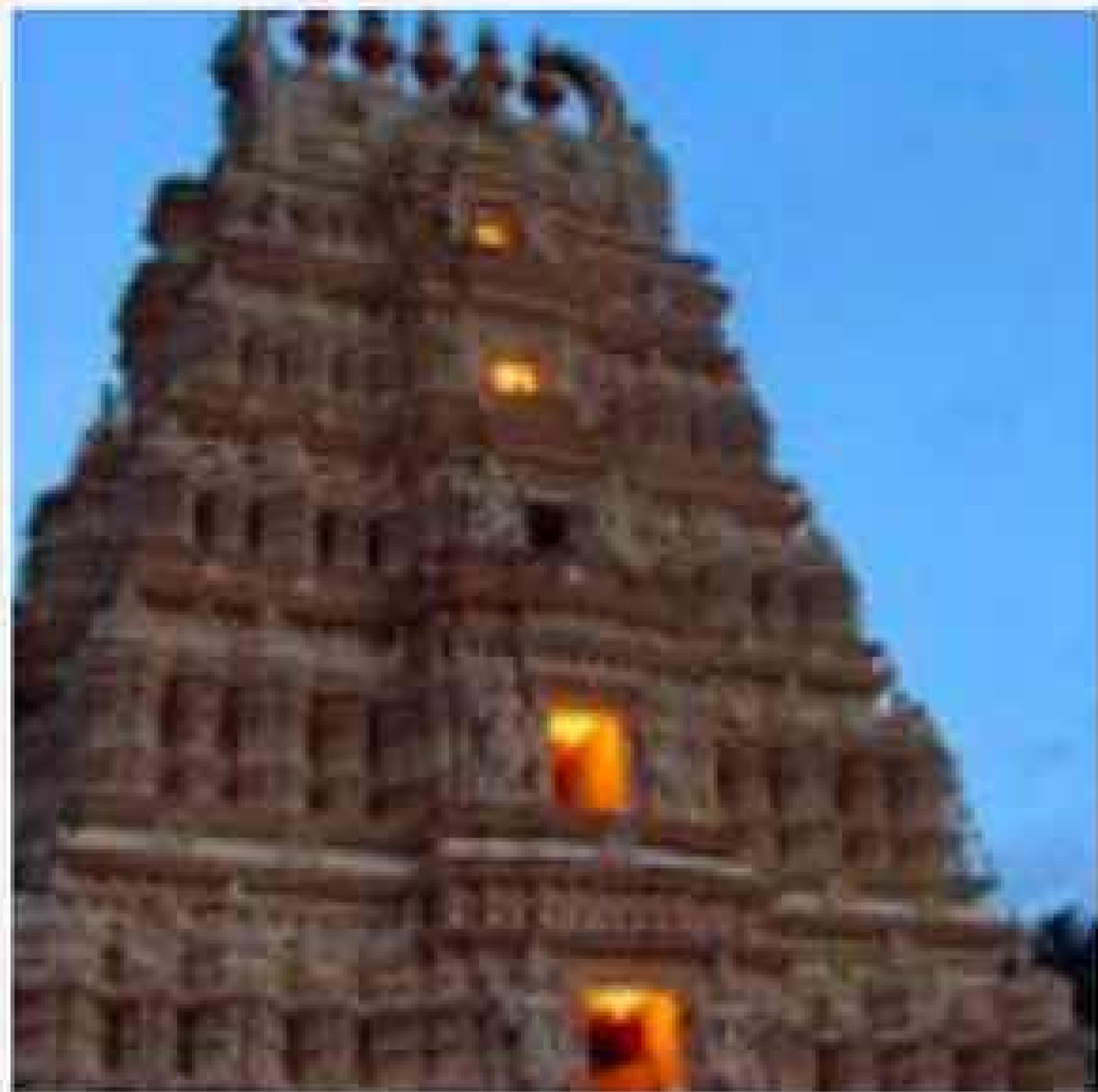


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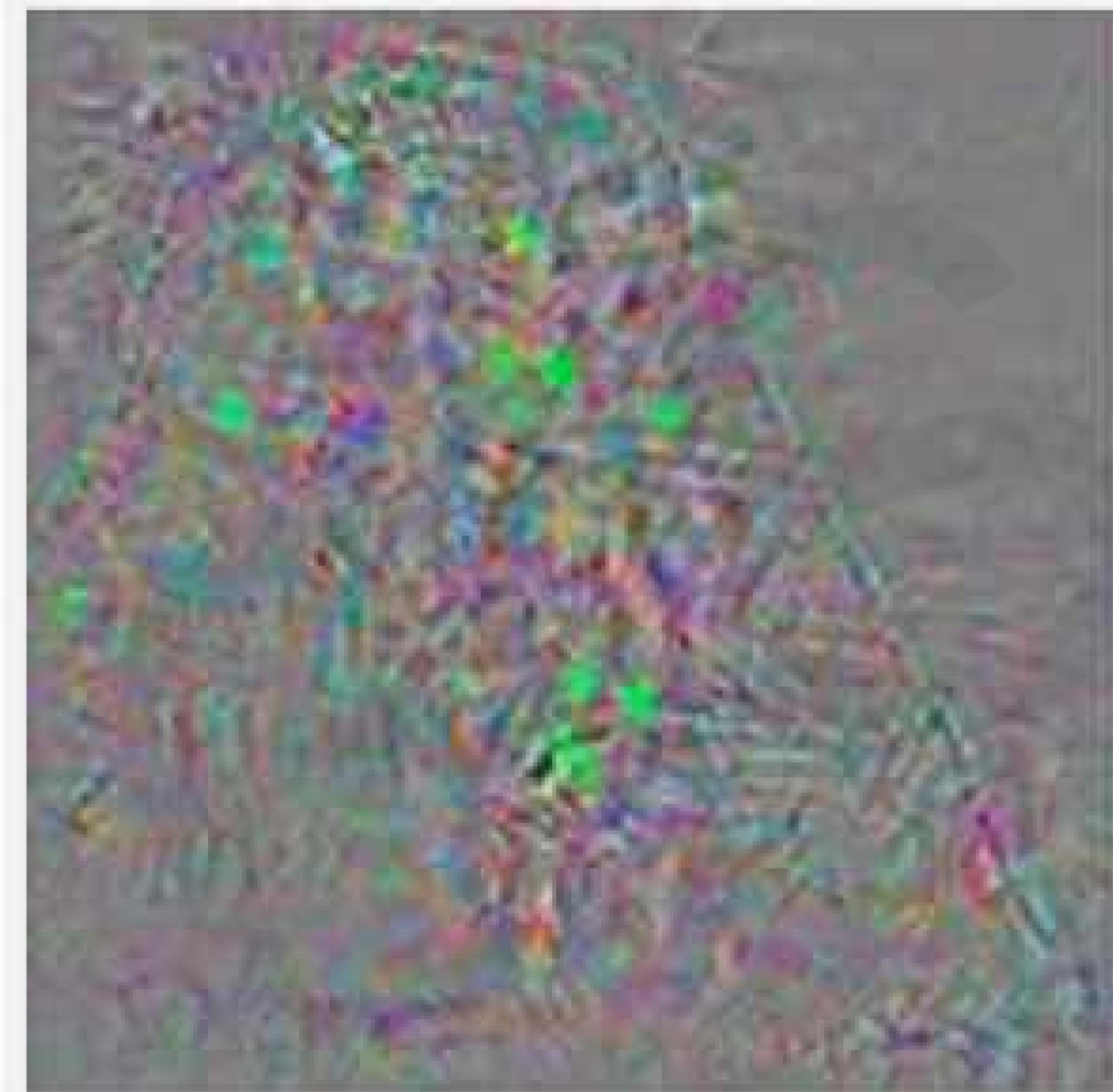
6.S191 Lecture

# Neural Network Failure Modes, Part III



Original image

Temple (97%)



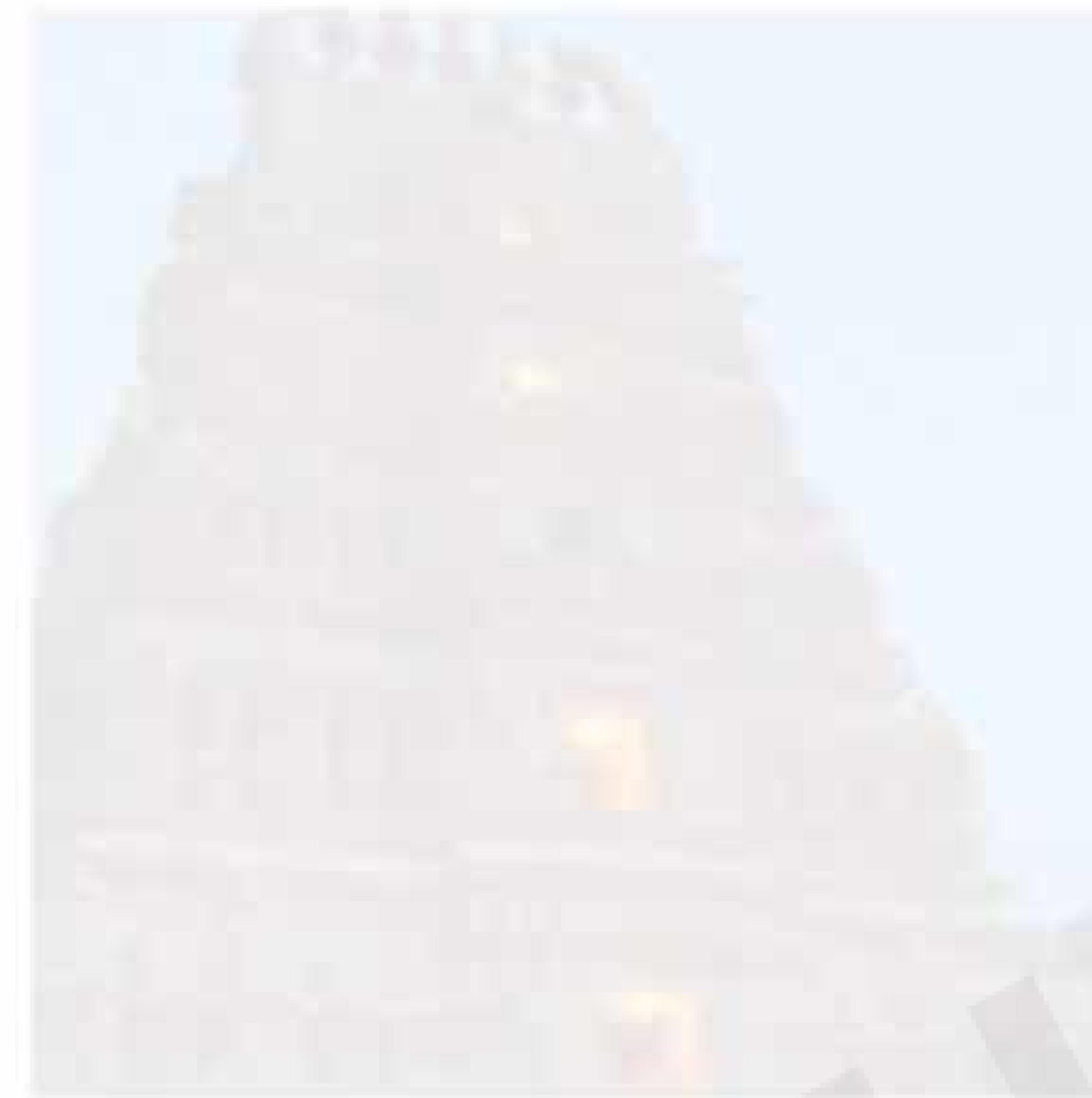
Perturbations



Adversarial example

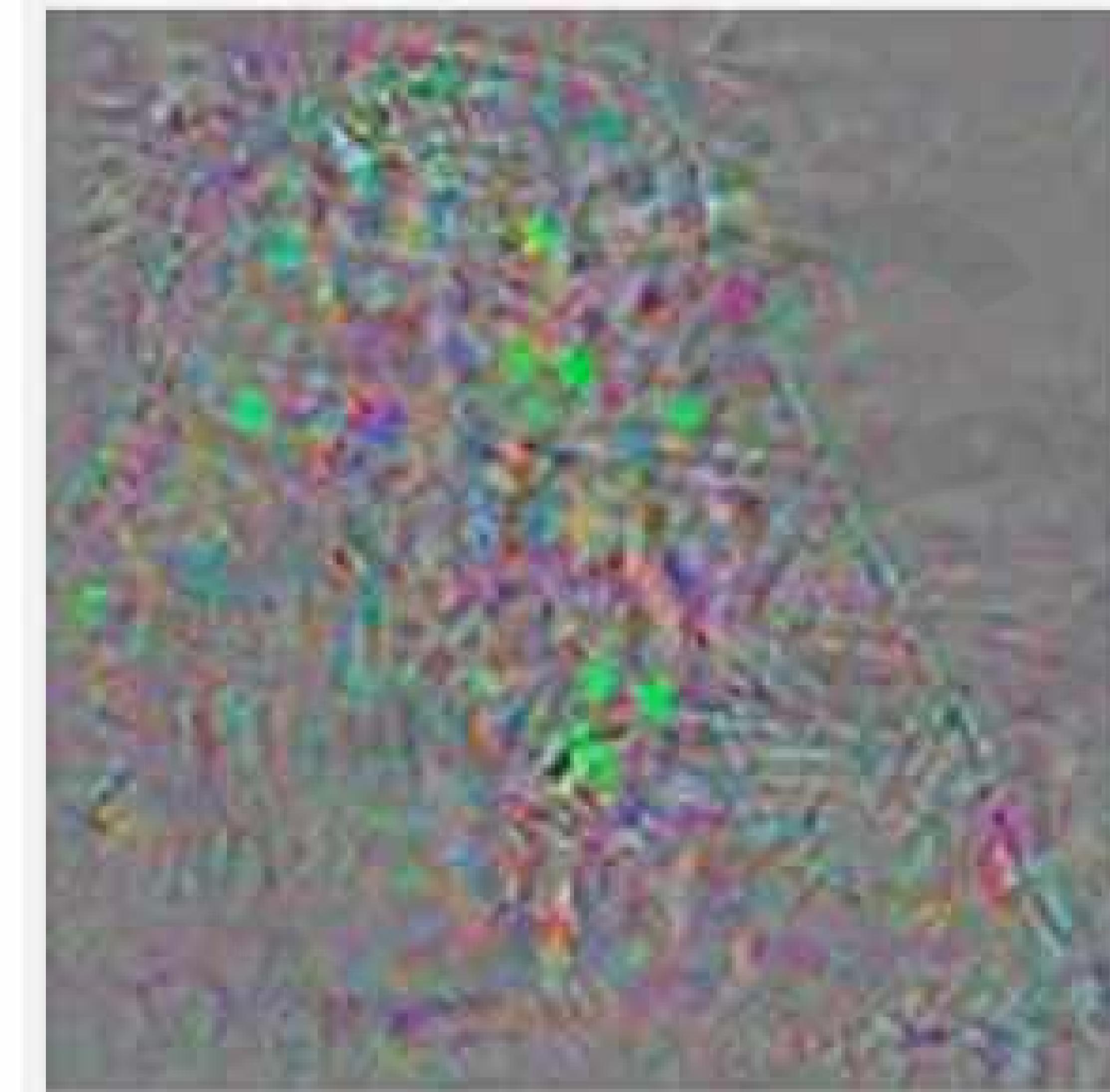
Ostrich (98%)

# Adversarial Attacks on Neural Networks



Original image

Temple (97%)



Perturbations



Adversarial example

Ostrich (98%)

# Adversarial Attacks on Neural Networks

**Remember:**

We train our networks with gradient descent

$$W \leftarrow W - \eta \frac{\partial J(W, x, y)}{\partial W}$$

*“How does a small change in weights decrease our loss”*

# Adversarial Attacks on Neural Networks

## Remember:

We train our networks with gradient descent

$$W \leftarrow W - \eta \frac{\partial J(W, x, y)}{\partial W}$$

*“How does a small change in weights decrease our loss”*

# Adversarial Attacks on Neural Networks

## Remember:

We train our networks with gradient descent

$$W \leftarrow W - \eta \frac{\partial J(W, x, y)}{\partial W}$$

Fix your image  $x$ ,  
and true label  $y$

“How does a small change in weights decrease our loss”

# Adversarial Attacks on Neural Networks

## Adversarial Image:

Modify image to increase error

$$x \leftarrow x + \eta \frac{\partial J(W, x, y)}{\partial x}$$

*“How does a small change in the input increase our loss”*

# Adversarial Attacks on Neural Networks

## Adversarial Image:

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Fix your weights  $\theta$ ,  
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“How does a small change in the input increase our loss”

# Synthesizing Robust Adversarial Examples



■ classified as turtle   ■ classified as rifle  
■ classified as other

# Algorithmic Bias

Overcoming Racial Bias In AI Systems And Startlingly Even In AI Self-Driving Cars

## AI expert calls for end to UK use of 'racially biased' algorithms

### Gender bias in AI: building fairer algorithms

#### Millions of black people affected by racial bias in health-care algorithms

Study reveals rampant racism in decision-making software used by US hospitals — and highlights ways to correct it.

Google 'fixed' its racist algorithm by removing gorillas from its image-labeling tech

#### The Best Algorithms Struggle to Recognize Black Faces Equally

US government tests find even top-performing facial recognition systems misidentify blacks at rates five to 10 times higher than they do whites.

Racial bias in a medical algorithm favors white patients over sicker black patients

### AI Bias Could Put Women's Lives At Risk - A Challenge For Regulators

#### Bias in AI: A problem recognized but still unresolved

Amazon, Apple, Google, IBM, and Microsoft worse at transcribing black people's voices than white people's with AI voice recognition, study finds

#### When It Comes to Gorillas, Google Photos Remains Blind

Google promised a fix after its photo-categorization software labeled black people as gorillas in 2015. More than two years later, it hasn't found one.

### *The Week in Tech: Algorithmic Bias Is Bad. Uncovering It Is Good.*

Artificial Intelligence has a gender bias problem – just ask Siri



6.S191 Lab



Massachusetts  
Institute of  
Technology

# Neural Network Limitations...

- Very **data hungry** (eg. often millions of examples)
- **Computationally intensive** to train and deploy (tractably requires GPUs)
- Easily fooled by **adversarial examples**
- Can be subject to **algorithmic bias**
- Poor at **representing uncertainty** (how do you know what the model knows?)
- Uninterpretable **black boxes**, difficult to trust
- Difficult to **encode structure** and prior knowledge during learning
- **Finicky to optimize**: non-convex, choice of architecture, learning parameters
- Often require **expert knowledge** to design, fine tune architectures

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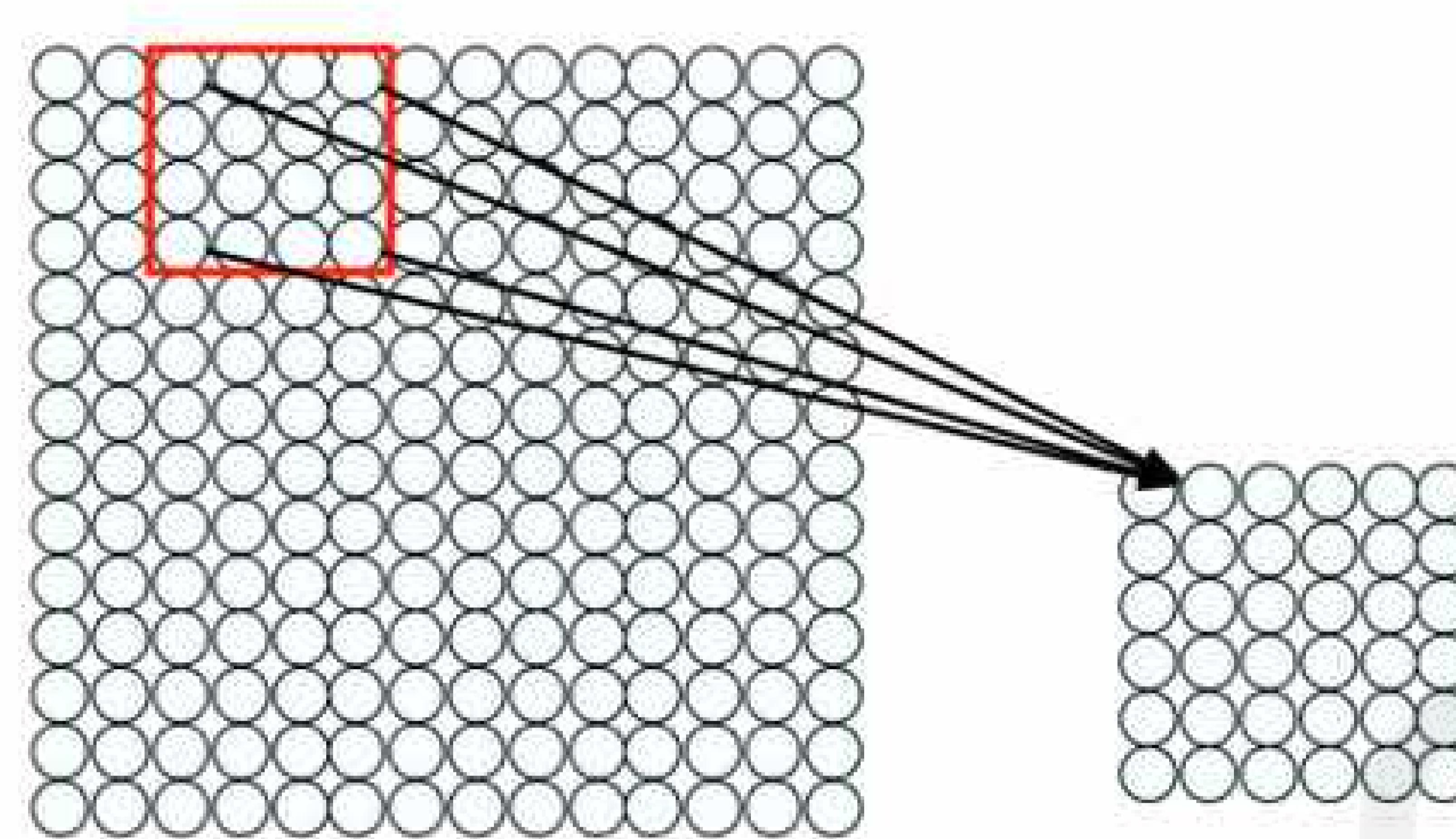
**6.S191 Lab  
+ Lecture**

# Neural Network Limitations...

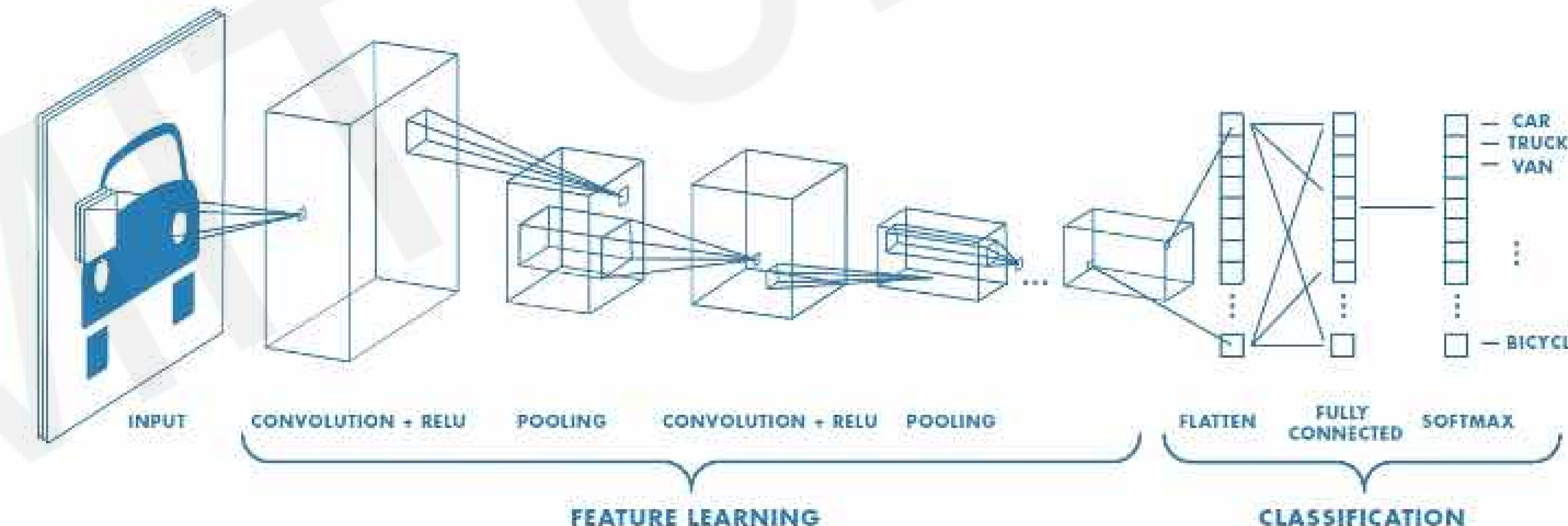
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# New Frontiers I: Encoding Structure into Deep Learning

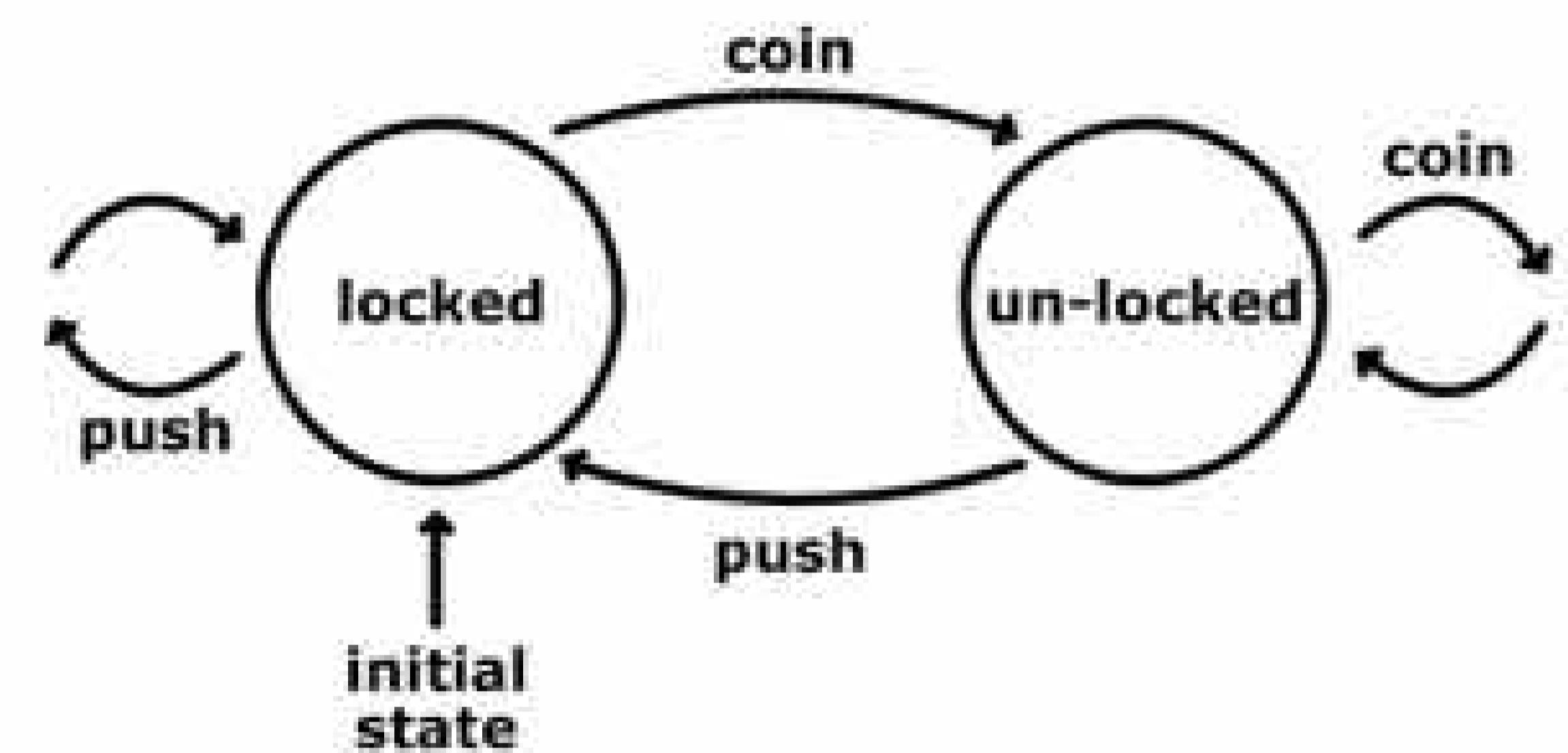
# CNNs: Using Spatial Structure



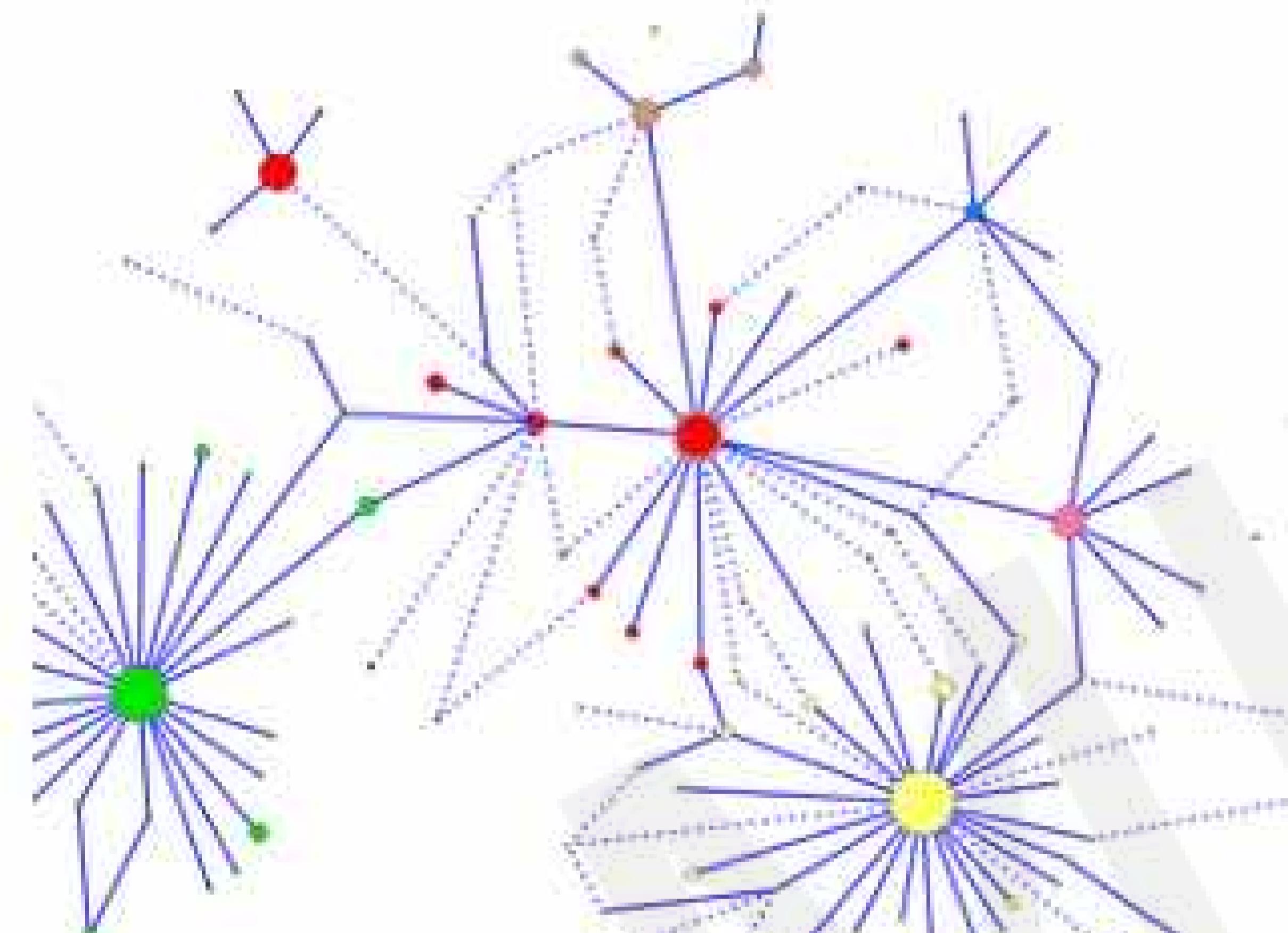
- 1) Apply a set of weights to extract **local features**
- 2) Use **multiple filters** to extract different features
- 3) **Spatially share** parameters of each filter



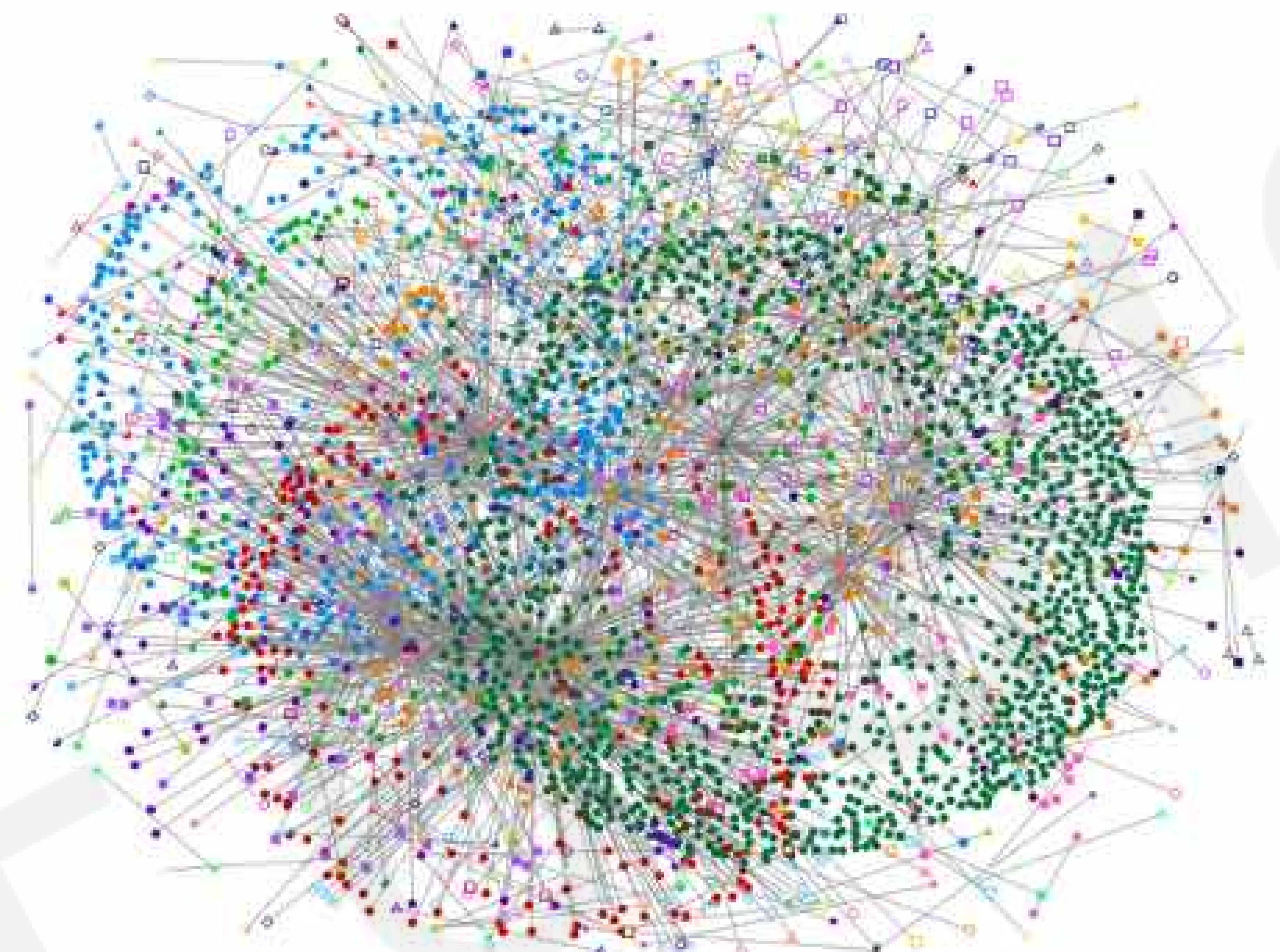
# Graphs as a Structure for Representing Data



# State Machines

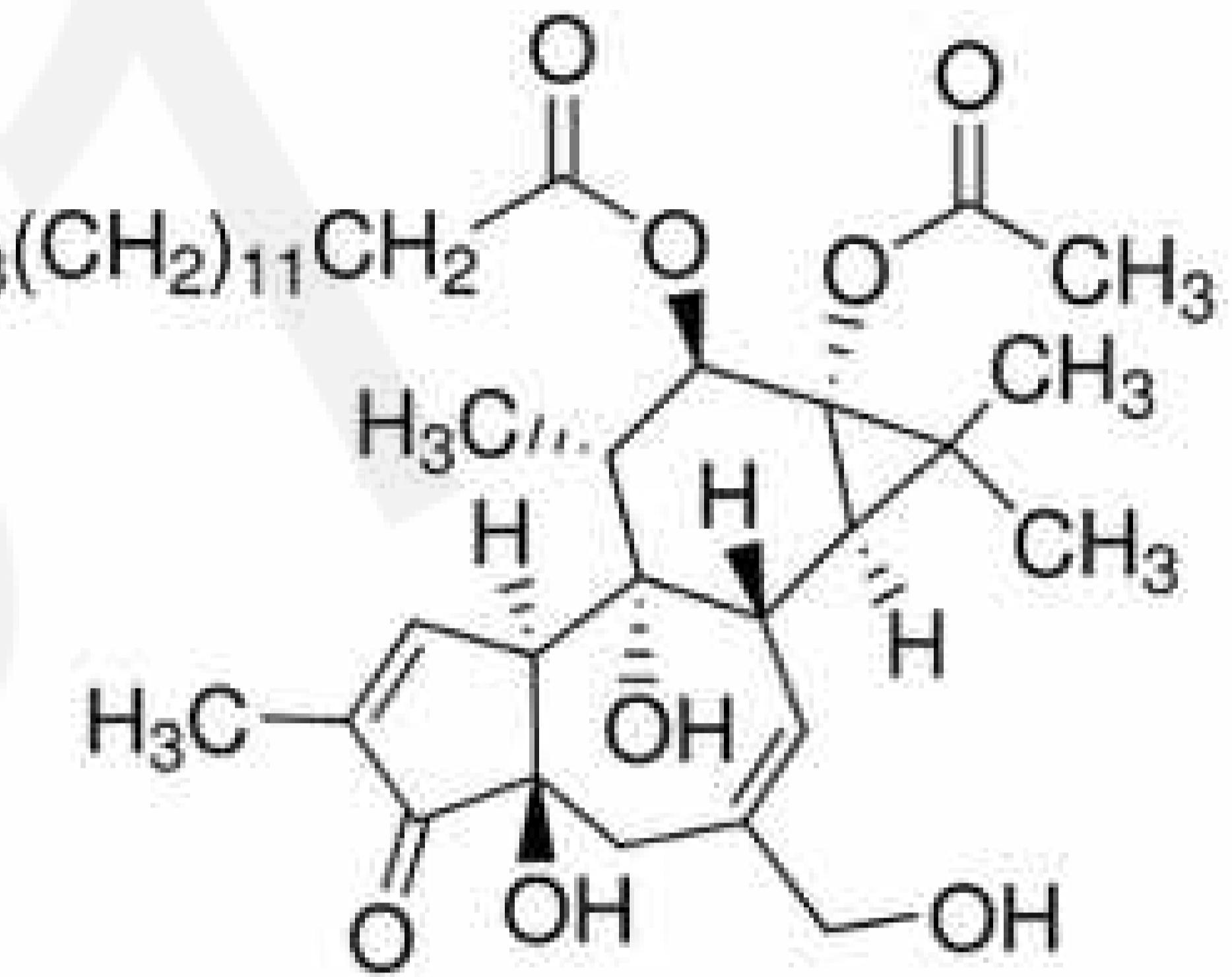


# Biological Networks



# Social Networks

Many real-world data – such as networks – cannot be captured by “standard” encodings or Euclidean geometries



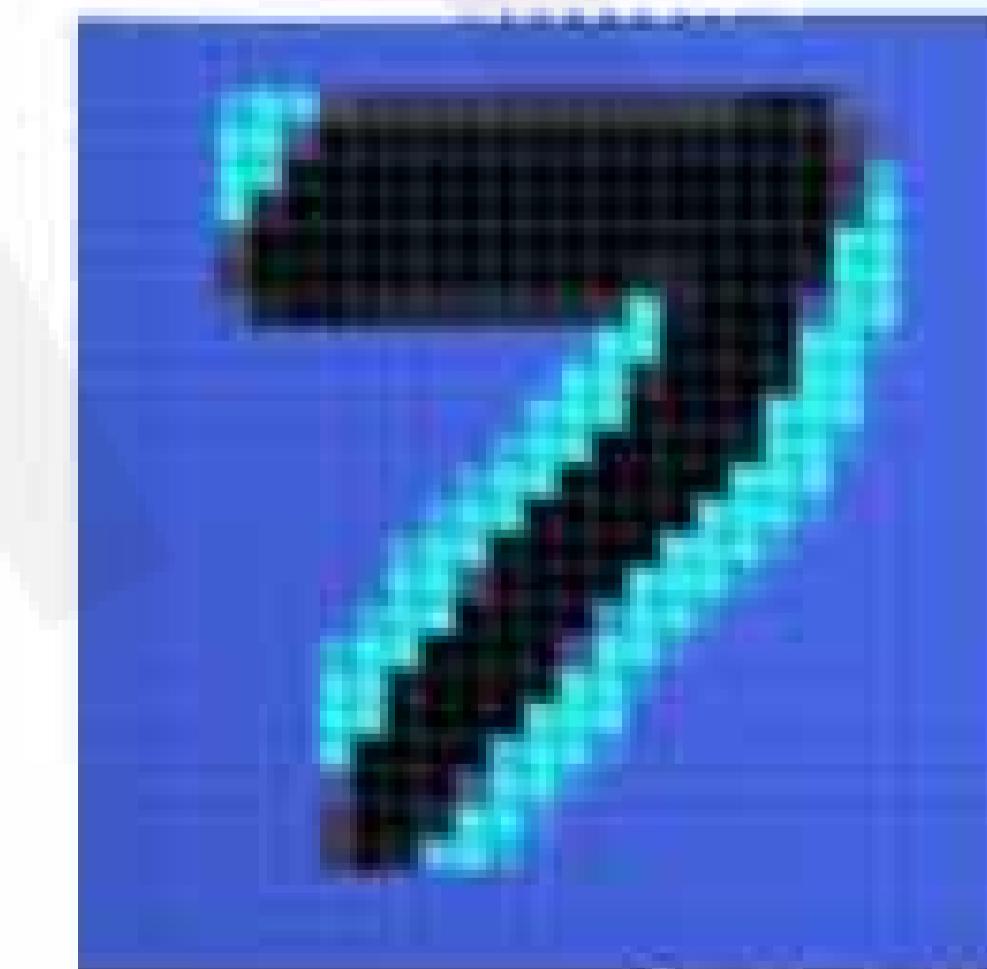
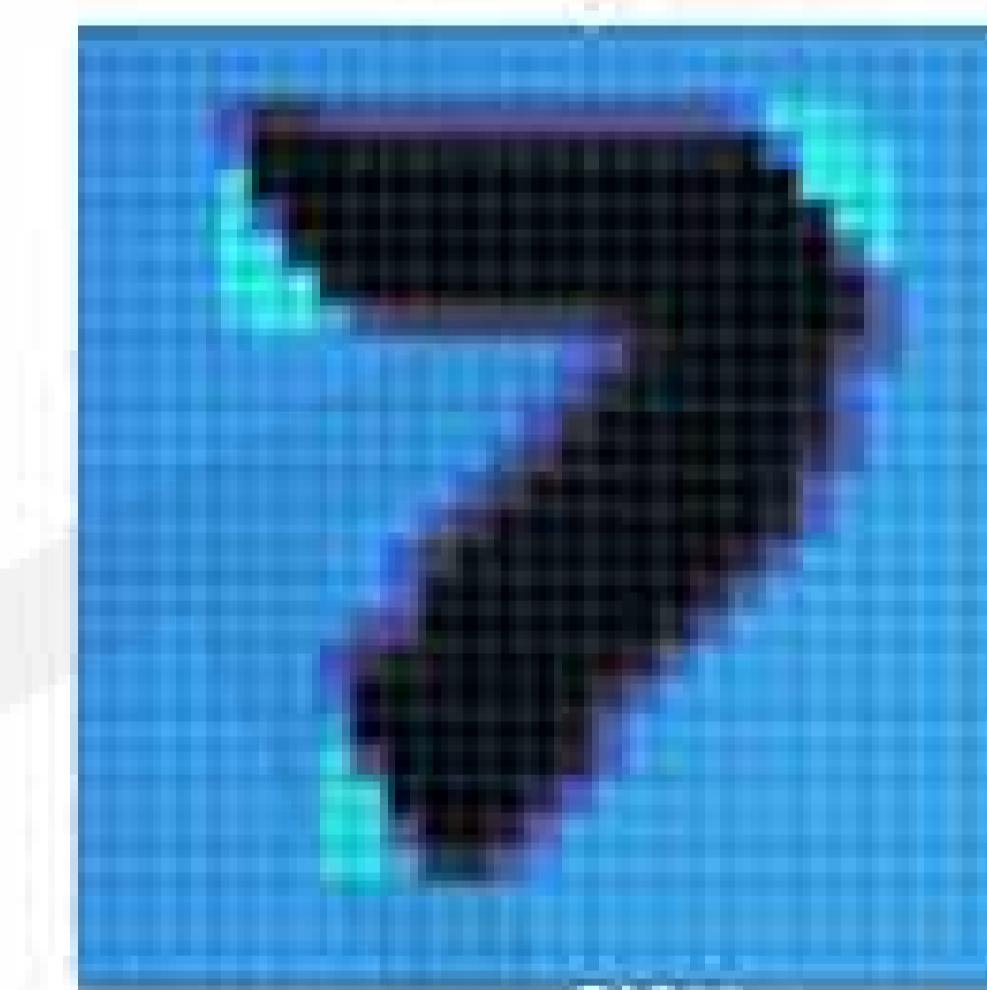
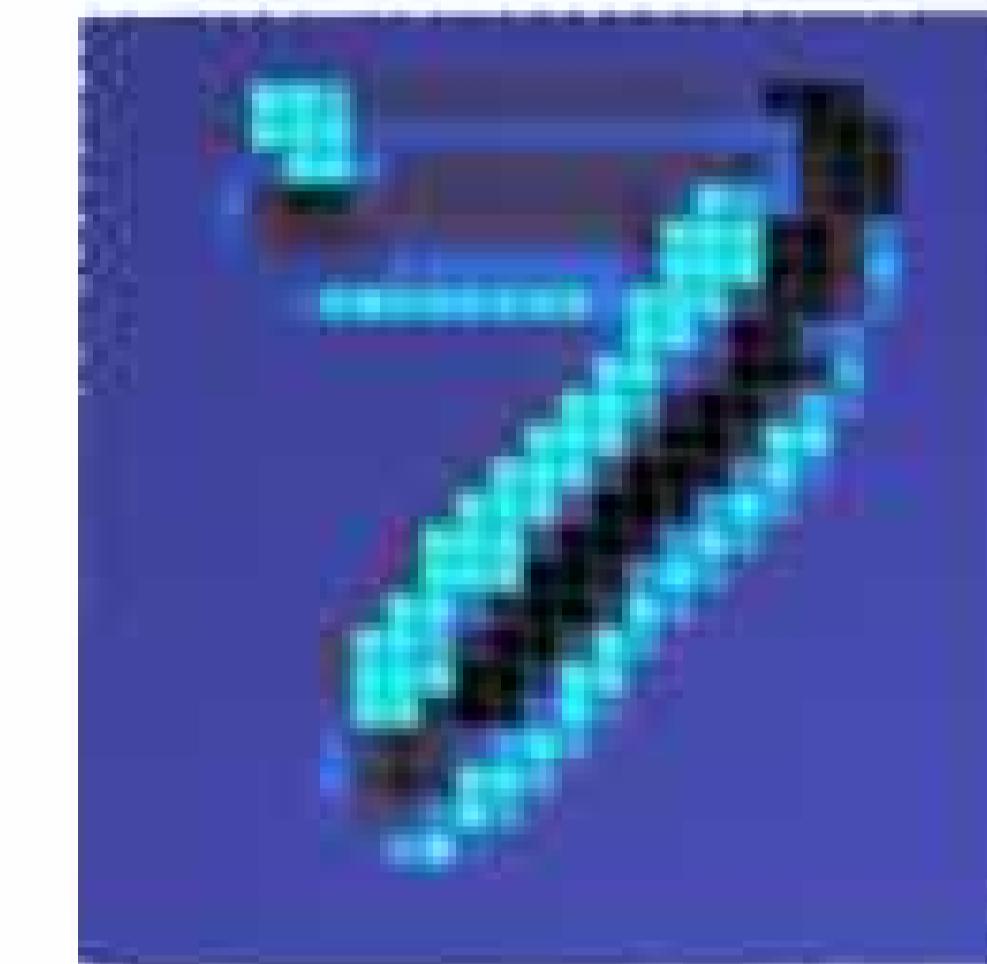
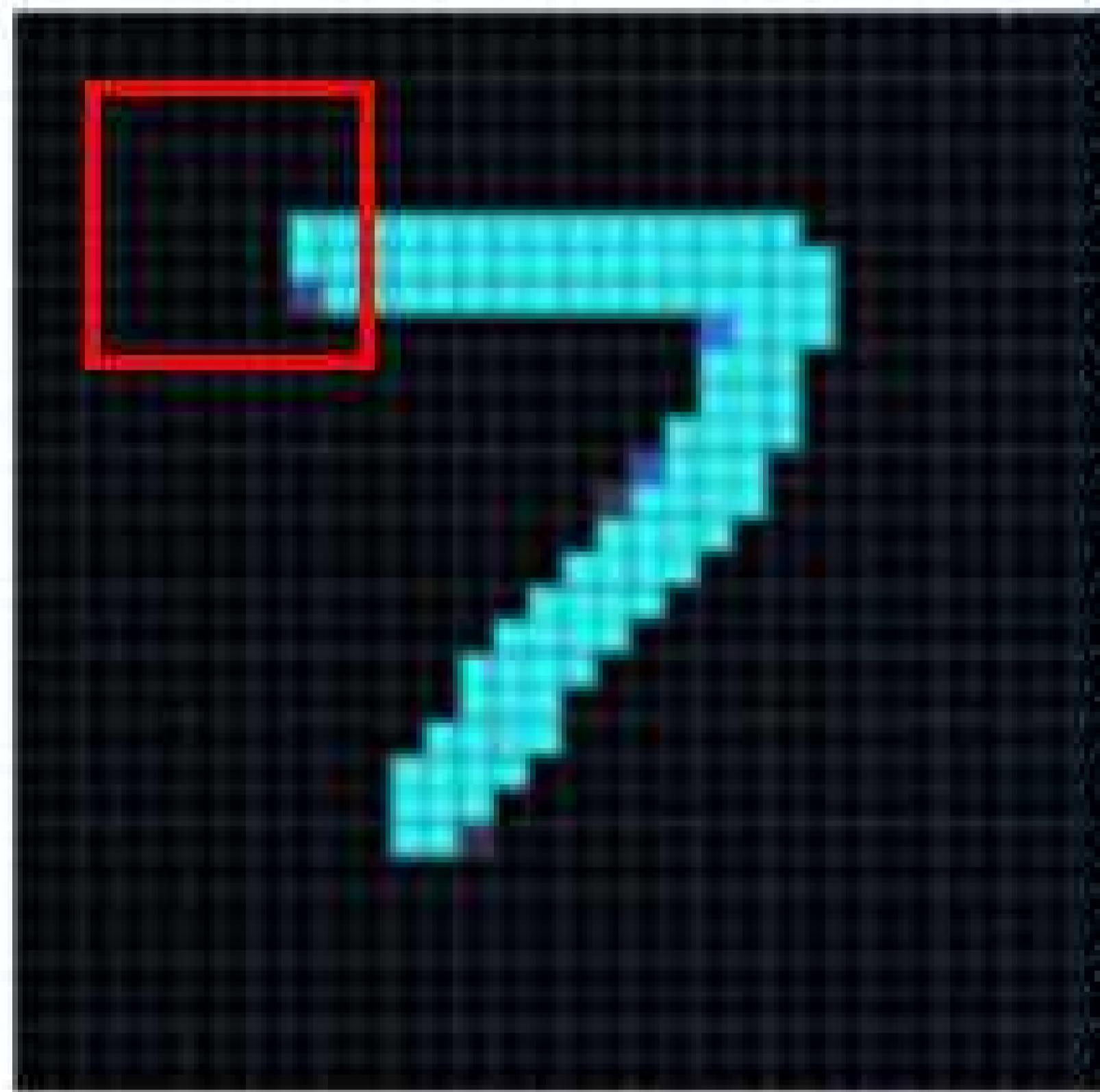
## Molecules



# Mobility & Transport

# Graph Convolutional Networks

## Convolutional Networks

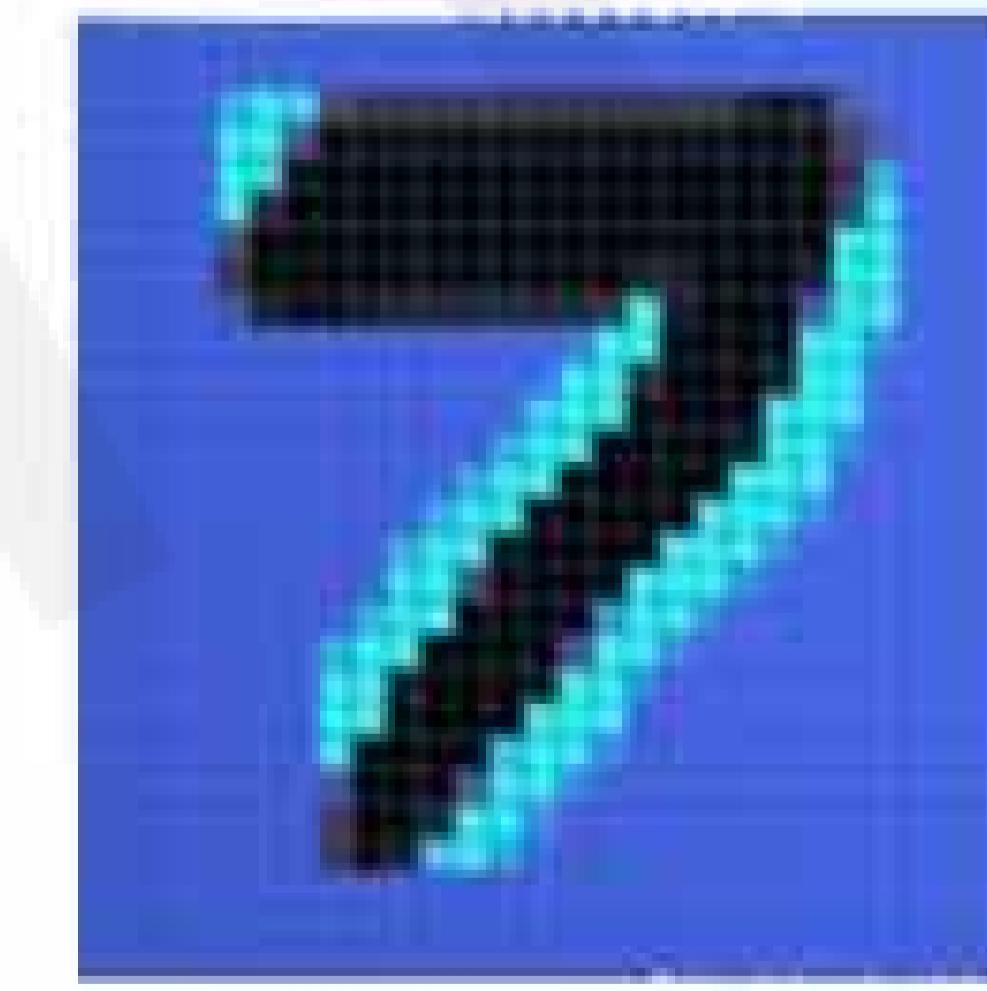
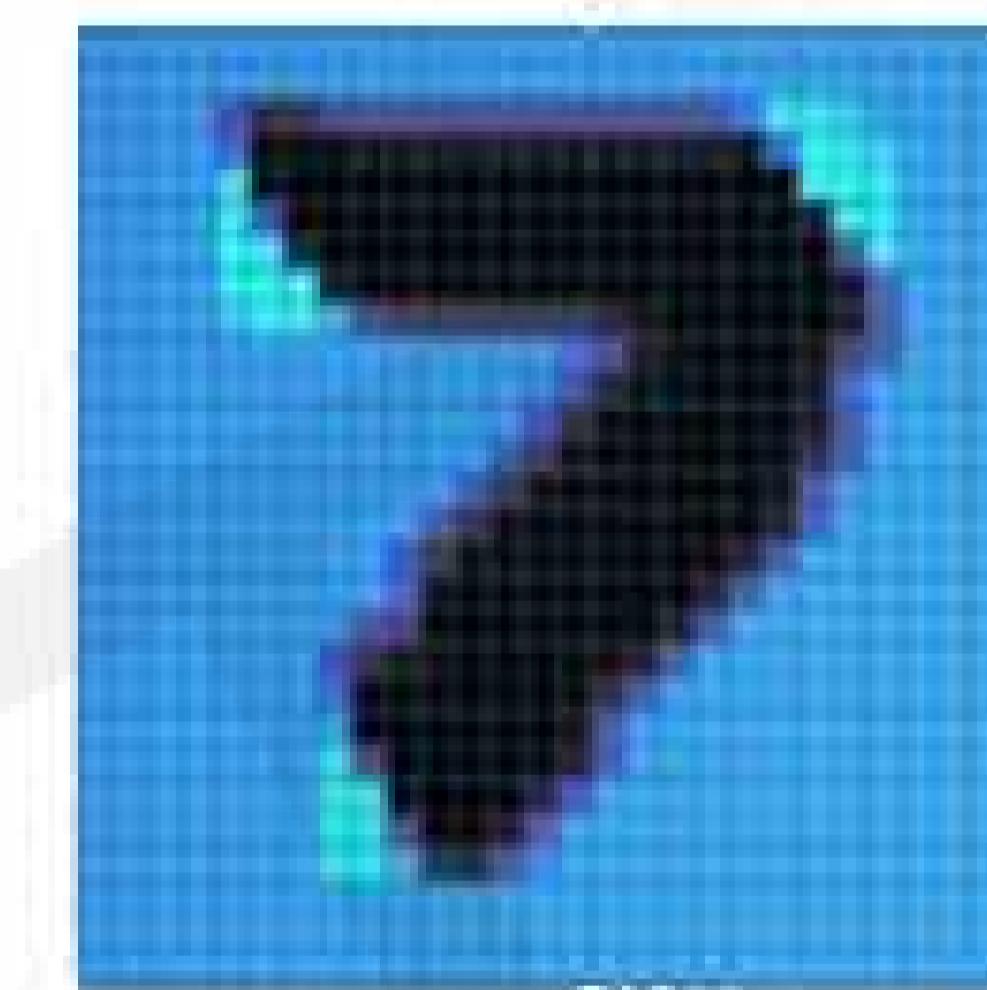
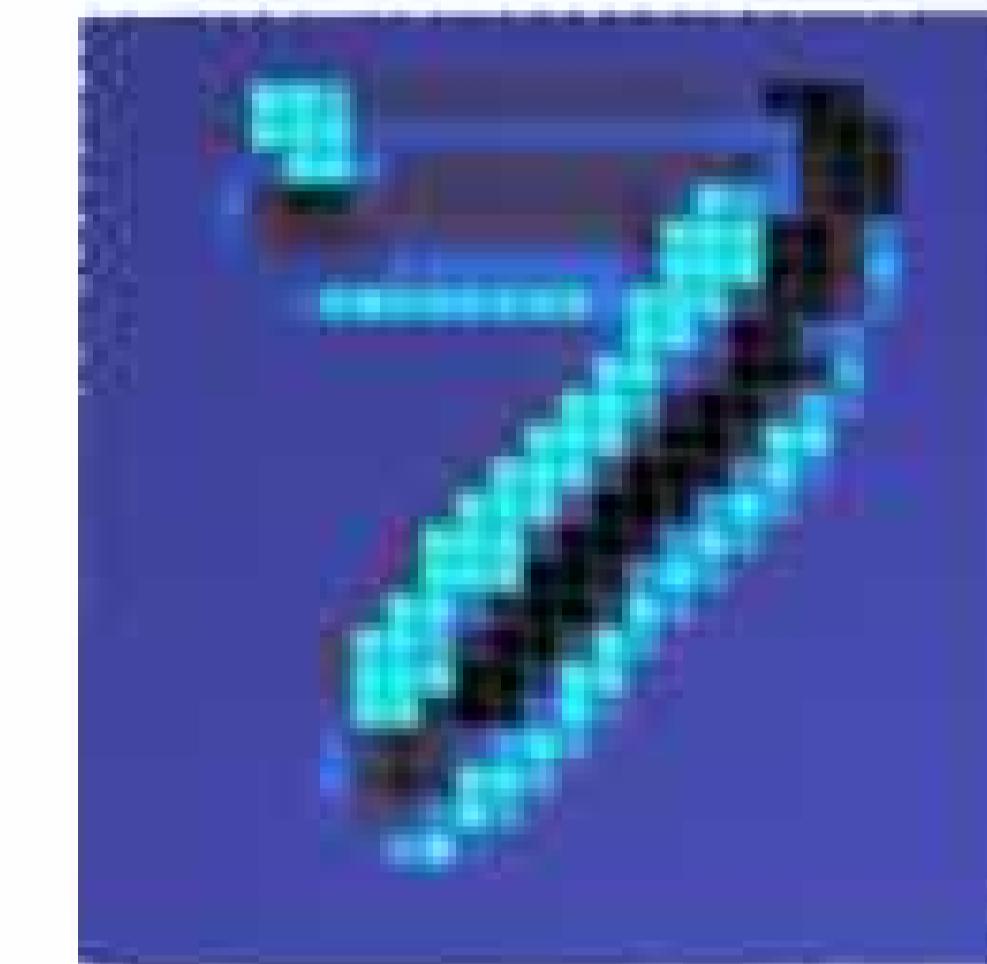


## Graph Convolutional Networks (GCNs)



# Graph Convolutional Networks

## Convolutional Networks

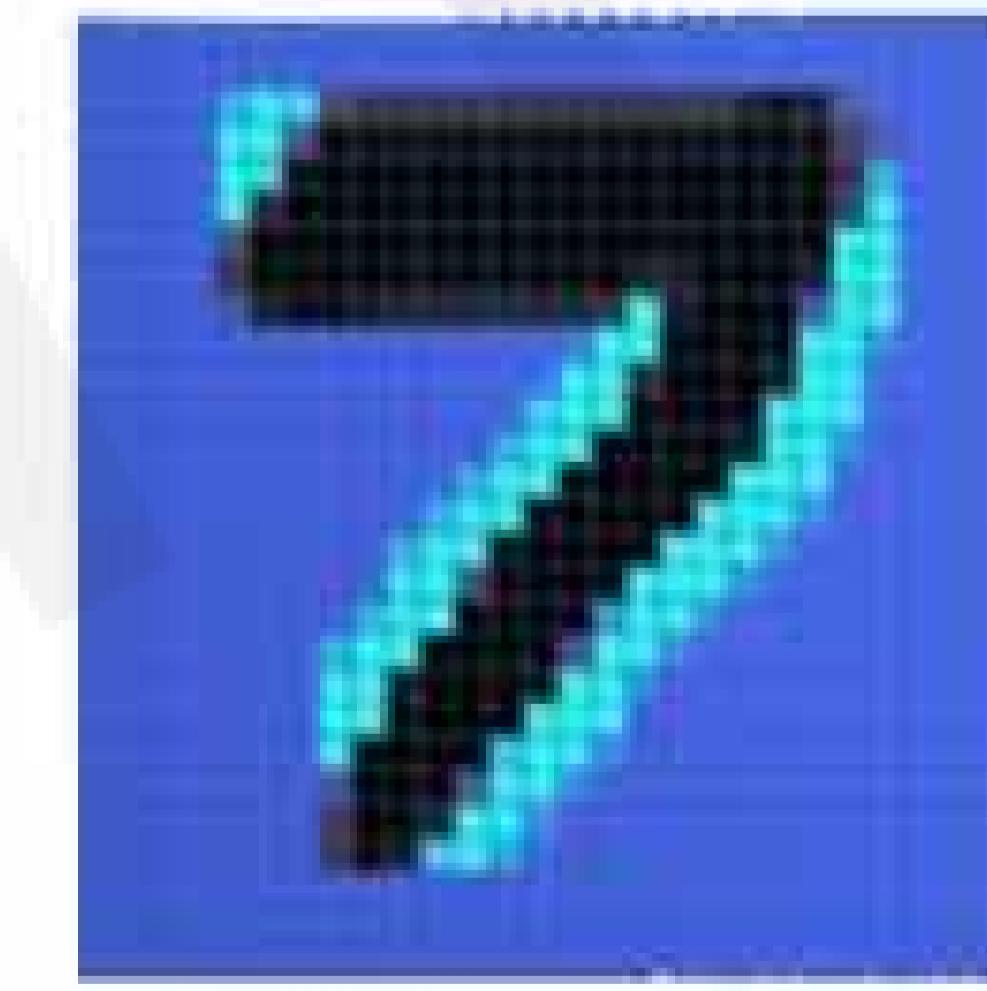
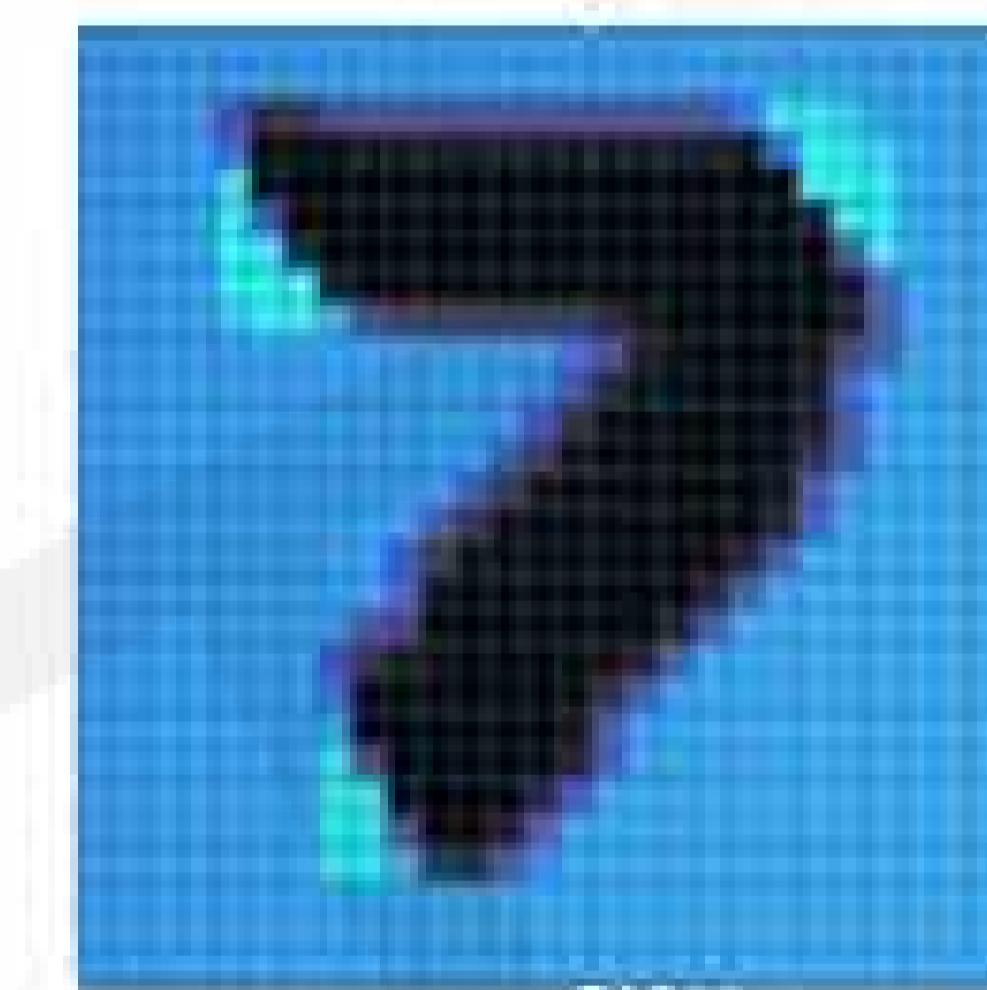
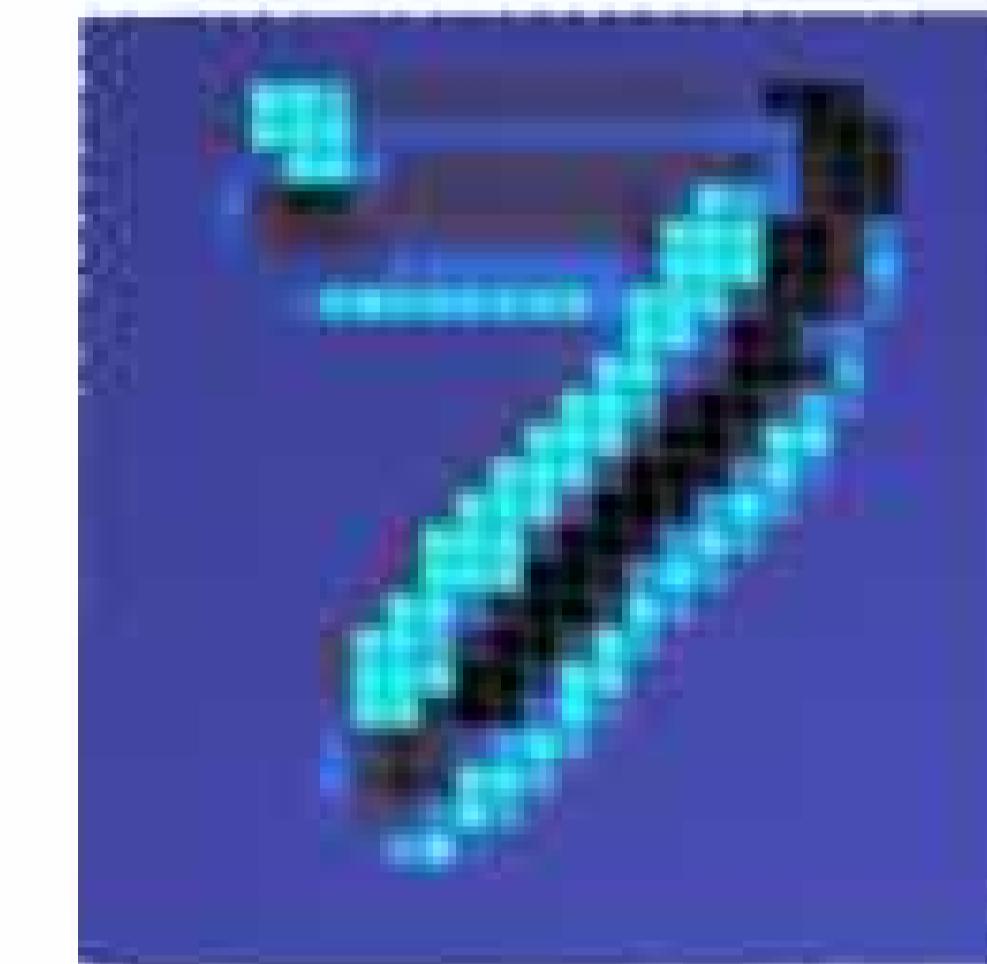
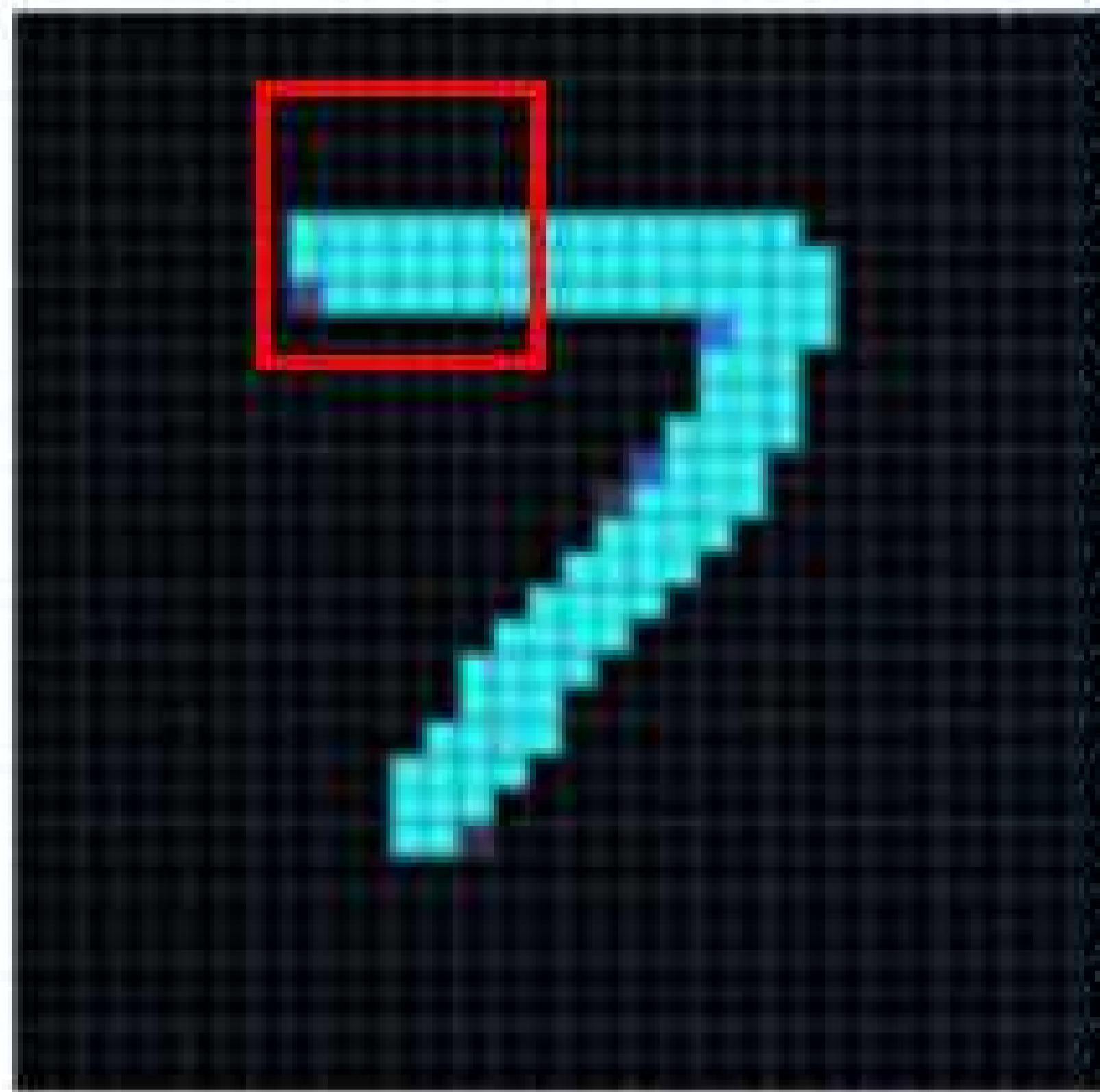


## Graph Convolutional Networks (GCNs)



# Graph Convolutional Networks

## Convolutional Networks

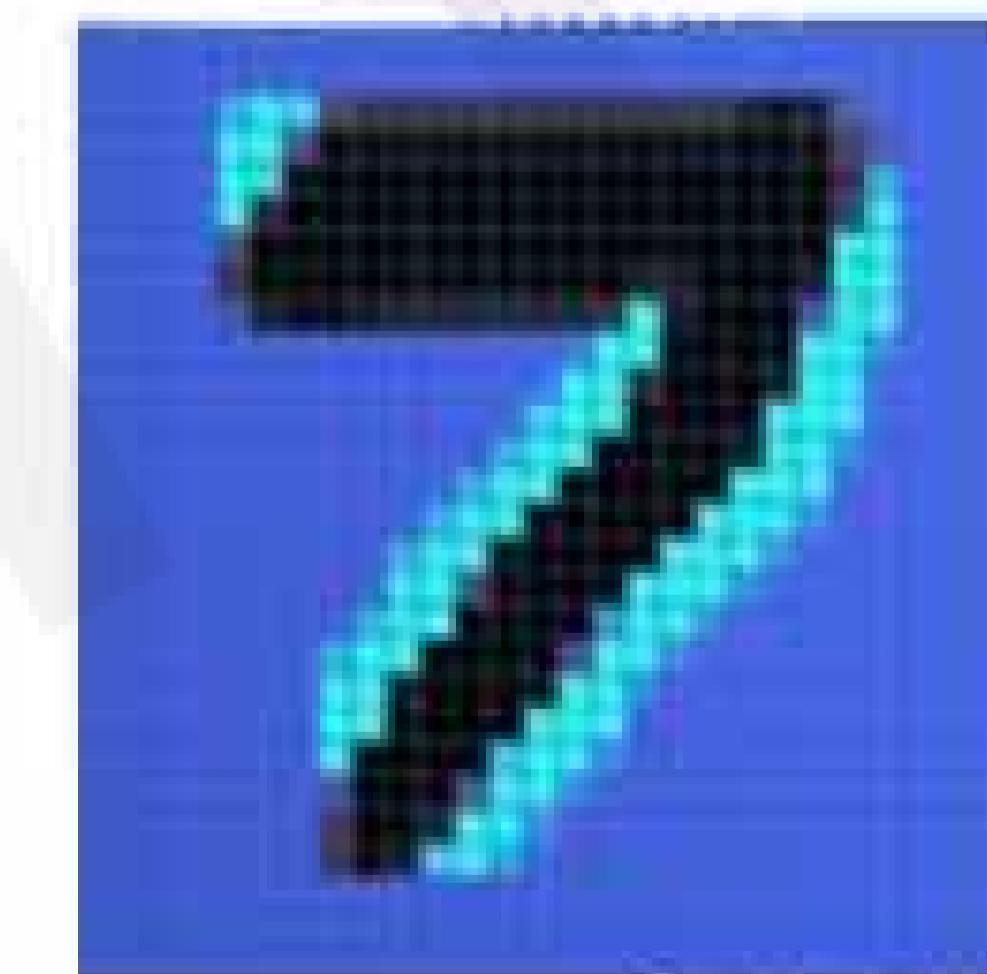
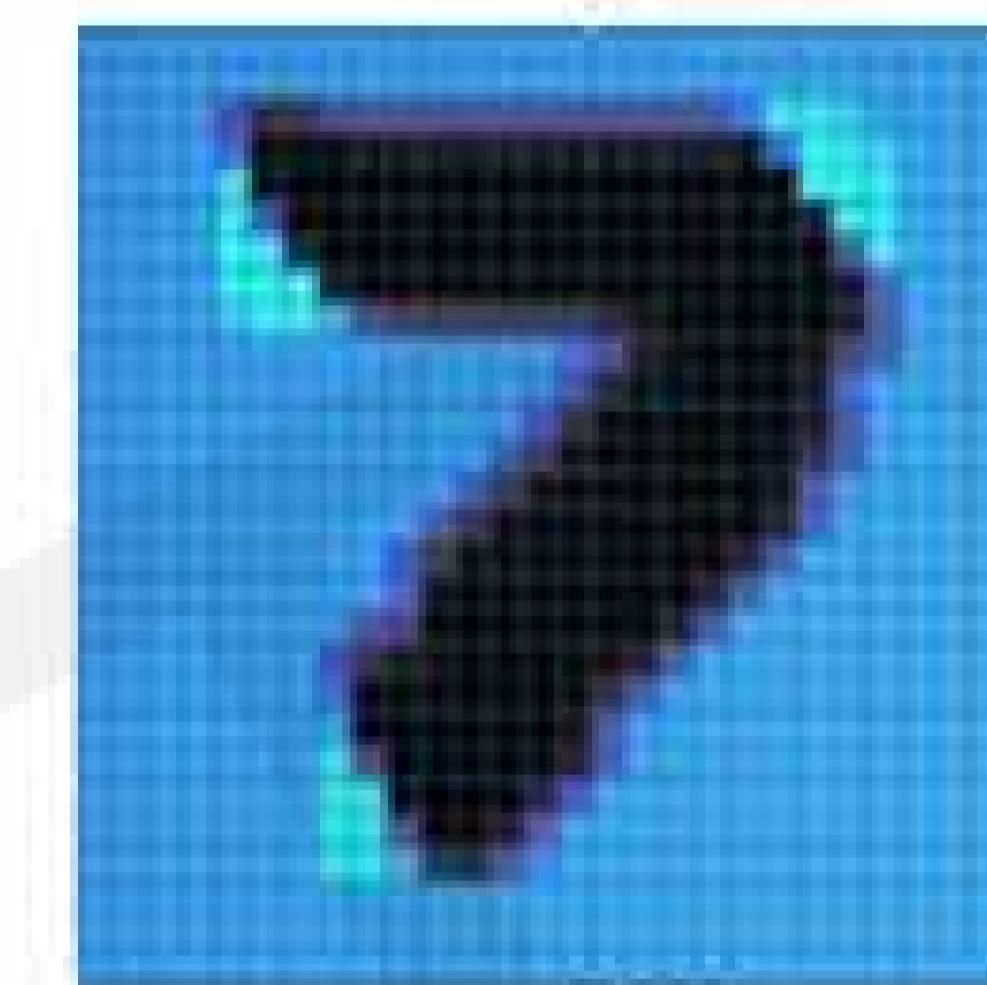
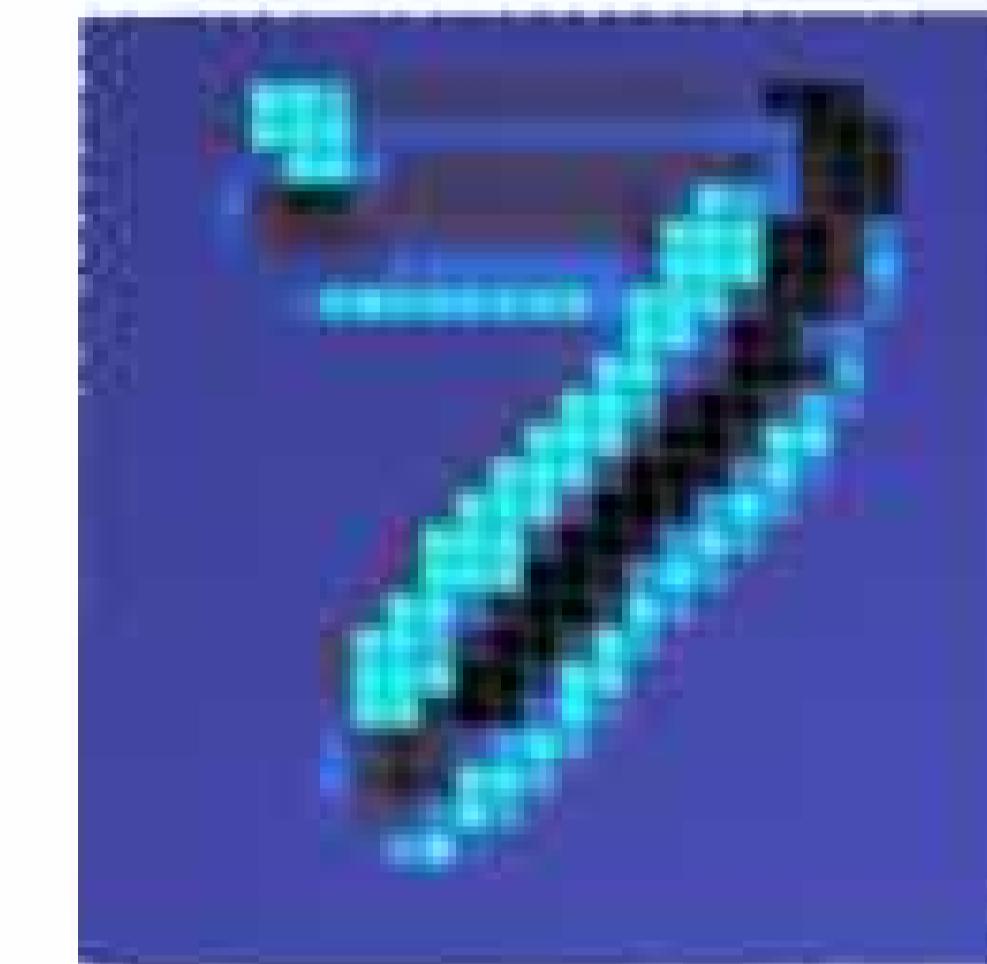
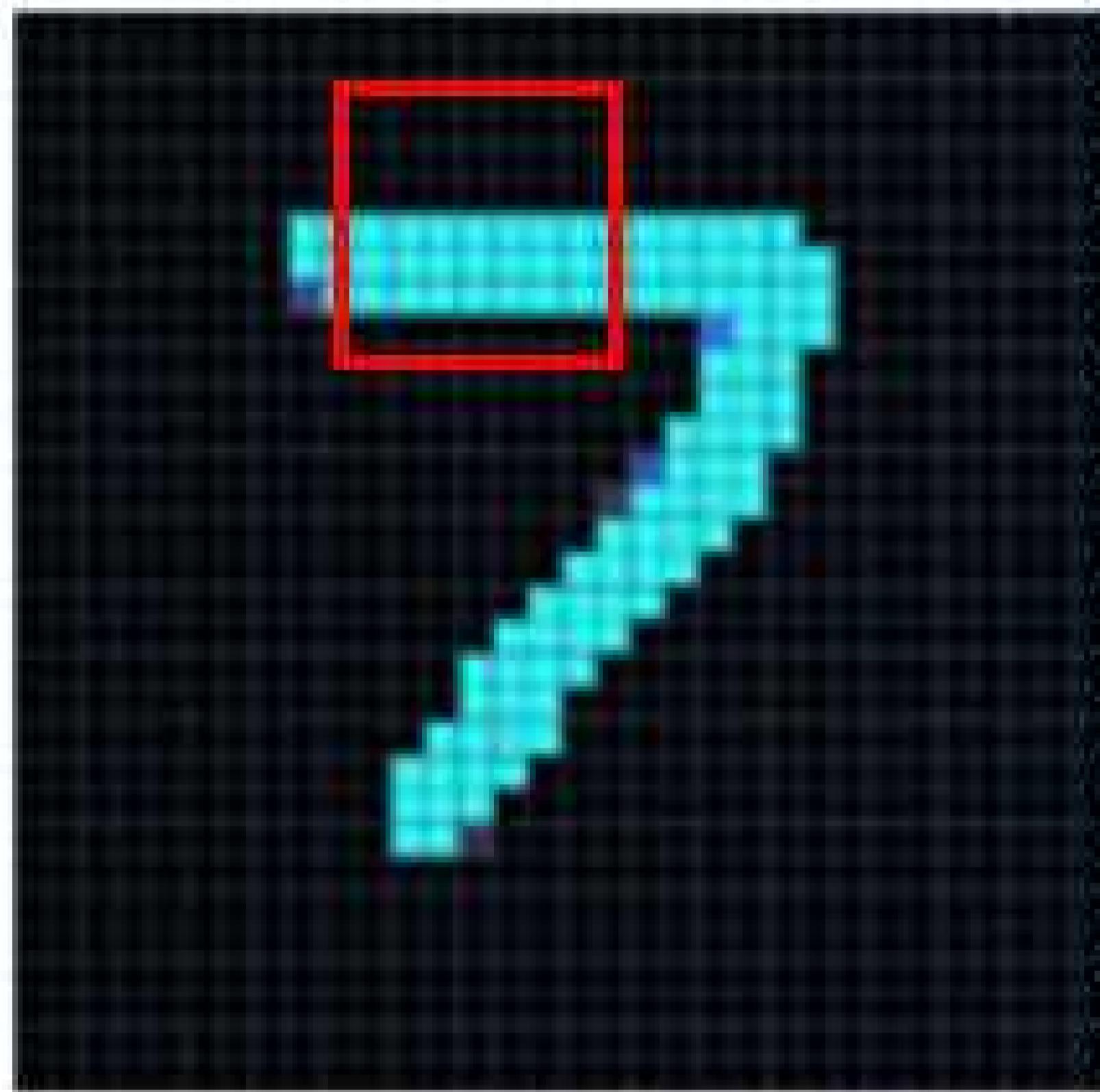


## Graph Convolutional Networks (GCNs)



# Graph Convolutional Networks

## Convolutional Networks

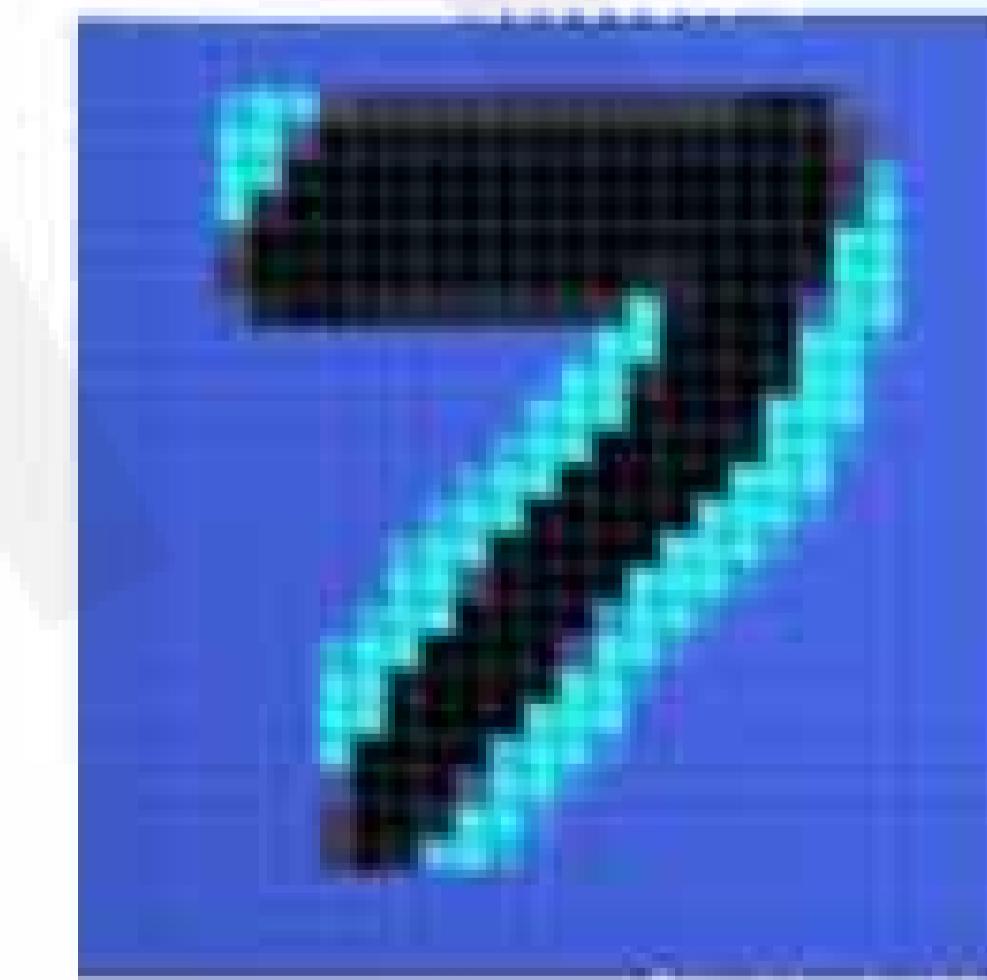
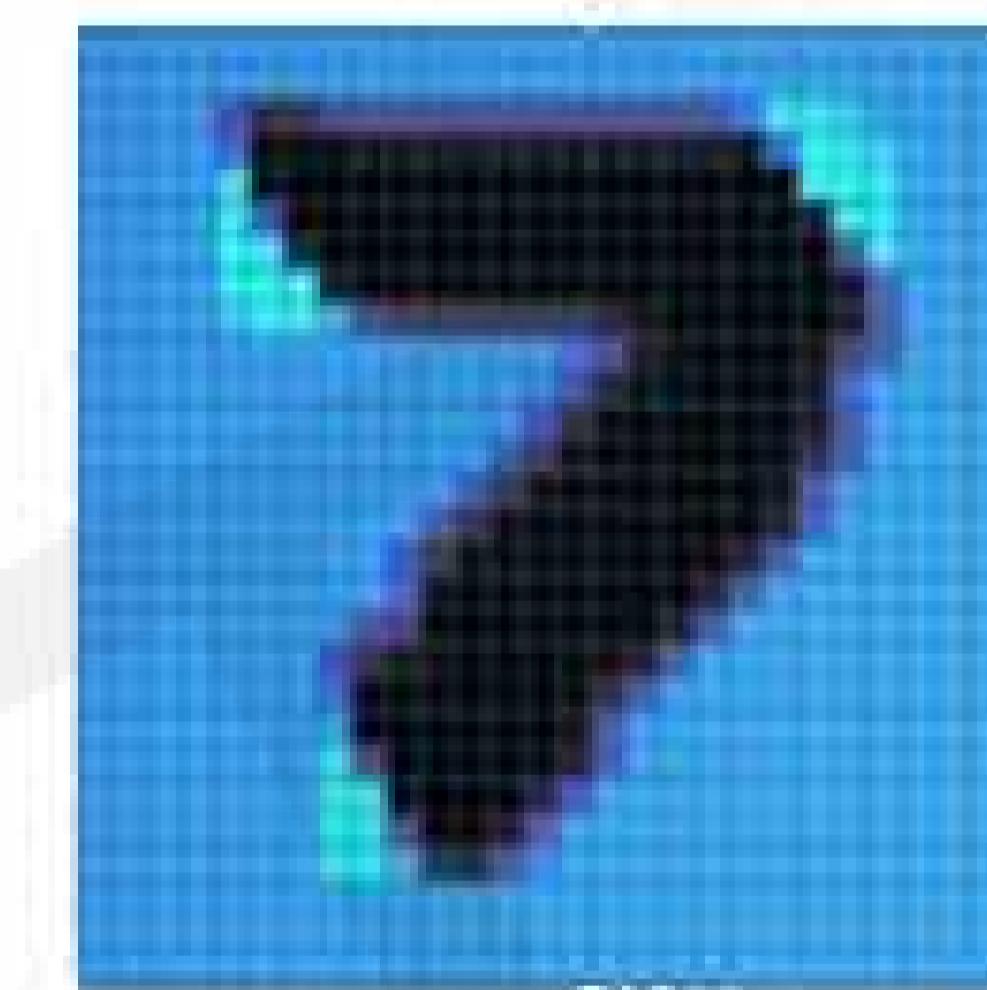
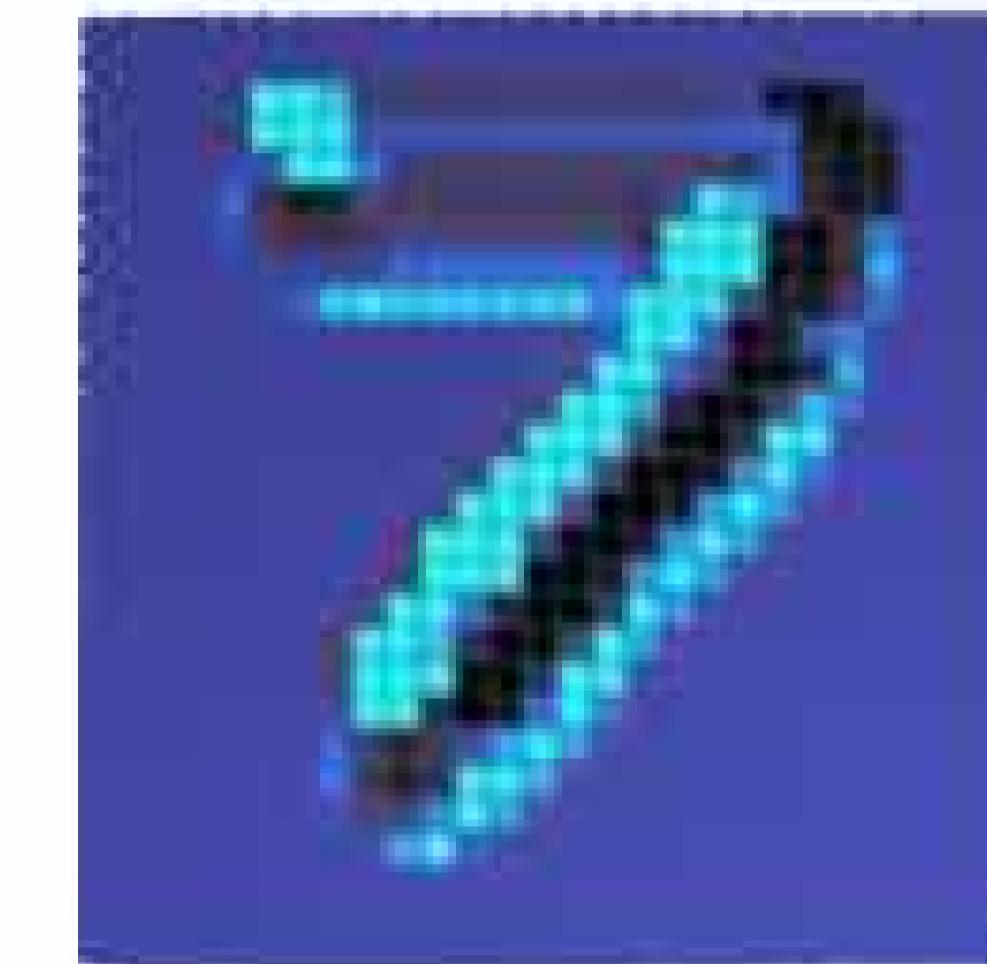
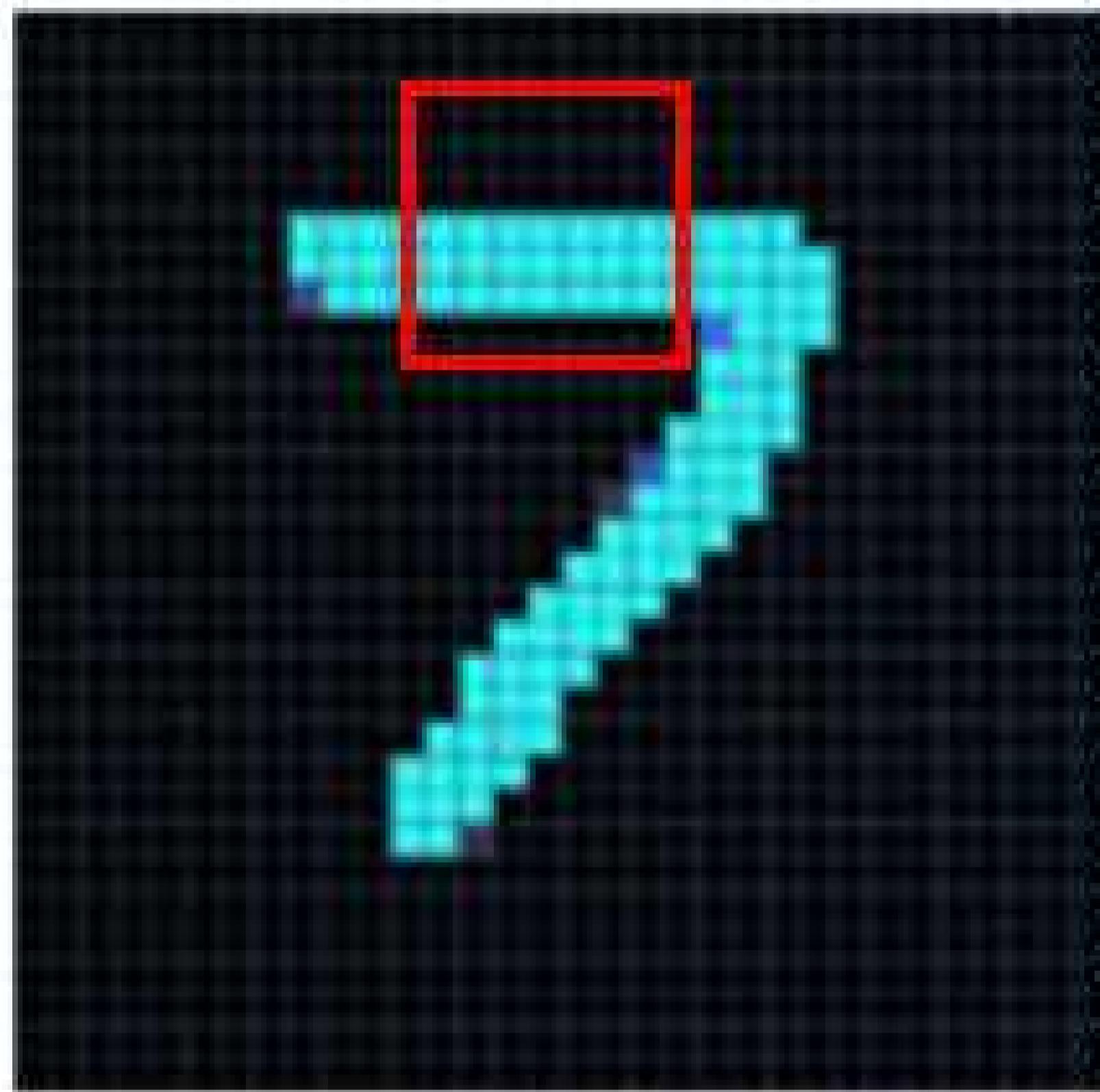


## Graph Convolutional Networks (GCNs)



# Graph Convolutional Networks

## Convolutional Networks



## Graph Convolutional Networks (GCNs)

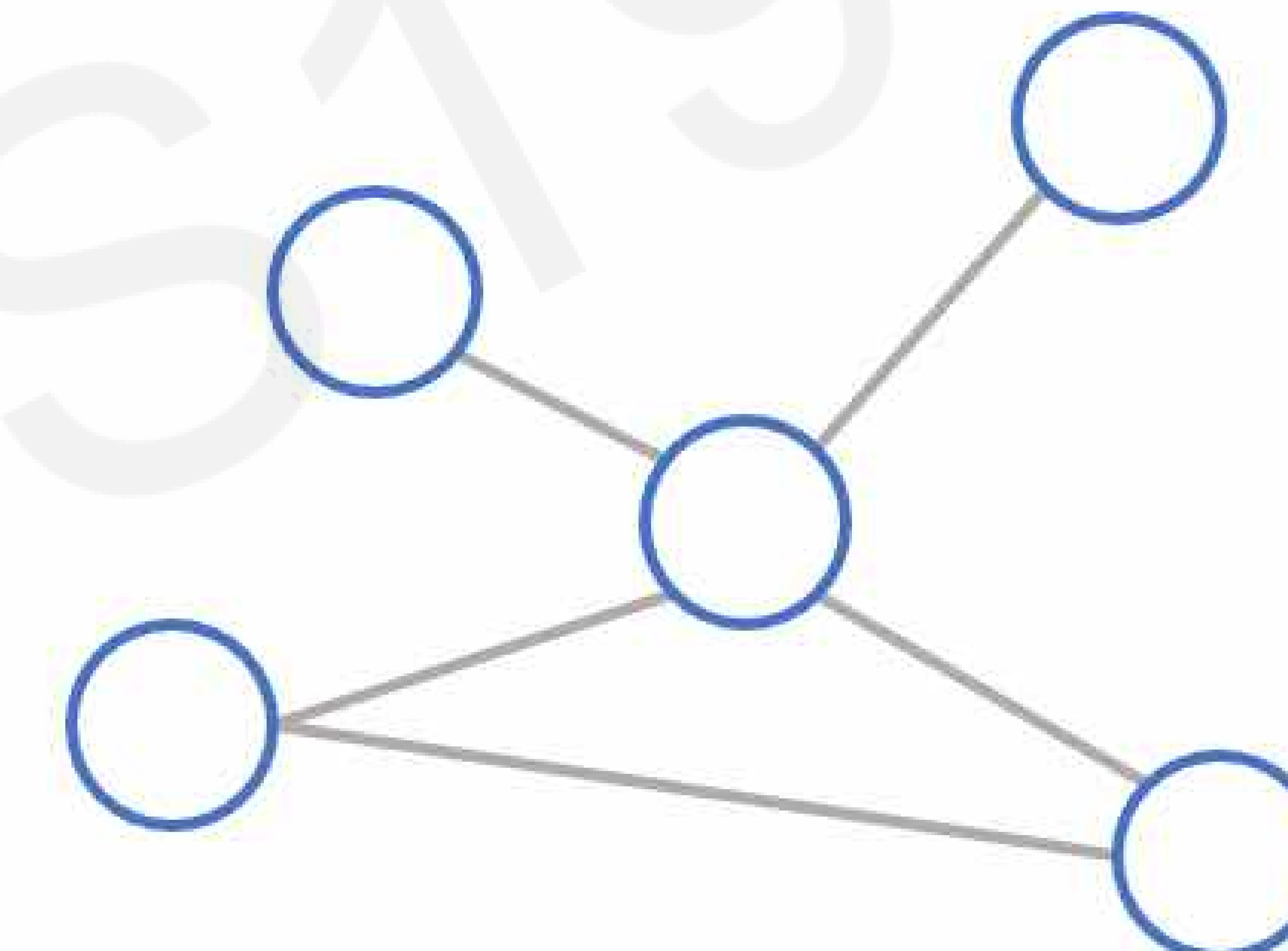


# Graph Convolutional Networks

Convolutional Networks

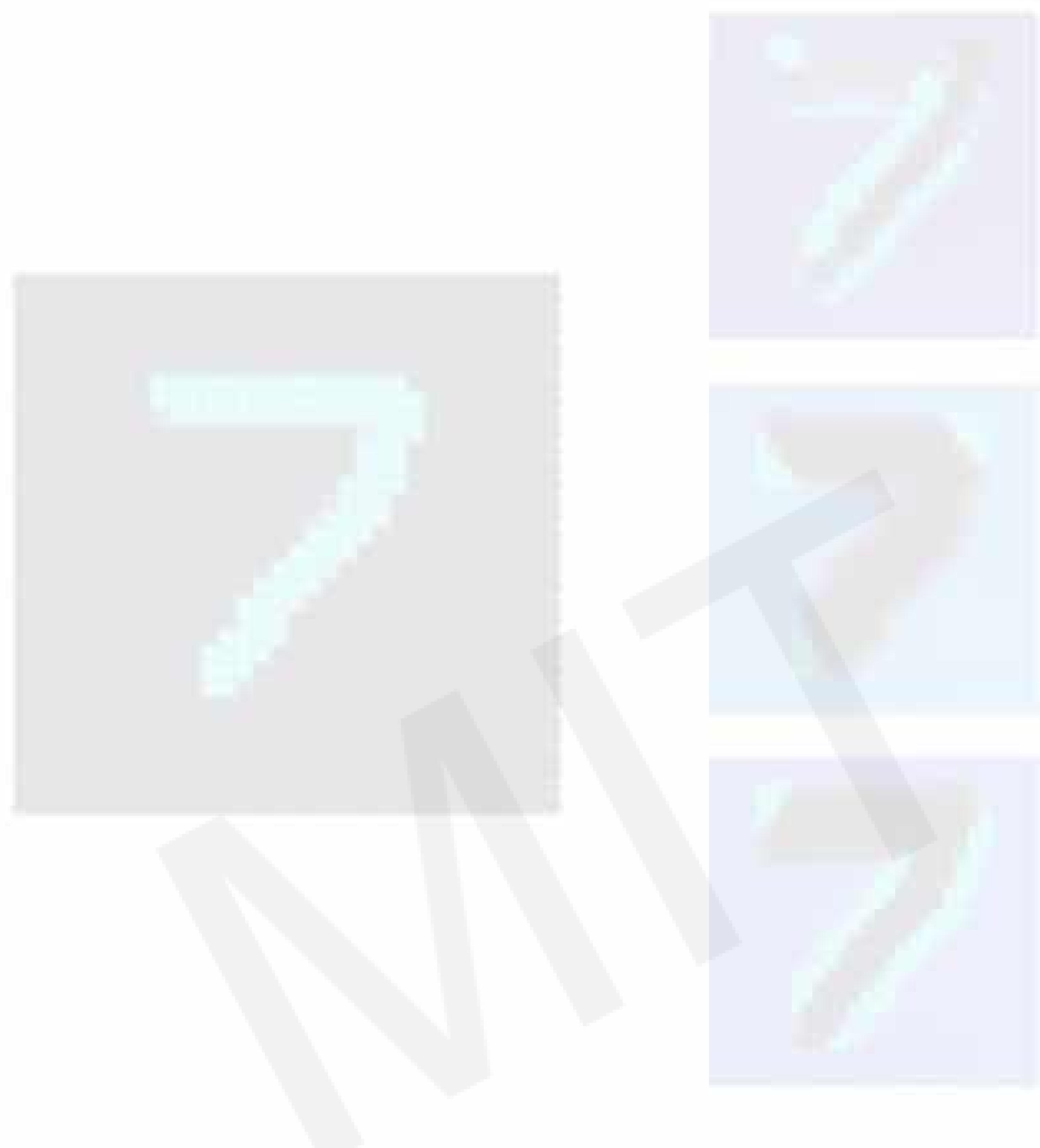


Graph Convolutional Networks (GCNs)

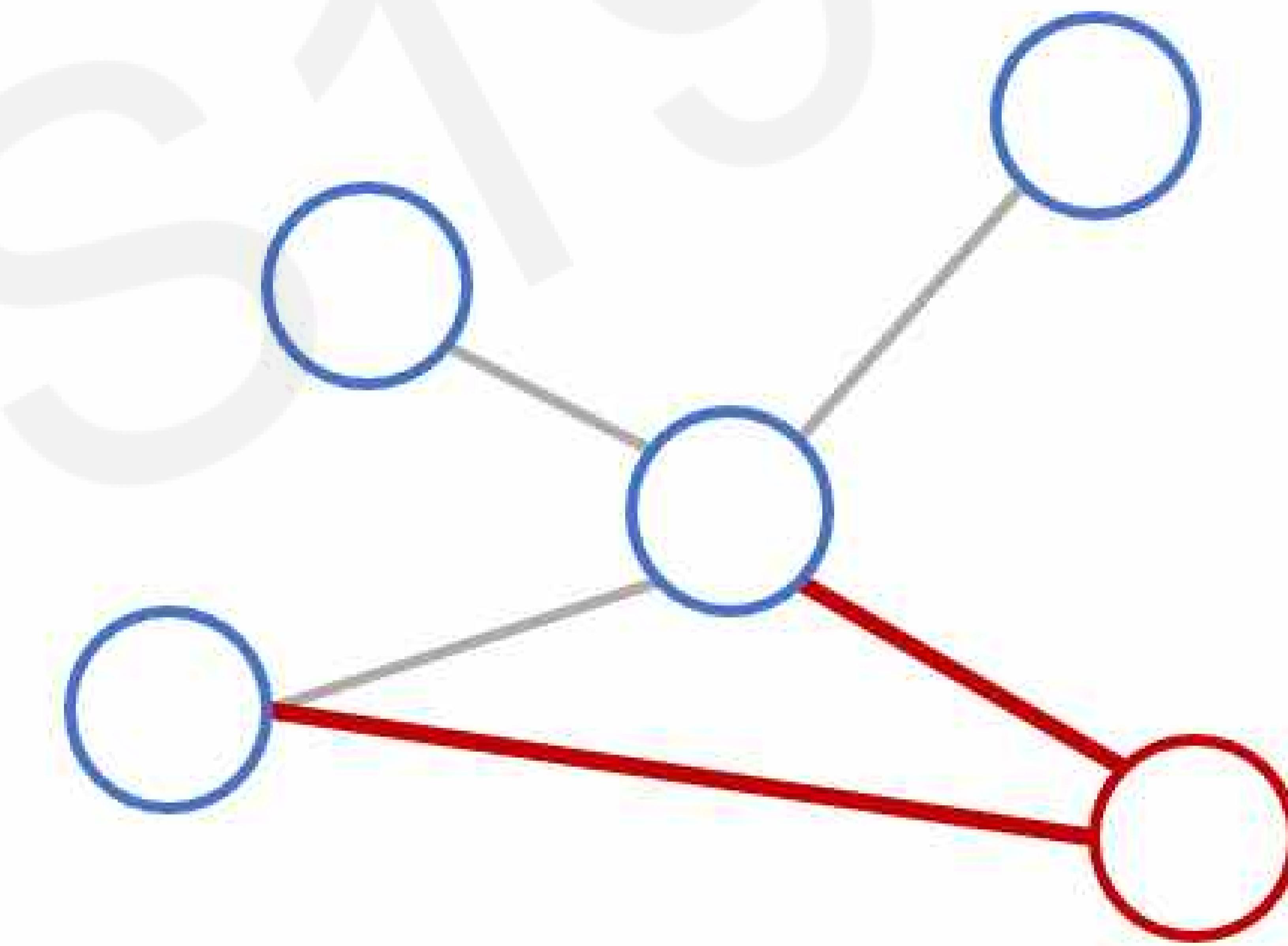


# Graph Convolutional Networks

Convolutional Networks

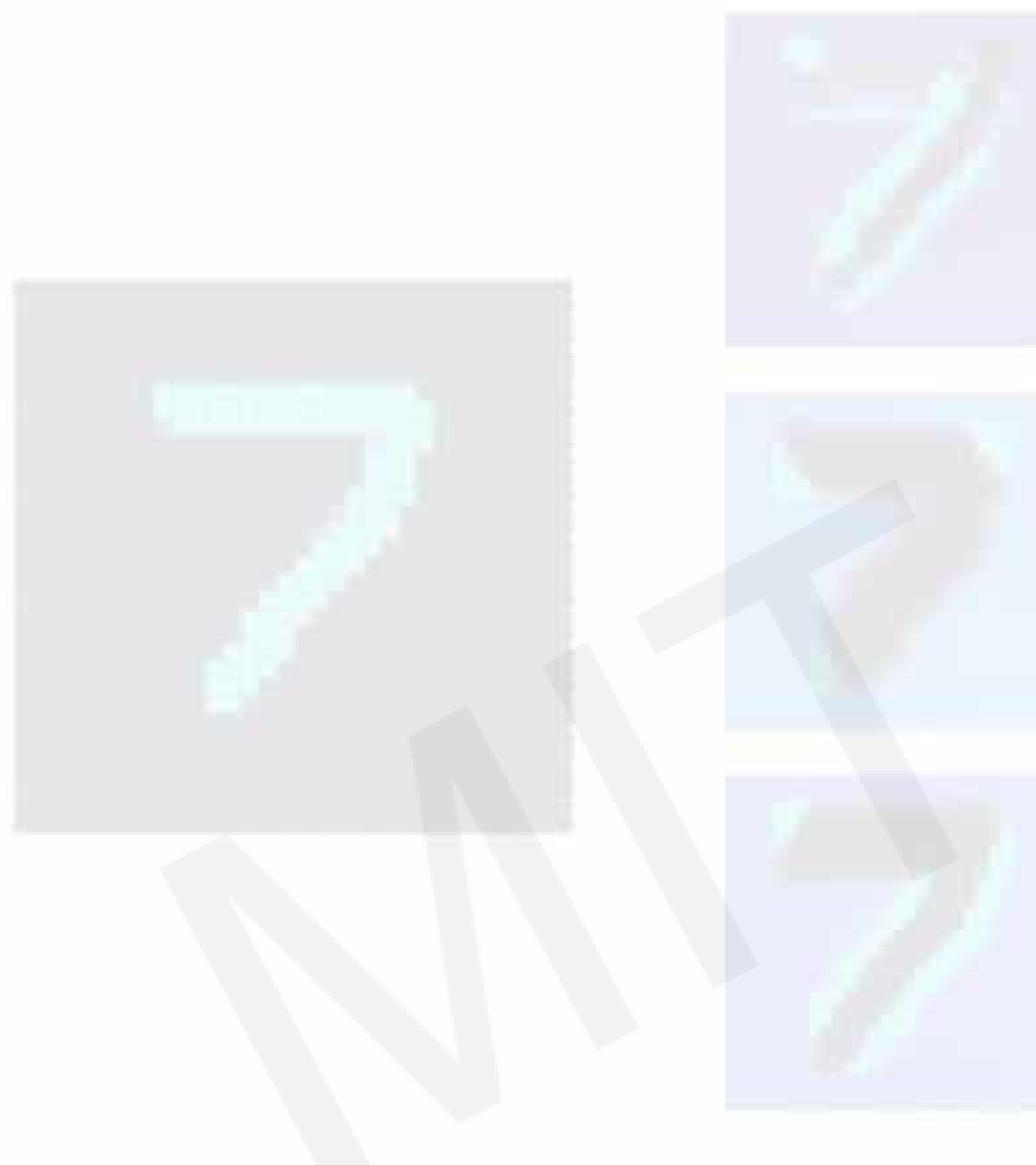


Graph Convolutional Networks (GCNs)

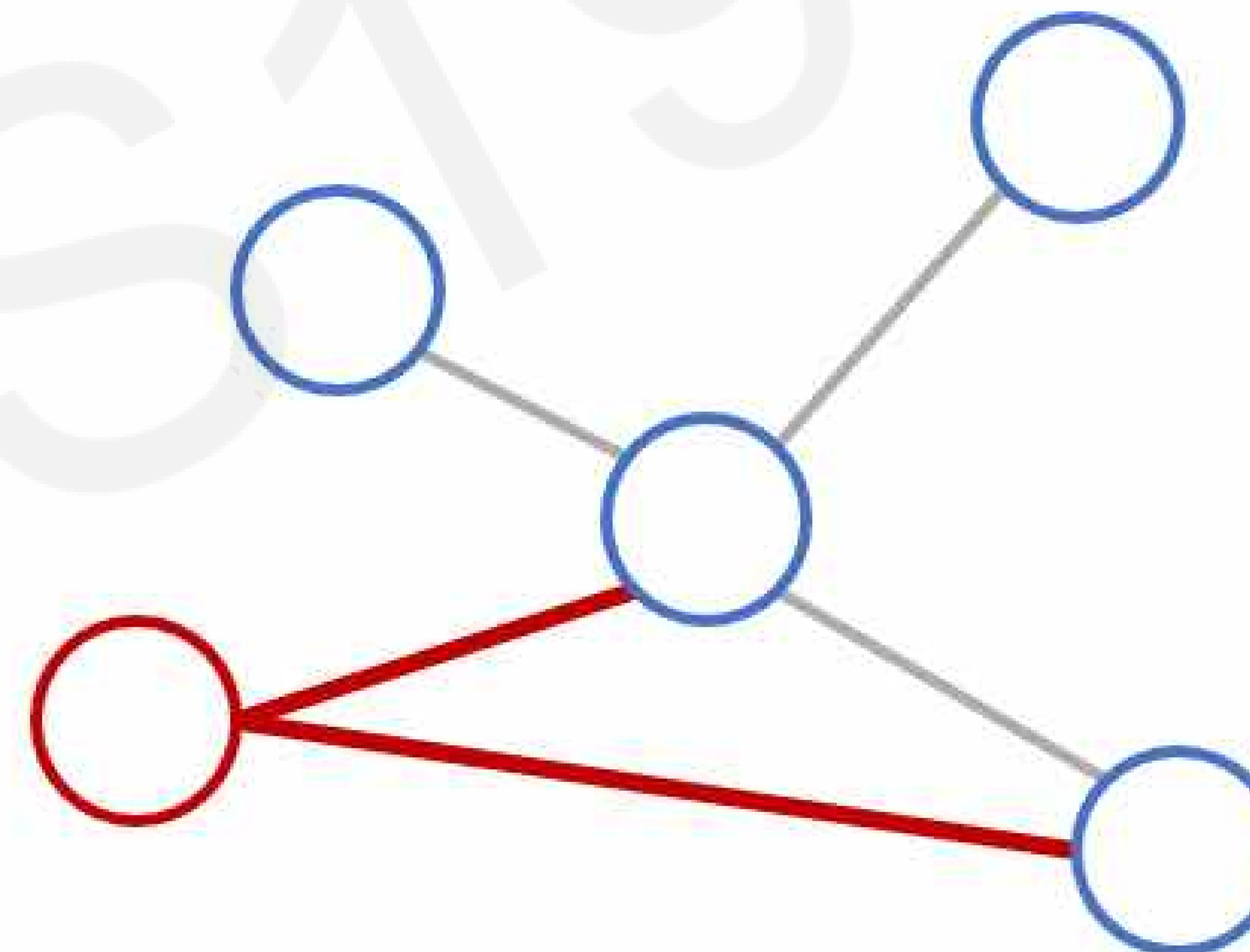


# Graph Convolutional Networks

Convolutional Networks



Graph Convolutional Networks (GCNs)

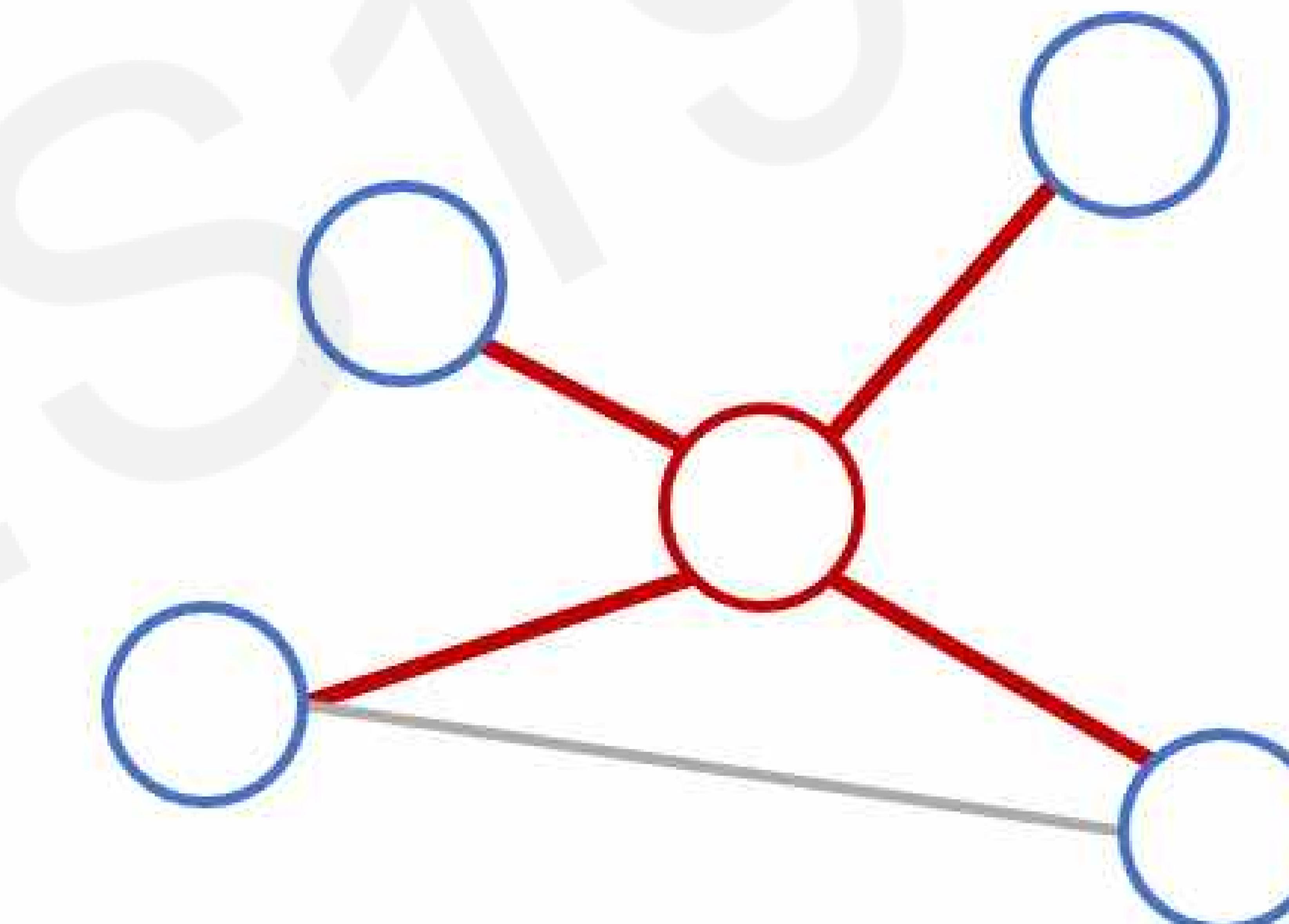


# Graph Convolutional Networks

Convolutional Networks



Graph Convolutional Networks (GCNs)

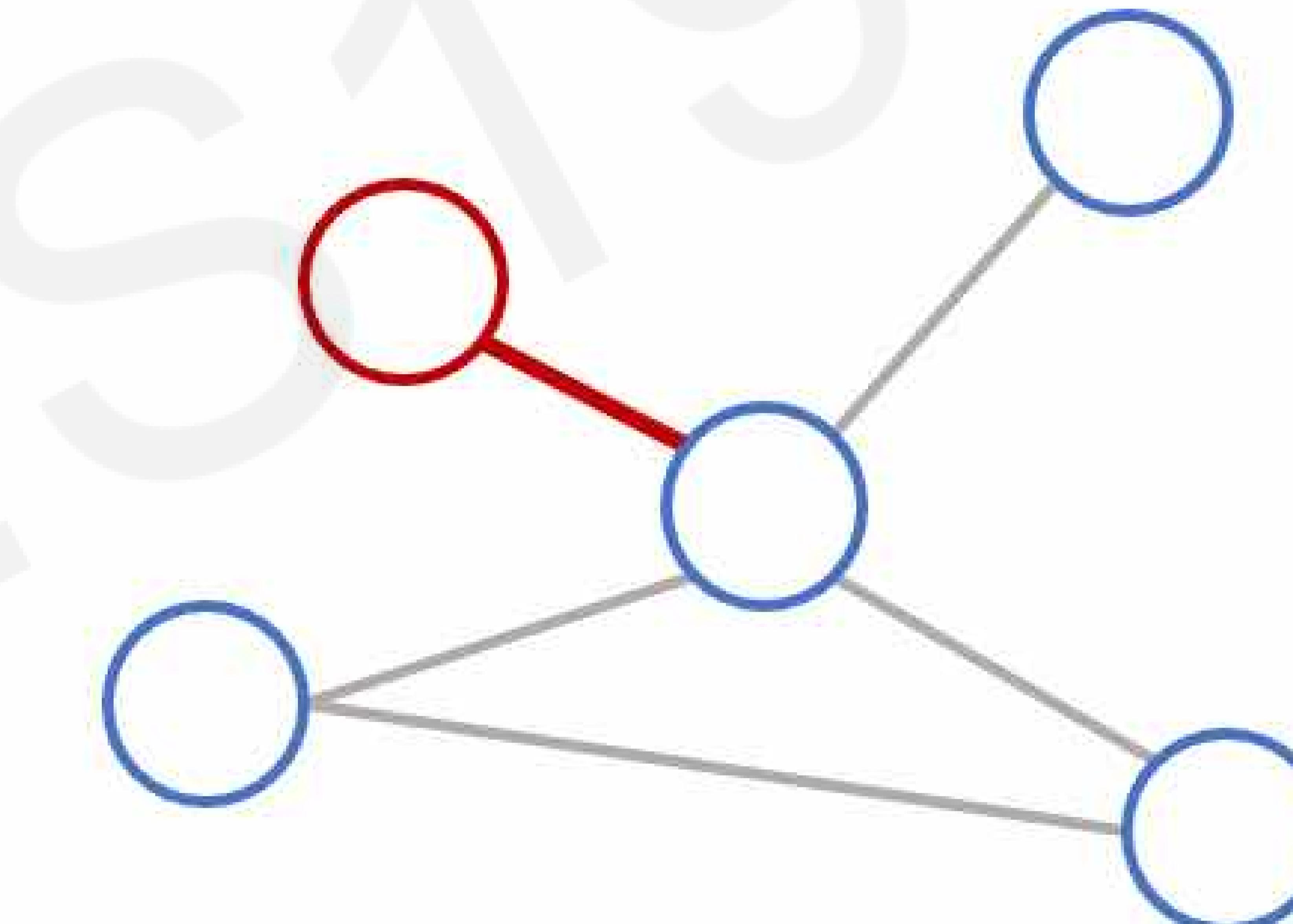


# Graph Convolutional Networks

Convolutional Networks

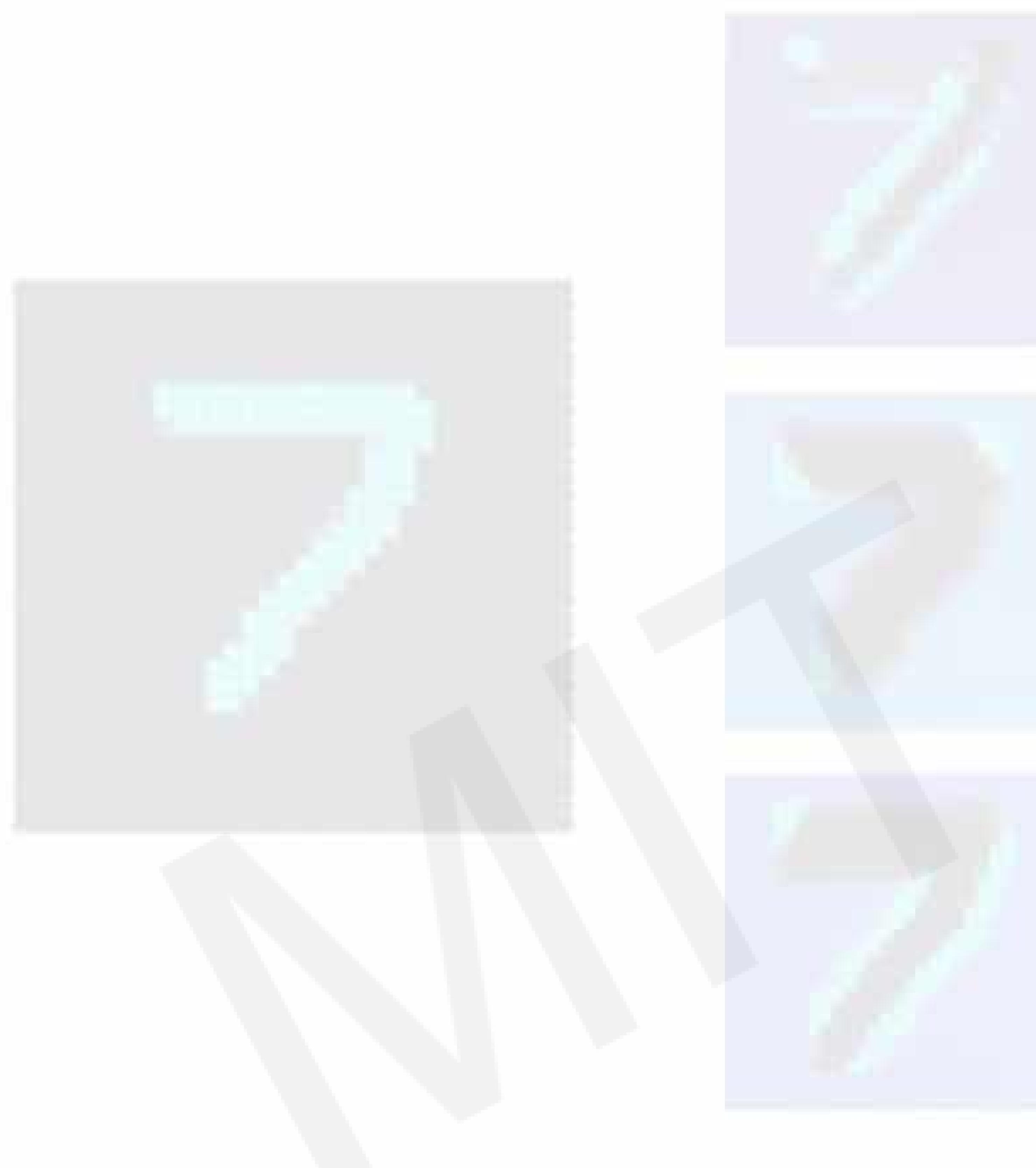


Graph Convolutional Networks (GCNs)

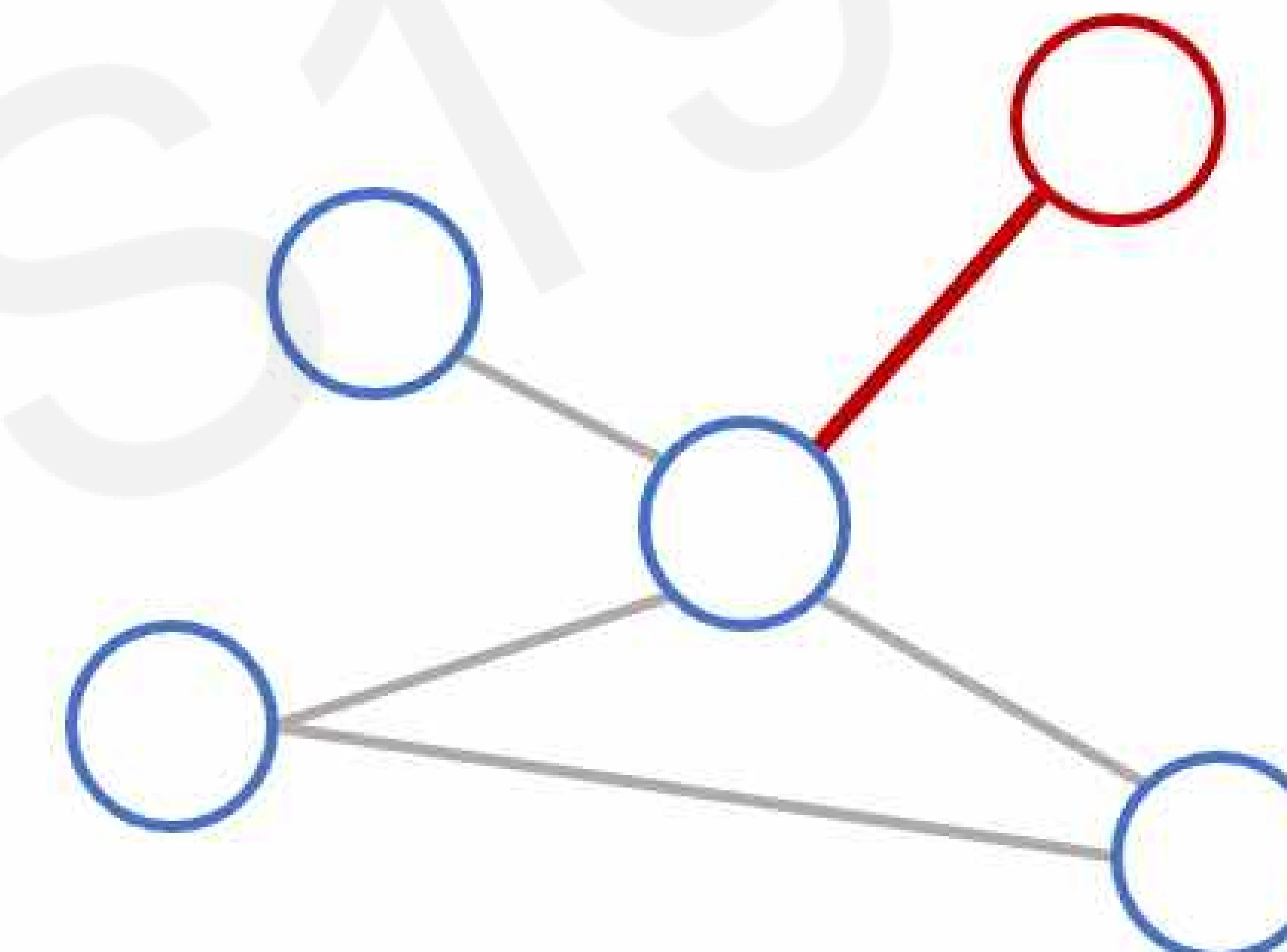


# Graph Convolutional Networks

Convolutional Networks



Graph Convolutional Networks (GCNs)

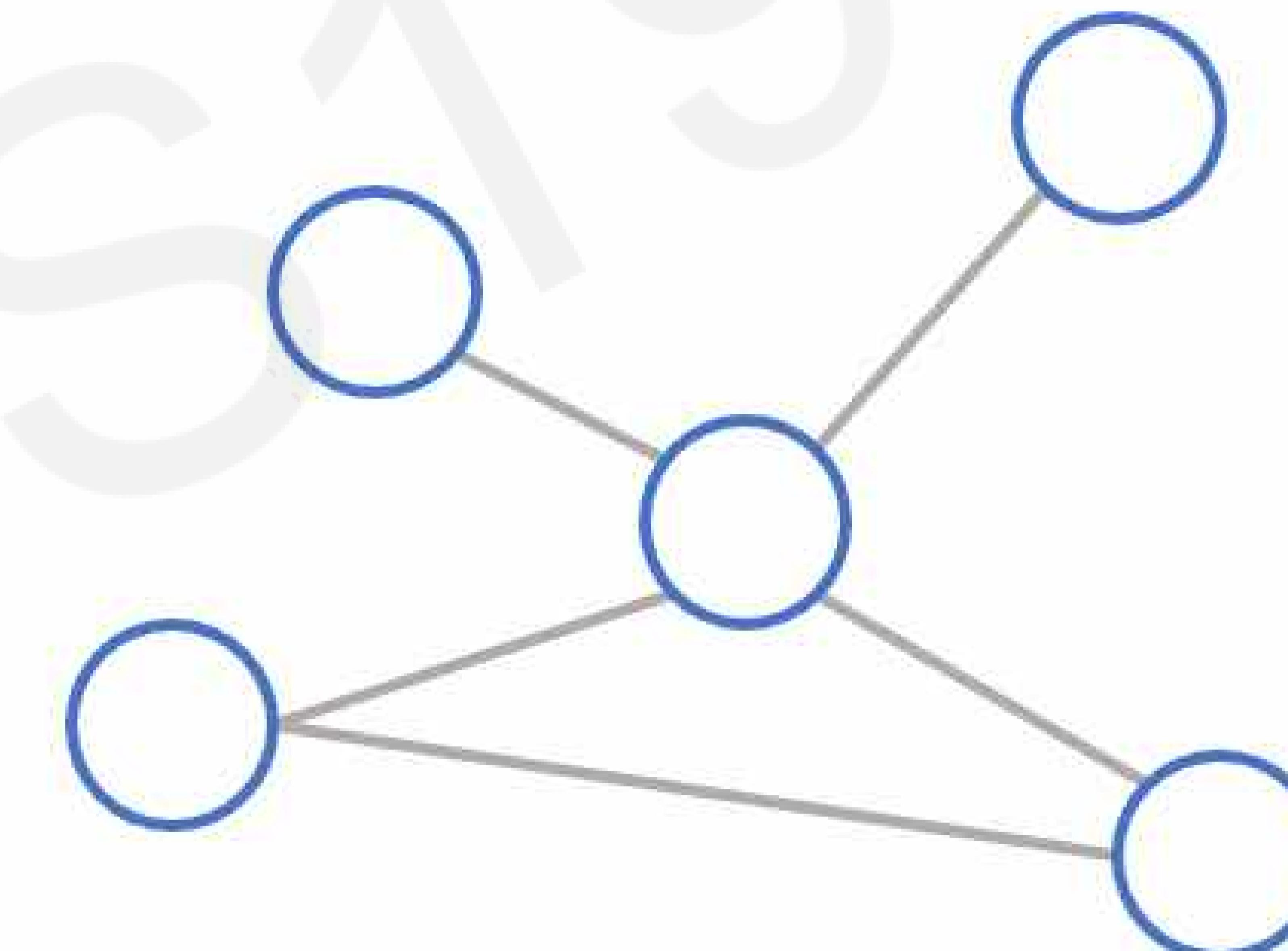


# Graph Convolutional Networks

Convolutional Networks

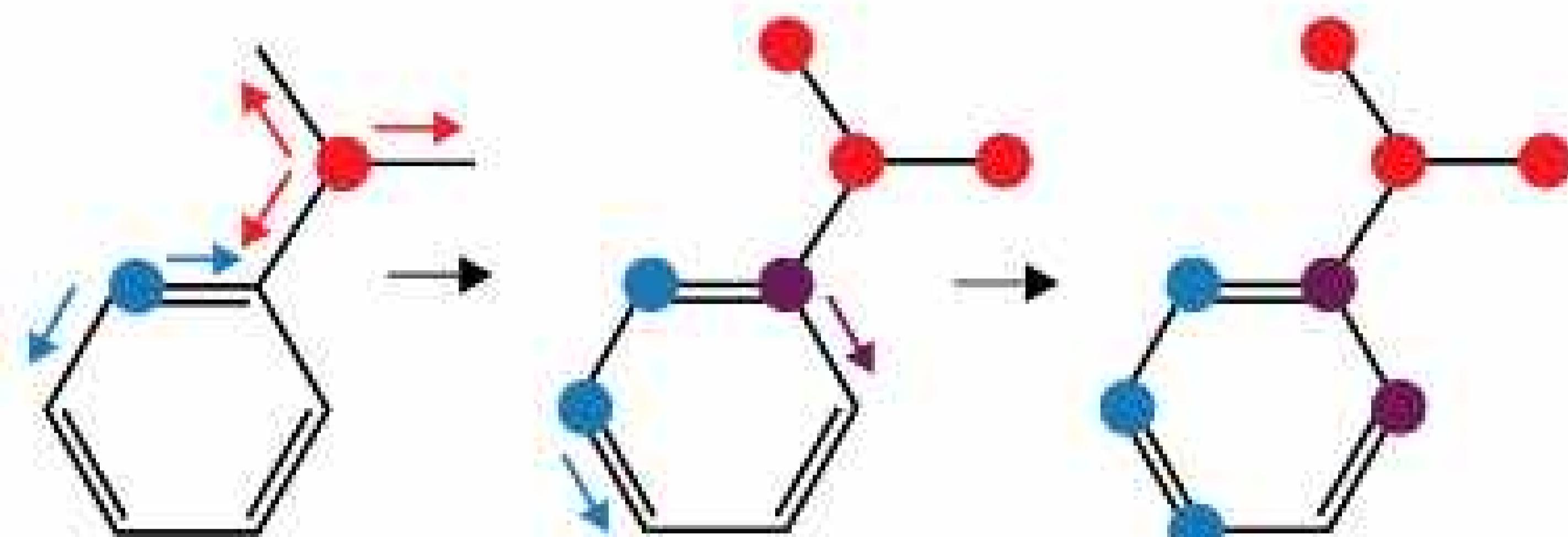


Graph Convolutional Networks (GCNs)



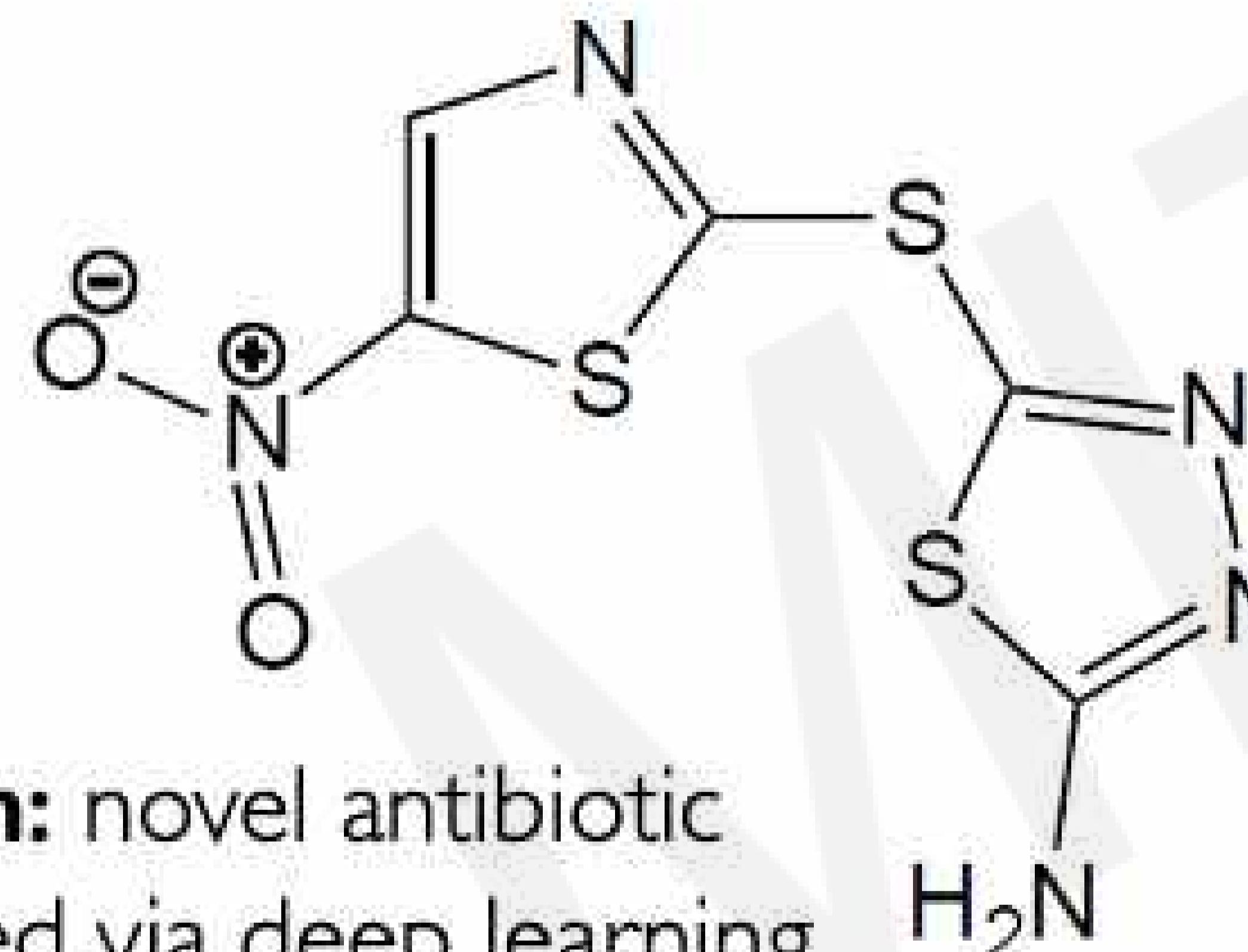
# Applications of Graph Neural Networks

## Molecular Discovery



Message-passing neural network

Jin+ *JCIM* 2019; Soleimany+ *ACS Cent Sci* 2021



Halicin: novel antibiotic discovered via deep learning

Stokes+ *Cell* 2020

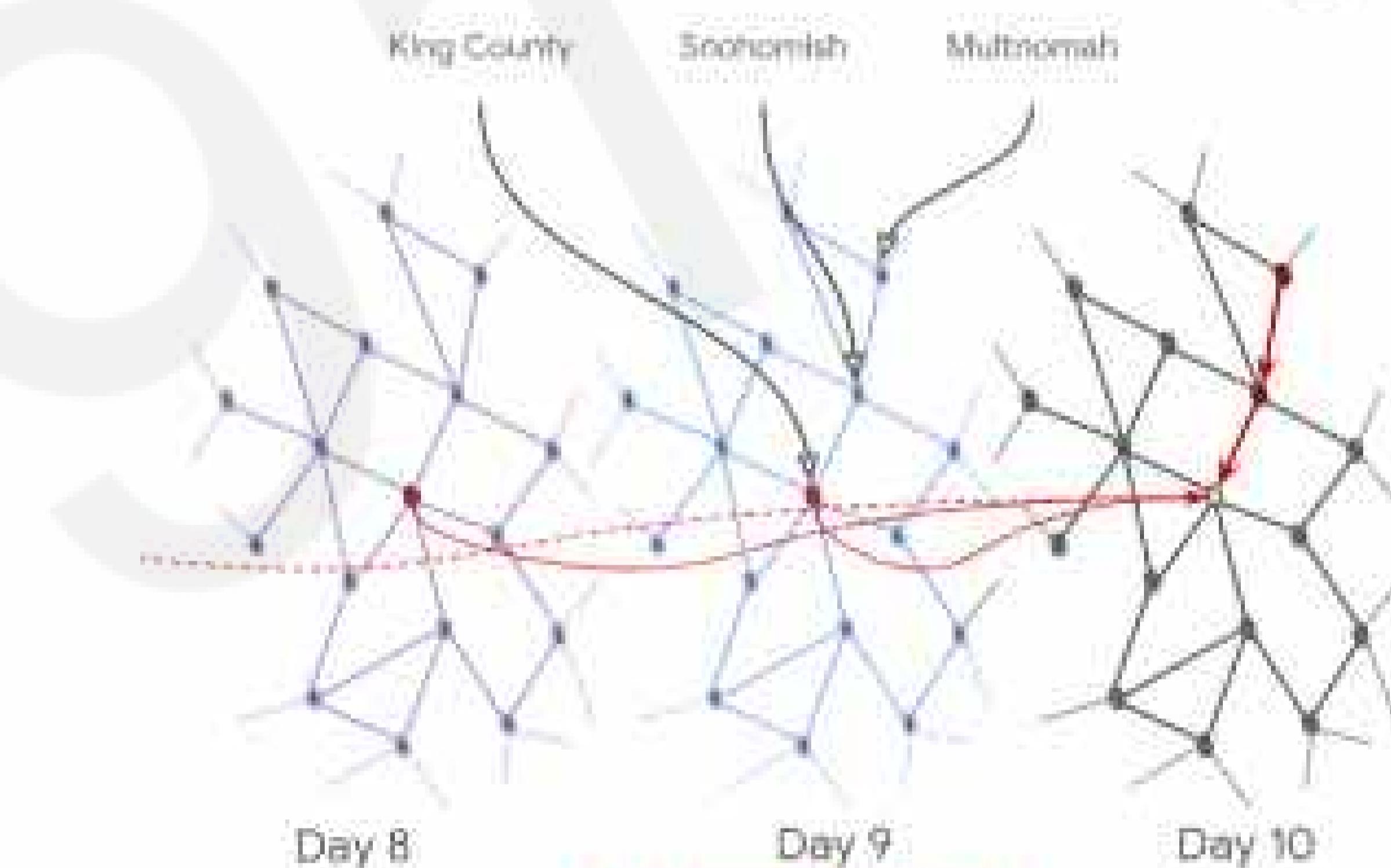
## Traffic Prediction

ETA Improvements with GoogleMaps

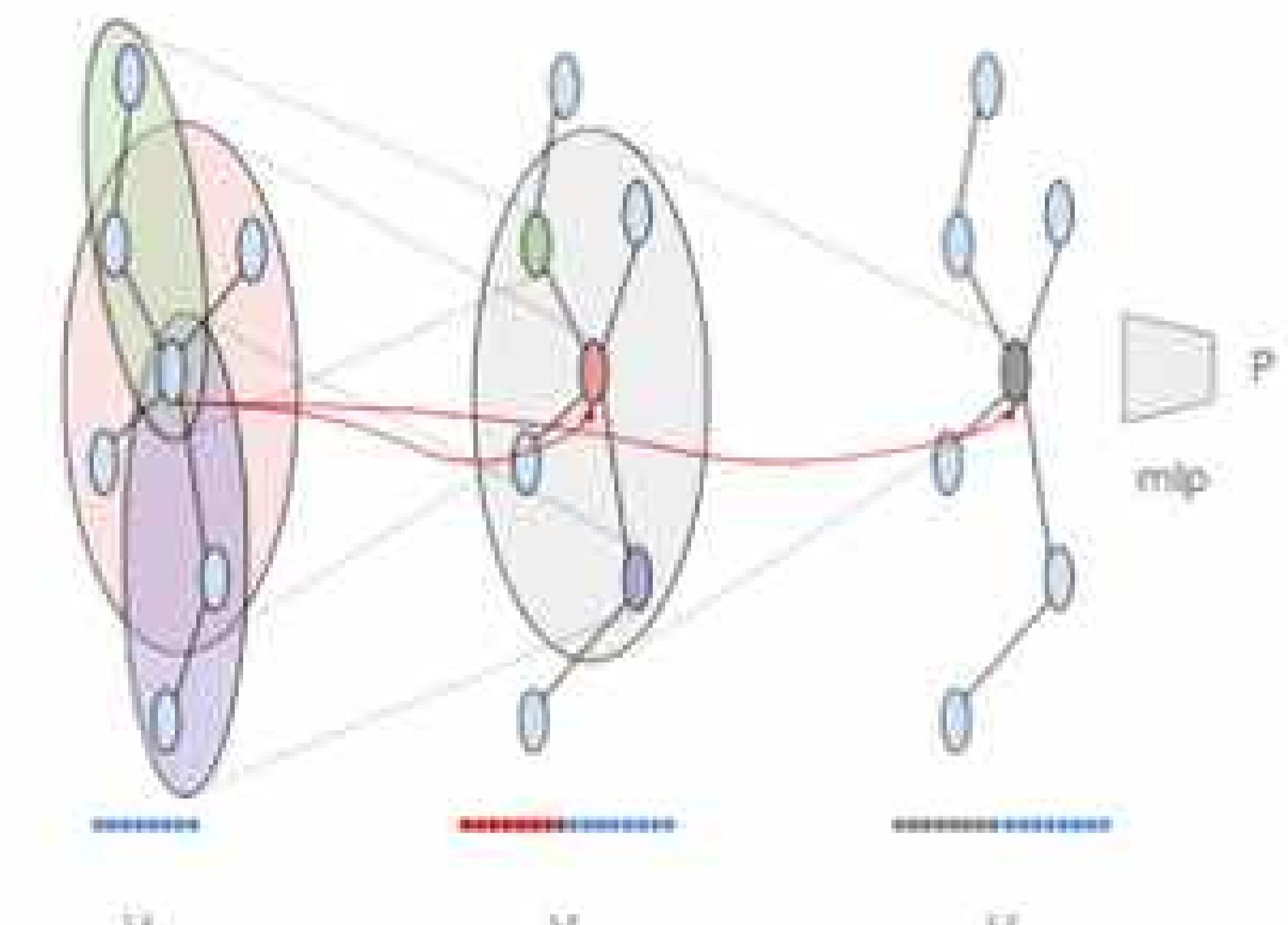


DeepMind + GoogleMaps

## COVID-19 Forecasting



Spatio-temporal data



Graph network + temporal embedding

Kapoor+ *KDD* 2020

# Learning From 3D Data

Point clouds are **unordered sets** with **spatial dependence** between points



mug?

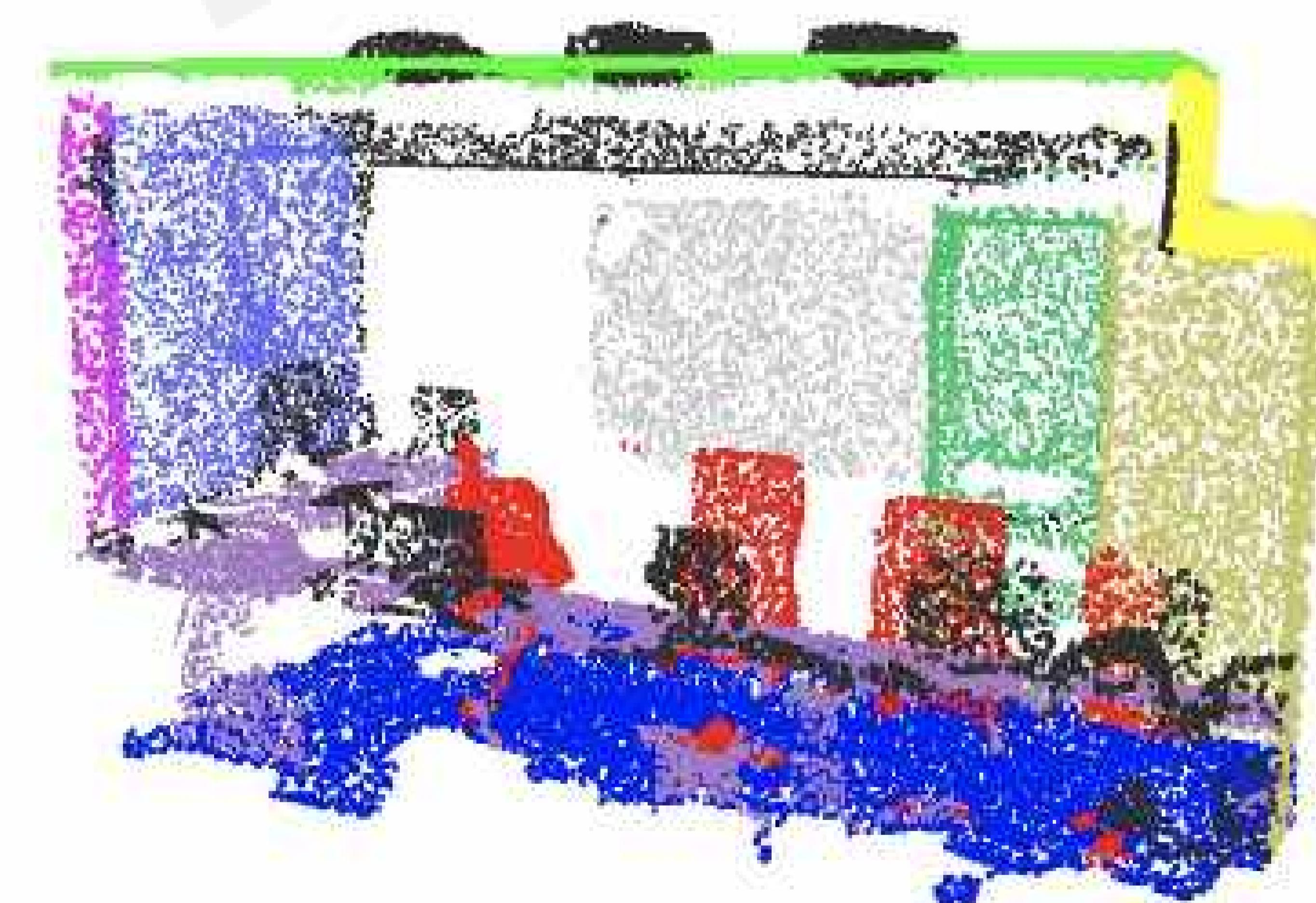


table?

car?

Classification

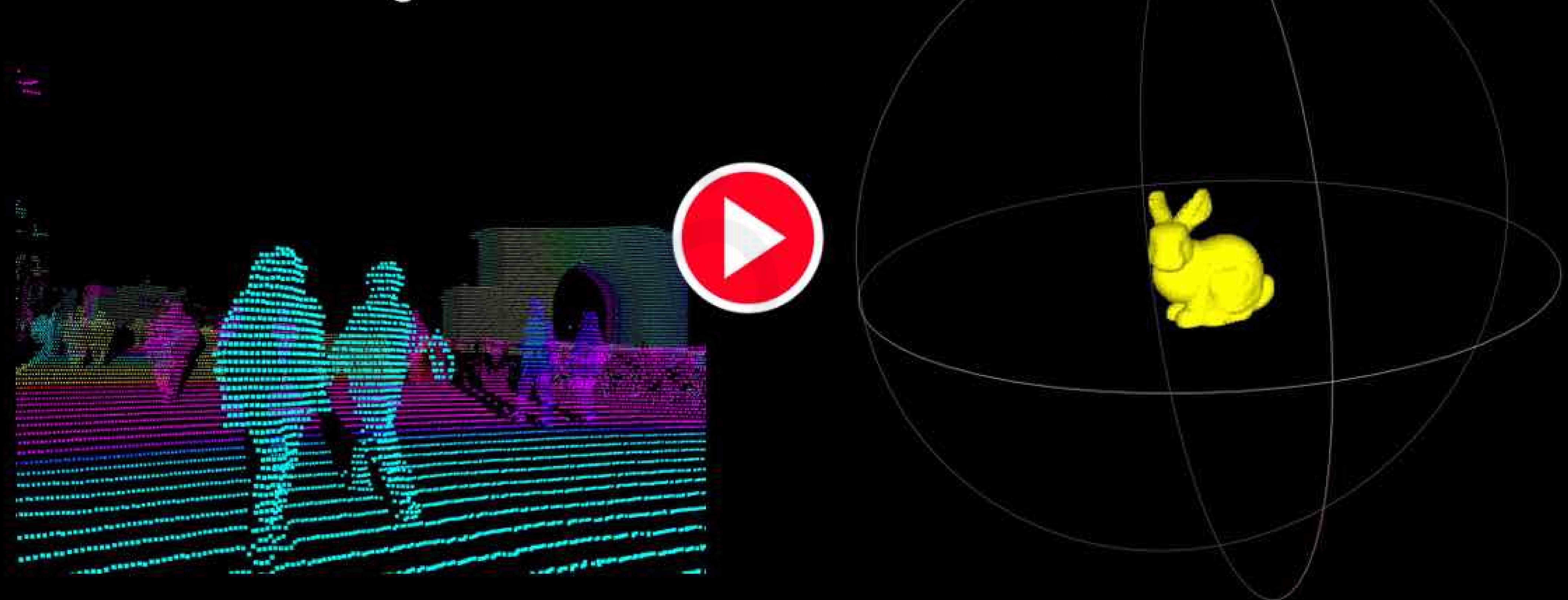
Part Segmentation



Semantic Segmentation

# Extending Graph CNNs to Pointclouds

Capture local geometric features of point clouds while maintaining order invariance

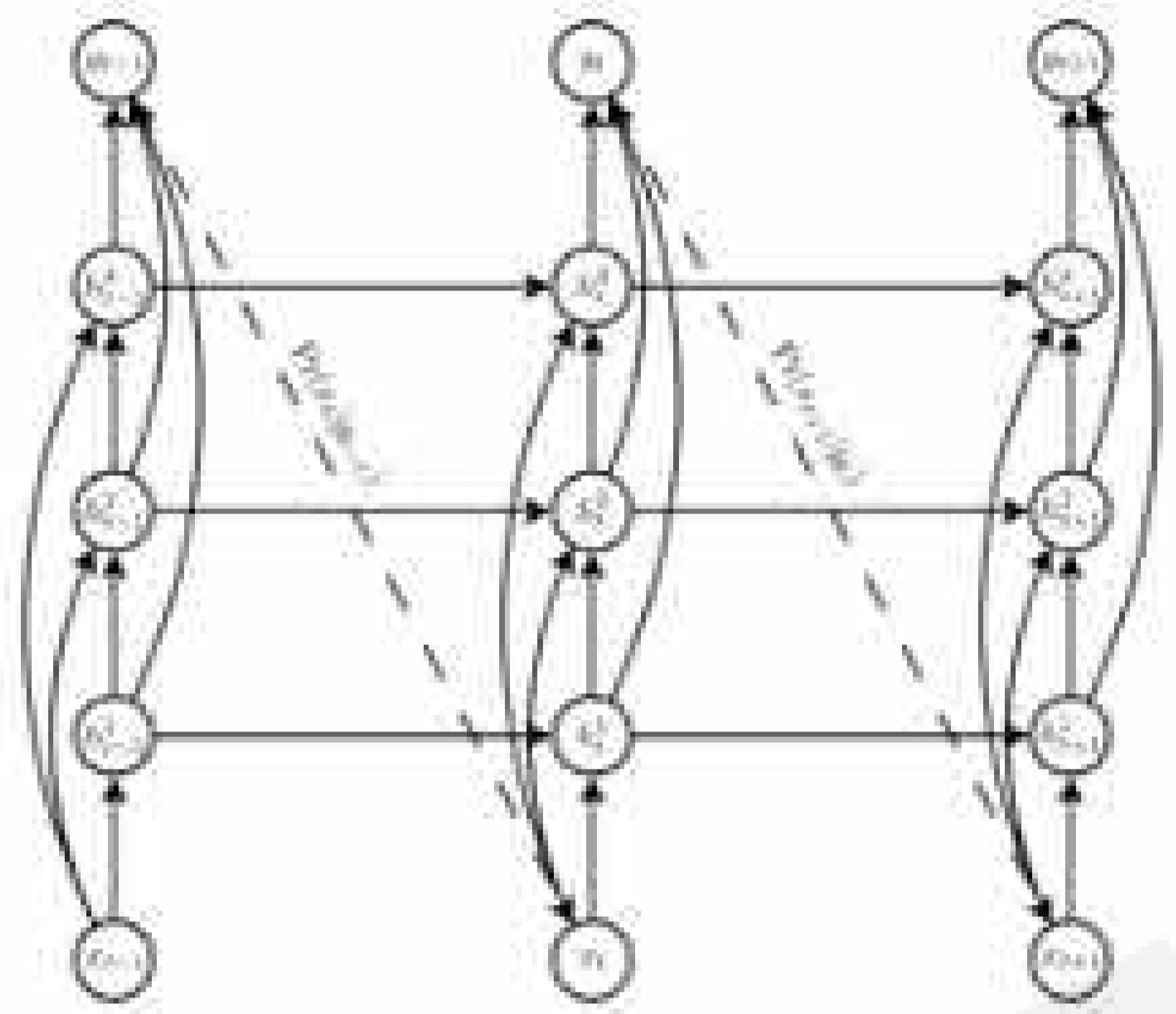


# New Frontiers II: Automated Machine Learning & AI

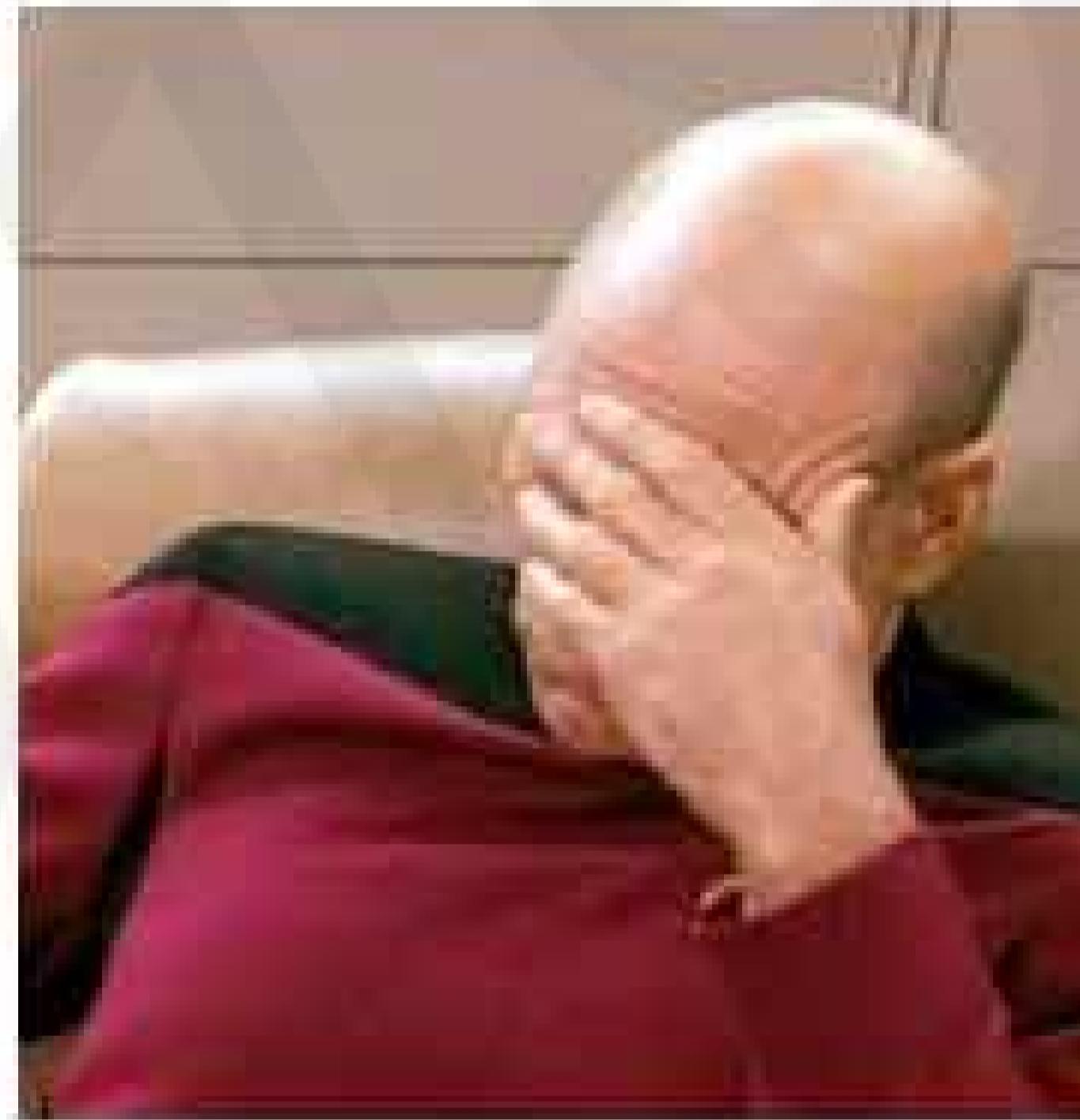


# Motivation: Automated Machine Learning

Standard deep neural networks are optimized for **a single task**



Complexity of models increases



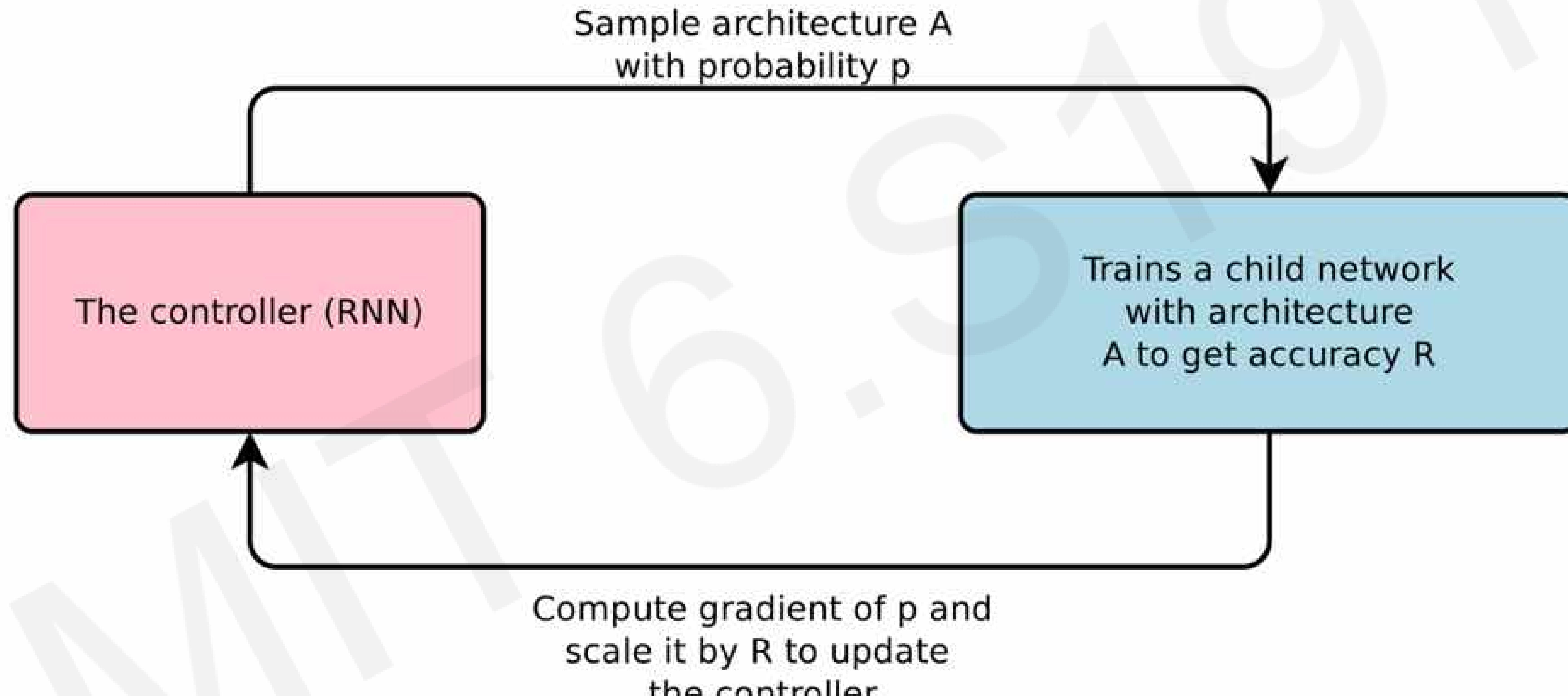
Greater need for specialized engineers

Often require **expert knowledge** to build an architecture for a given task

Build a learning algorithm that **learns which model** to use to solve a given problem

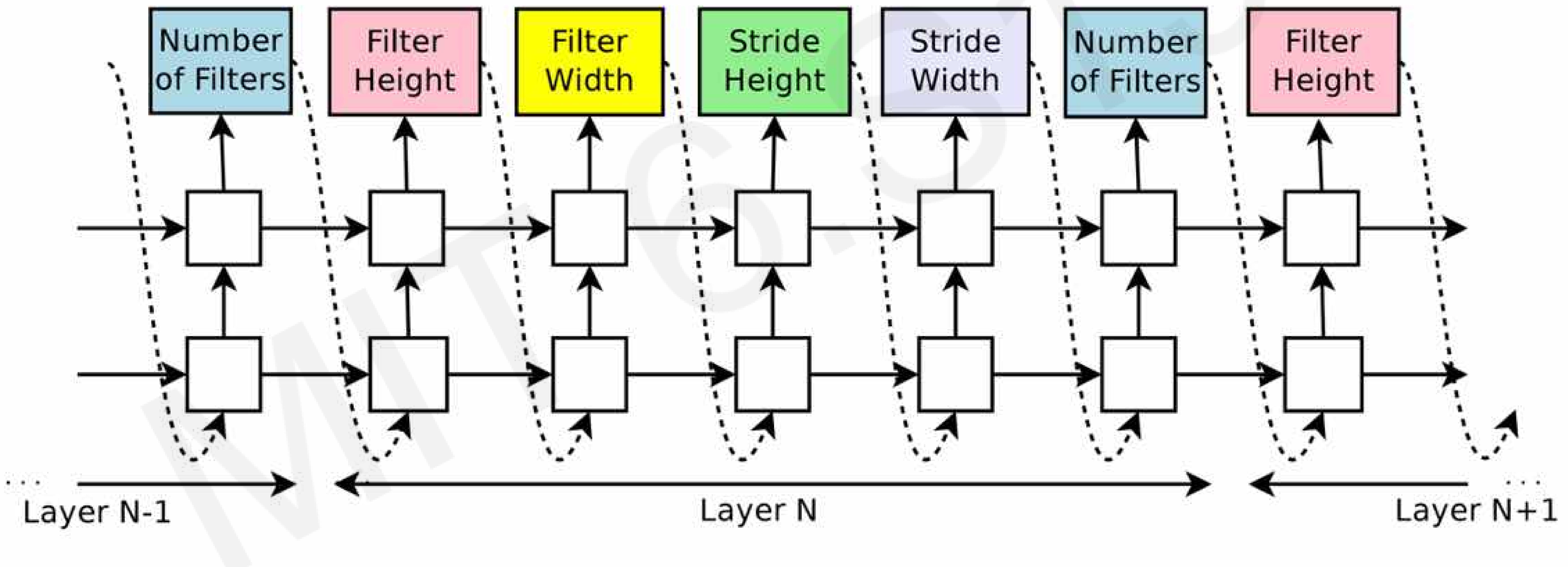
## AutoML

# Automated Machine Learning (AutoML)

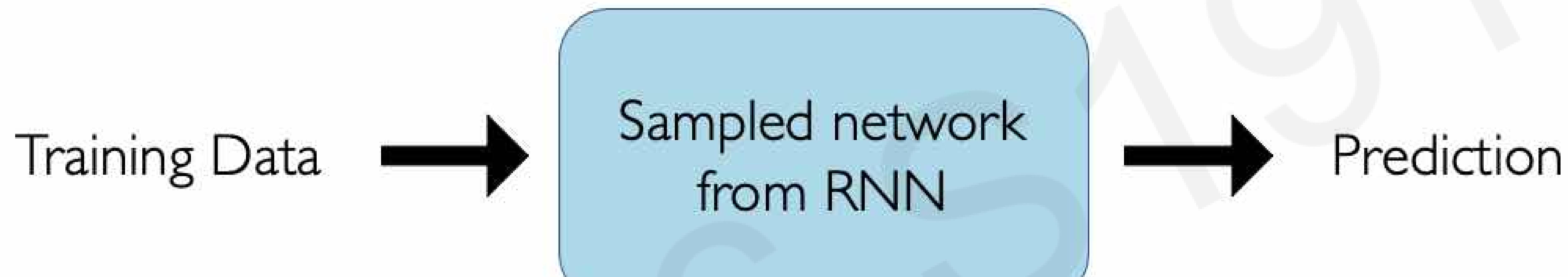


# AutoML: Model Controller

At each step, the model samples a brand new network



# AutoML: The Child Network

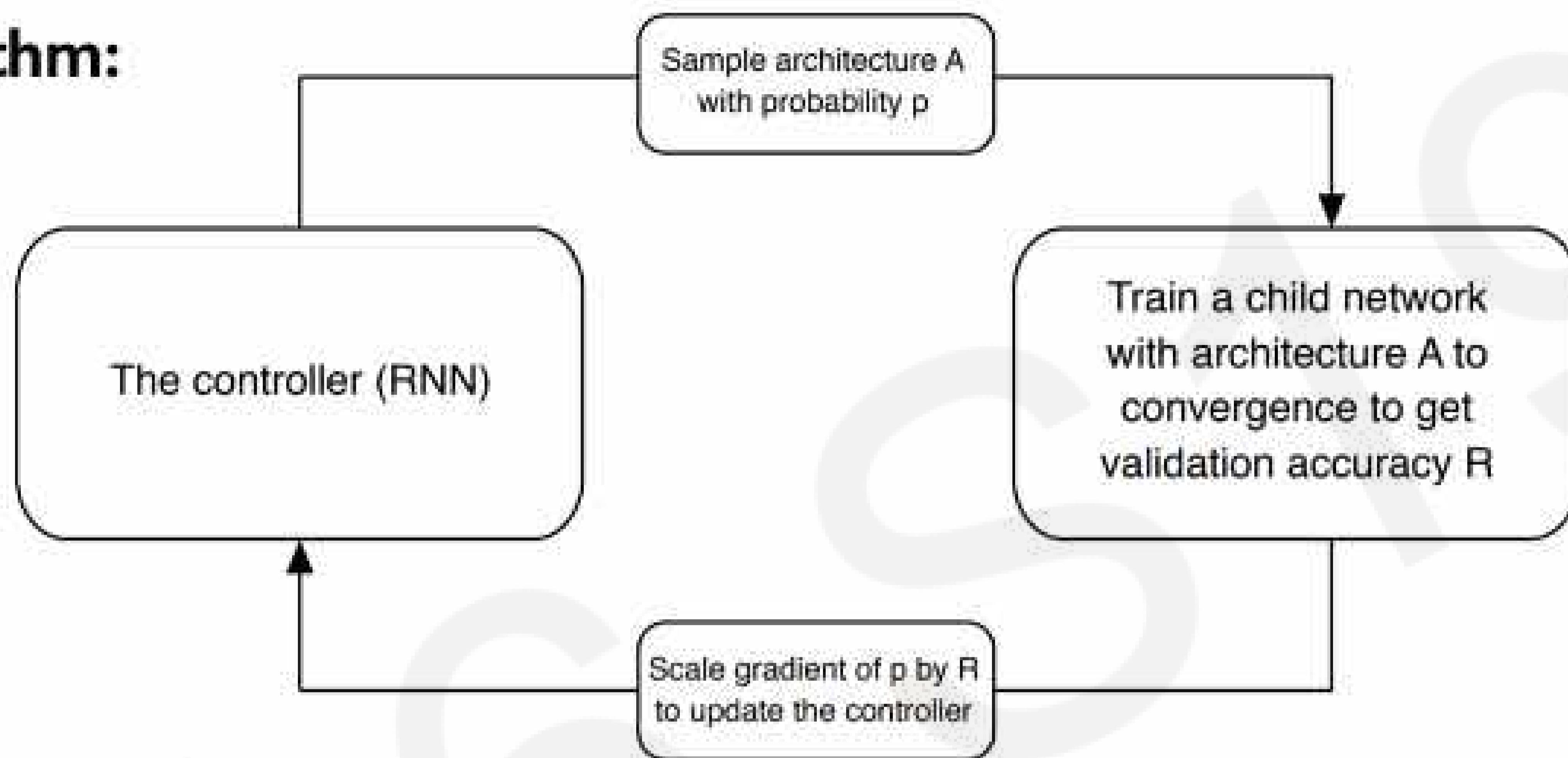


Compute final accuracy on this dataset.

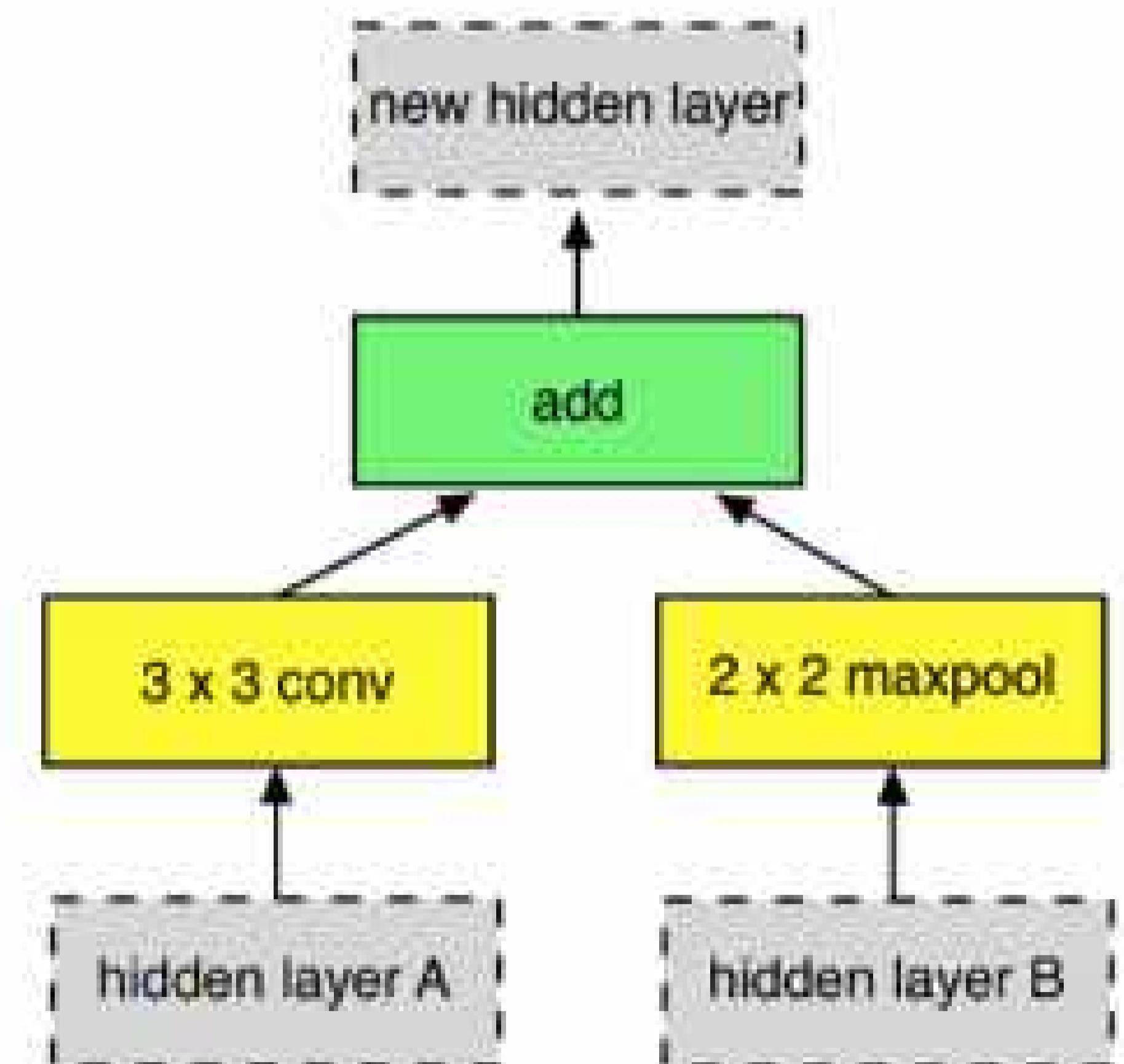
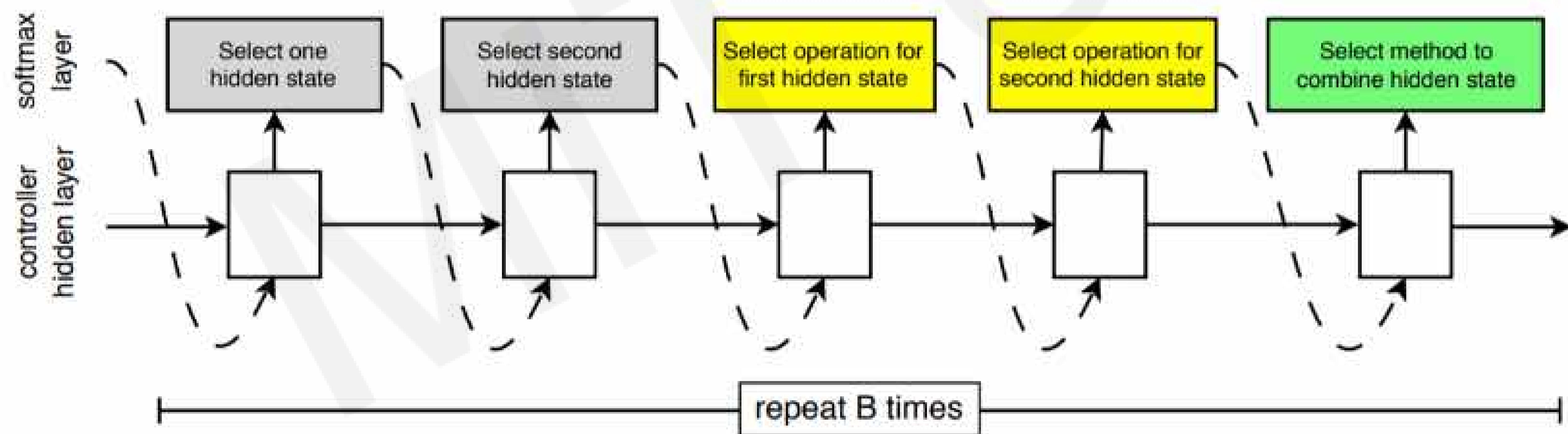
Update RNN controller based on the accuracy of the child network after training.

# Learning Architectures for Image Recognition

## Neural architecture search algorithm:

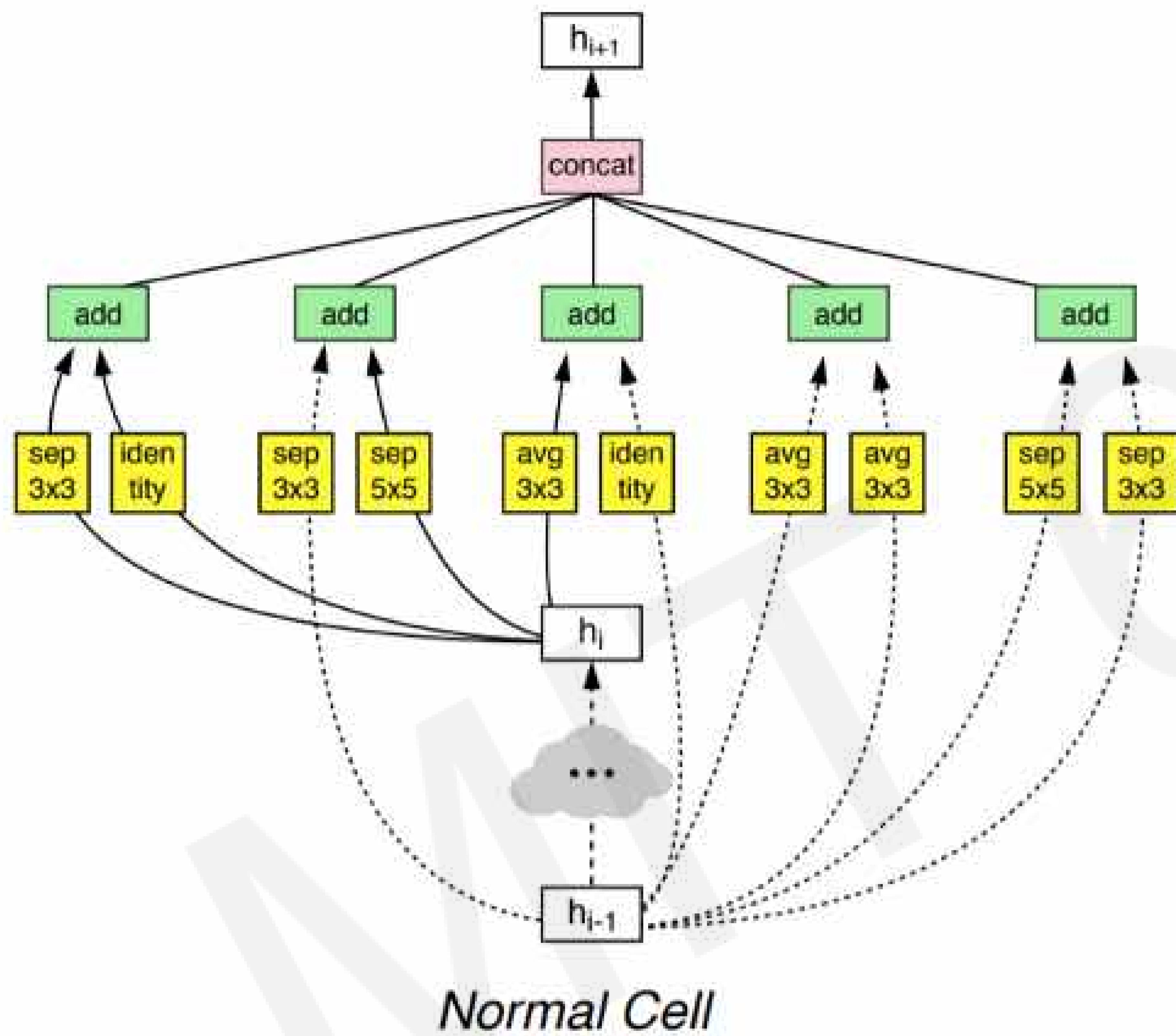


## Controller architecture for constructing convolutional layers:

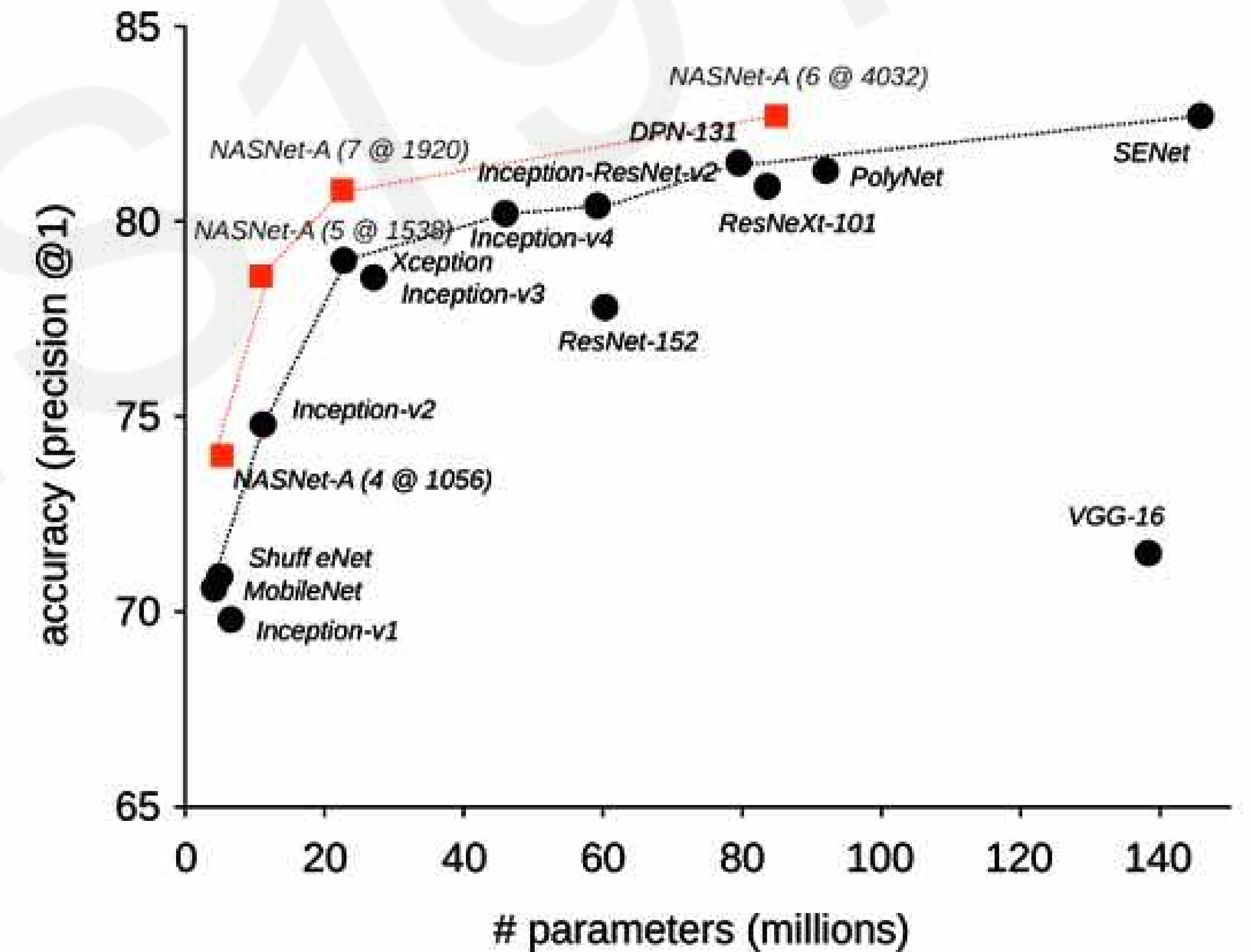


# Learning Architectures for Image Recognition

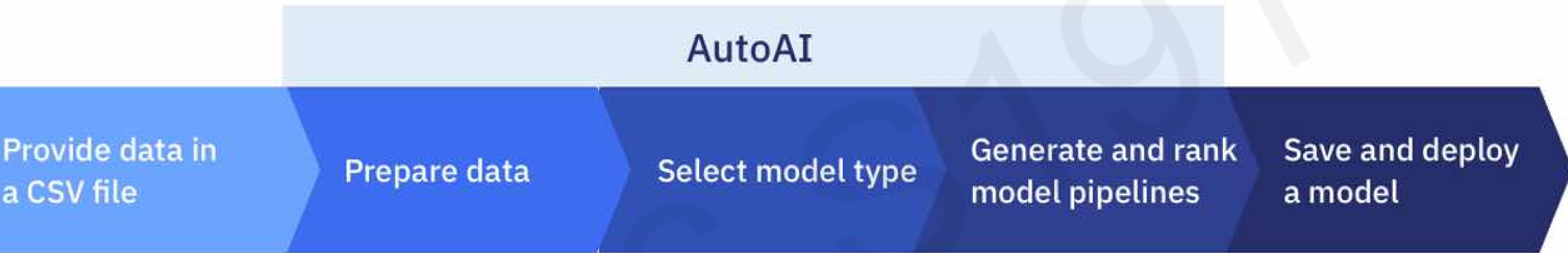
Learned architecture for convolutional cell



Model performance on ImageNet



# From AutoML to AutoAI





# AutoAI Spawns a Powerful Idea

- Design an AI pipeline that can build new models capable of solving a task
- Reduces the need for experienced engineers to design the networks
- Makes deep learning more accessible to the public

Connections and distinctions  
between artificial and human  
intelligence



# 6.S191:

## Introduction to Deep Learning

### Lab 3: Reinforcement Learning

Link to download labs:  
<http://introtodeeplearning.com#schedule>

1. Open the lab in Google Colab
2. Start executing code blocks and filling in the #TODOs
3. Need help? Come to 10-250/Gather.Town!