From Neural Networks to Graph Neural Networks

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Outline

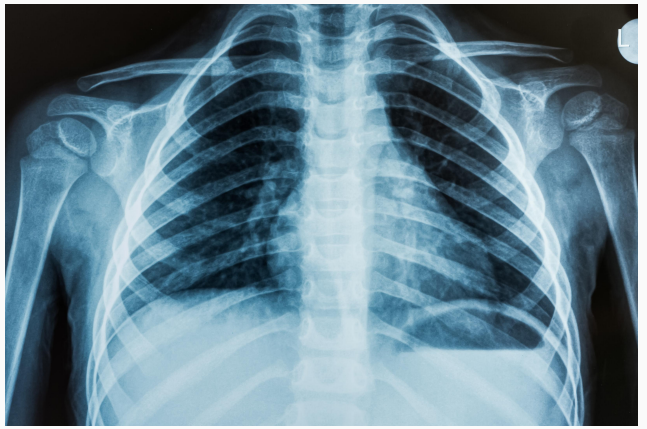
- **Motivation**
  - Supervised learning as function approximation
  - From feature engineering to deep learning
- **Multi-Layer Perceptrons (MLPs)**
  - Perceptron and multi-layer perceptrons
  - Activation functions and output layers
  - Training, generalization, and expressivity
- **Learning on Graphs**
  - Graphs as relational data
  - Node-, edge-, and graph-level tasks
  - Why MLPs are not enough
- **Graph Neural Networks**
  - Message passing
  - Graph Convolutional Networks (GCNs)
  - Limitations: over-smoothing, over-squashing, expressivity
- **Research directions in our group**

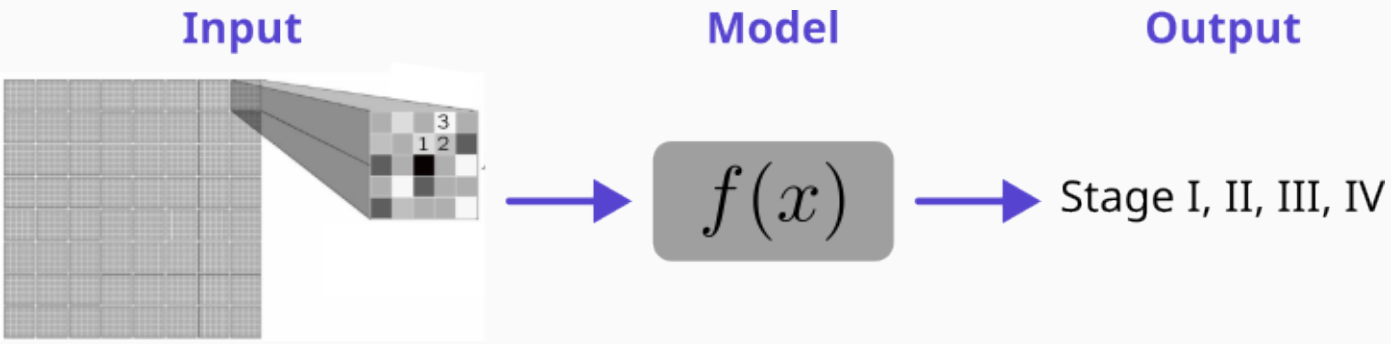
Motivation

A Real Problem [Motivation]

Given an X-ray image:

$\rightarrow$ determine the stage of a tumor





A Real Problem [Motivation]

Formally, we consider an input space $\mathcal{X}$ and an output space $\mathcal{Y}$:

$$x \in \mathcal{X} \qquad y \in \mathcal{Y}$$

We assume that there exists an unknown function:

$$f^\star : \mathcal{X} \to \mathcal{Y}$$

and we are given samples:

$$(x_i, y_i) \sim \mathcal{D}$$

Our goal is to learn a function f_θ such that:

$$f_\theta(x) \approx f^\star(x)$$

Learning Settings [Motivation]

Different learning paradigms arise depending on the available data.

- **Supervised learning**
  - data: $\{(x_i, y_i)\}_{i=1}^{n}$
  - goal: learn $f_\theta(x) \approx y$
  - e.g. tumor stage prediction, image classification

$\mathcal{X}$	$\mathcal{Y}$
	Bird
	Bird
	Dog
	Cat

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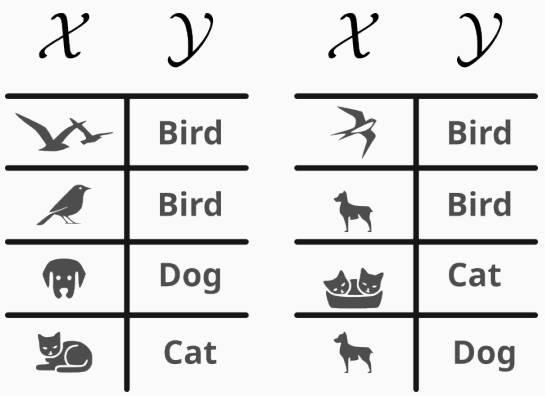

- **Unsupervised learning**
  - data: $\{x_i\}_{i=1}^n$
  - goal: discover hidden structure in the data
  - examples: clustering

In this talk, we focus on supervised learning.

The classical approach (pre deep learning) [Motivation]

In classical approaches, we decompose the problem as:

$$f(x) = g(\phi(x))$$

where:

- $\phi : \mathcal{X} \to \mathbb{R}^d$ is a feature map
- $g : \mathbb{R}^d \to \mathcal{Y}$ is a simple predictor

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- Detect contours
- Contrast
- Irregularity of regions

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How to design ϕ?

- Detect contours
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ϕ must be designed manually and this requires:

- domain knowledge
- trial and error

Moreover, the space of possible feature maps is extremely large, and there is no systematic way to choose a good one.

The deep learning approach [Motivation]

Deep learning changes this paradigm.

Instead of fixing ϕ, we parametrize both ϕ and g:

$$f_\theta(x) = g_{\theta_2}\big(\phi_{\theta_1}(x)\big)$$

where:

- ϕ_{θ_1} is a learned representation
- g_{θ_2} is a learned predictor

Equivalently, we consider a single parametric function:

$$f_\theta : \mathcal{X} \to \mathcal{Y}$$

and we learn all parameters jointly from data.

The deep learning approach [Motivation]

Deep learning tells us that, instead of manually designing features, we should learn a parametric function directly from data.

This raises a fundamental question:

How do we choose the family of functions f_θ?

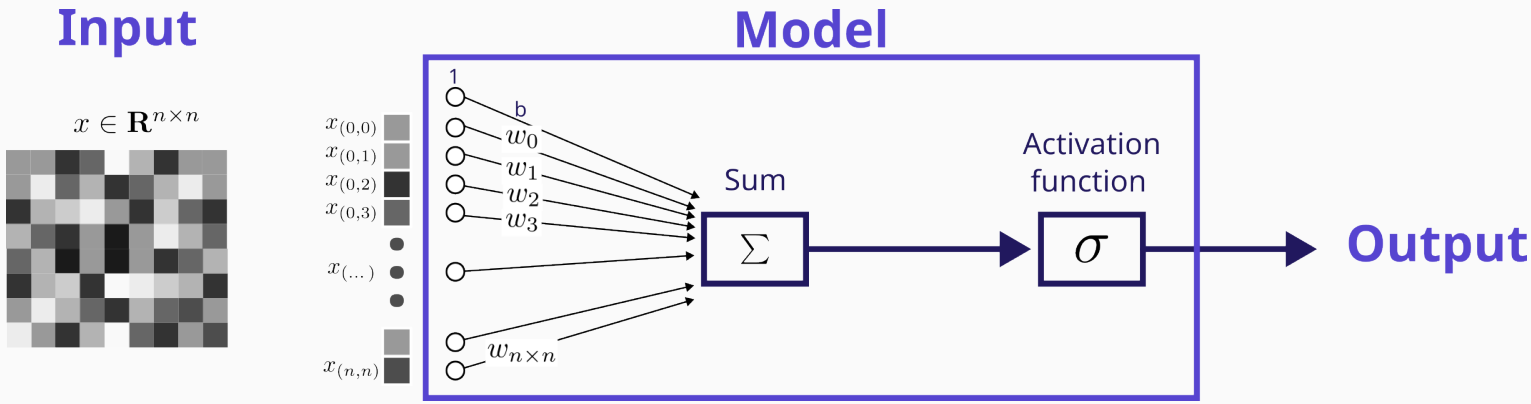
A natural answer is to consider **neural networks**, that is, highly flexible parametric models obtained by composing simple transformations.

The simplest and most classical example is the **Multi-Layer Perceptron (MLP)**.

Multi-Layer Perceptron (MLP)

Perceptron

We start from the simplest parametric model: the **Perceptron**.



Given an input $x \in \mathbb{R}^d$, the perceptron computes:

$$f_\theta(x) = w^\top x + b$$

and produces a prediction:

$$\hat{y} = \sigma(w^\top x + b)$$

where:

- $w \in \mathbb{R}^d$ are the weights
- $b \in \mathbb{R}$ is the bias
- σ is an activation function

Perceptron

The perceptron defines a linear decision boundary:

$$w^\top x + b = 0$$

Therefore, it can only model **linearly separable** problems.

However, many real-world tasks require modeling **nonlinear relationships**, which a single perceptron cannot capture.

Key idea: increase expressivity by composing multiple perceptrons...

Multi-Layer Perceptron (MLP)

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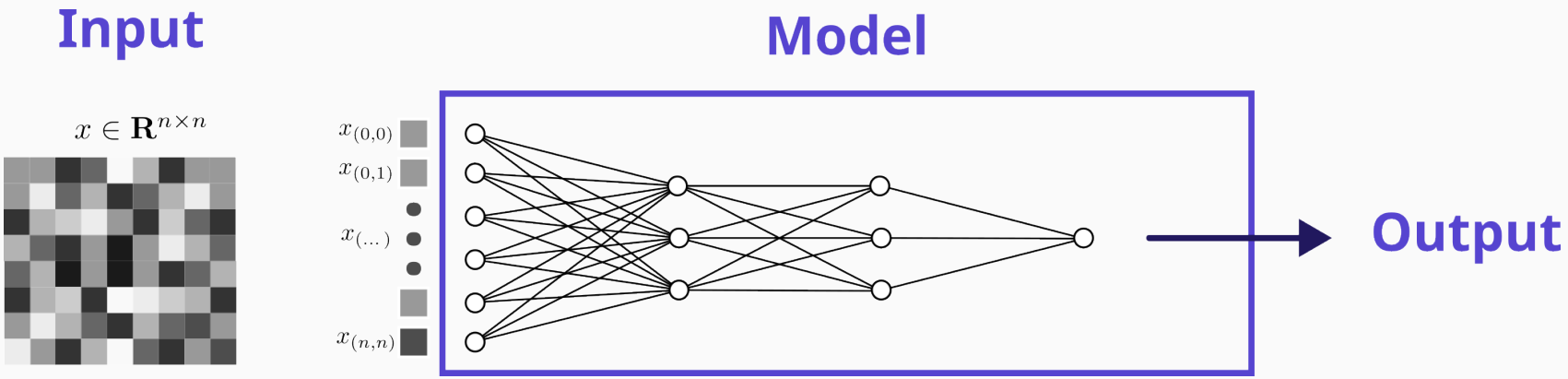
An MLP is obtained by stacking multiple perceptrons in layers.

Each layer takes as input the output of the previous one:

$$x \to h^{(1)} \to h^{(2)} \to \cdots \to \hat{y}$$



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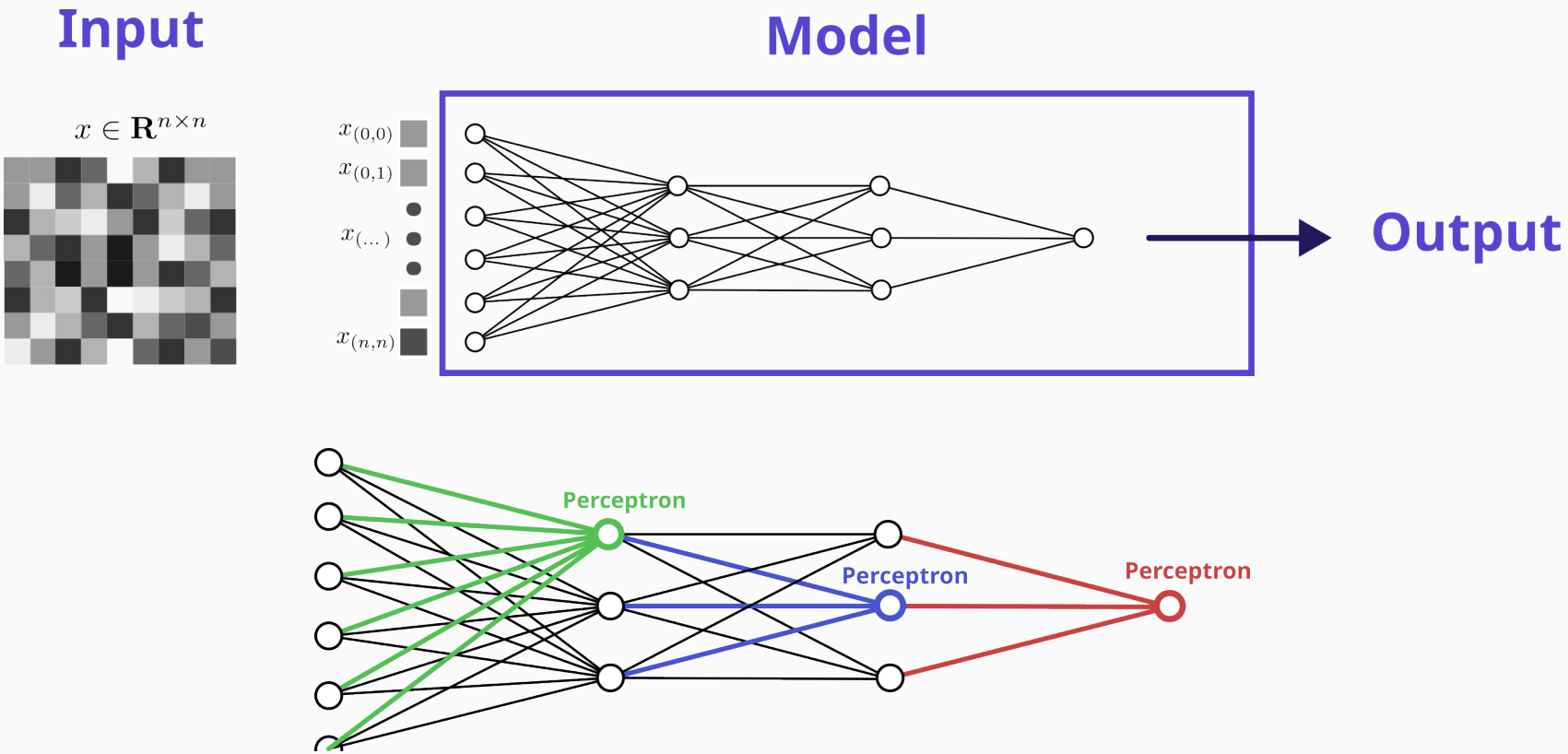


Multi-Layer Perceptron (MLP)

Formally, an MLP is a function defined by the composition of L layers.

$$
\begin{aligned}
h^{(0)} &= x \\
h^{(\ell)} &= \sigma\big(W^{(\ell)} h^{(\ell-1)} + b^{(\ell)}\big), \qquad \ell = 1, \dots, L-1 \\
f_\theta(x) &= W^{(L)} h^{(L-1)} + b^{(L)}
\end{aligned}
$$

The parameters are:

$$
\theta = \{W^{(\ell)}, b^{(\ell)}\}_{\ell=1}^{L}
$$

Multi-Layer Perceptron (MLP)

The MLP progressively builds internal representations of the input.

Each layer transforms the data into a more useful representation:

$$x \to h^{(1)} \to h^{(2)} \to \dots$$

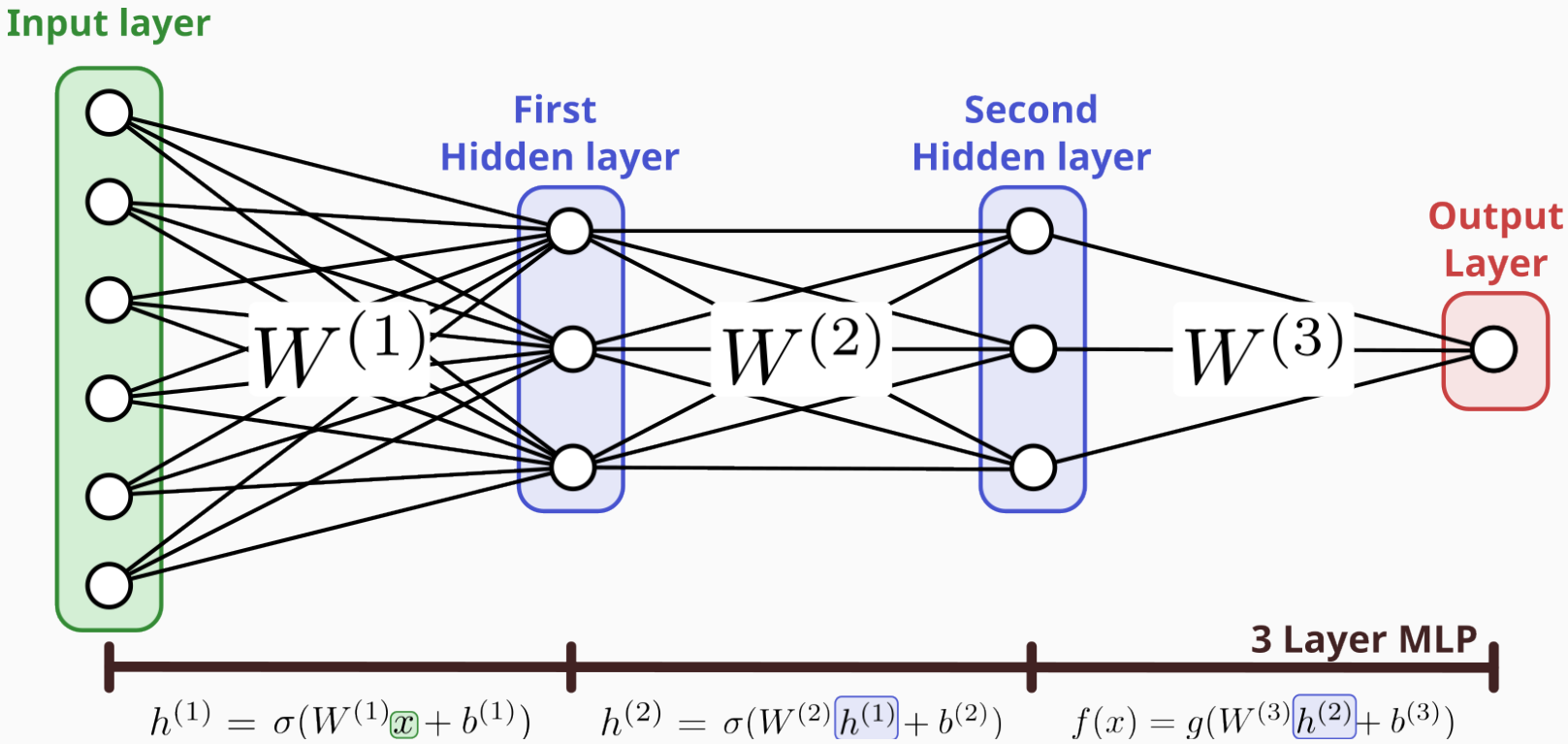
We can interpret:

$$\phi_\theta(x) = h^{(L-1)}$$

as a learned feature map, and the final layer as a predictor.

Thus, feature extraction and prediction are learned jointly from data.

Multi-Layer Perceptron (MLP) Visual



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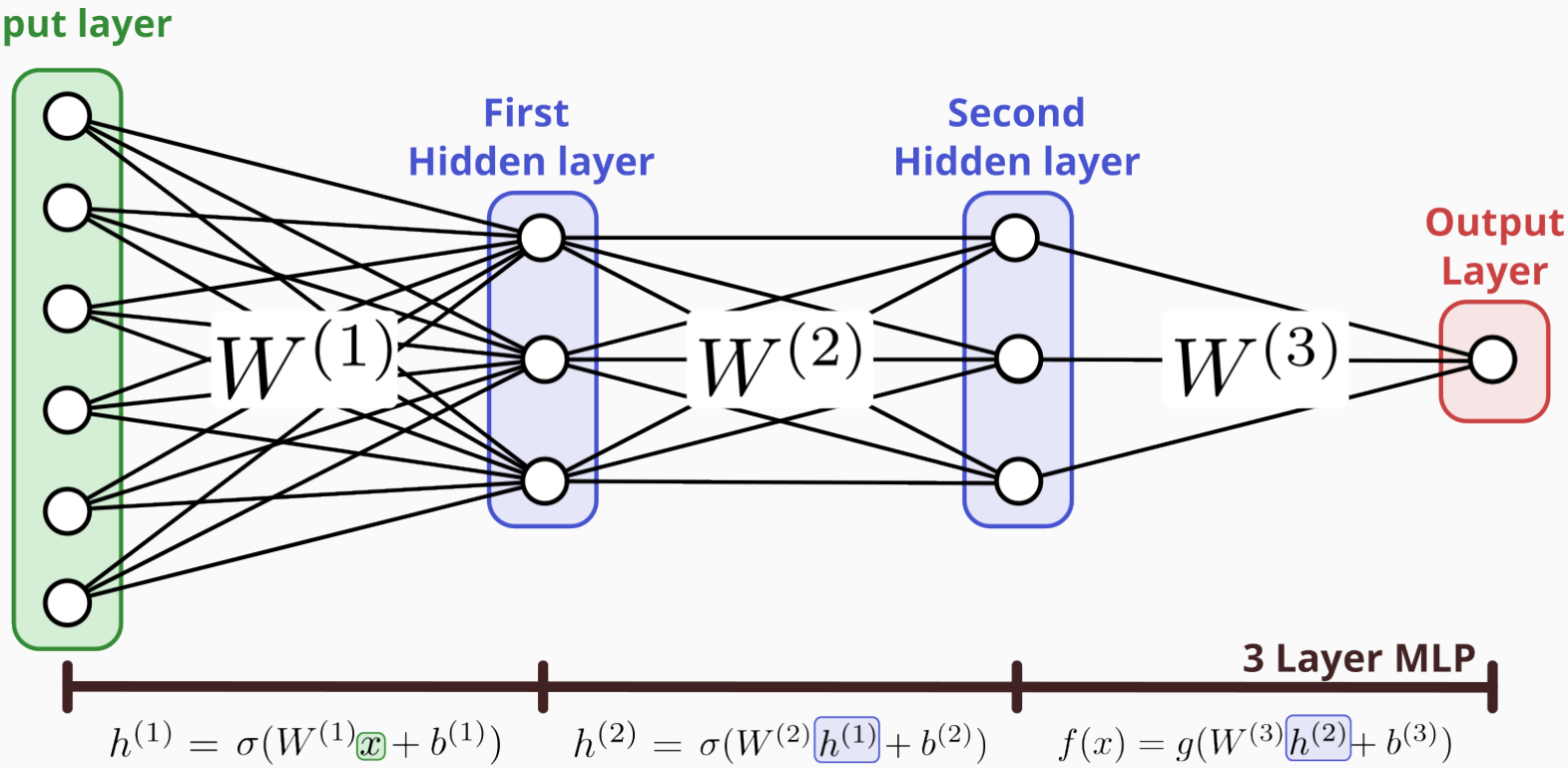

$$f(x) = g(W^{(3)}\sigma(W^{(2)}\sigma(W^{(1)}x + b^{(1)}) + b^{(2)}) + b^{(3)})$$

"Feature map"

Simple classifier

MLP: Activation Functions and Output Layers

Nonlinear activation functions σ. Common examples include:

ReLU:	**Tanh:**	**Sigmoid:**
$\sigma(x) = \max(0, x)$	$\sigma(x) = \tanh(x)$	$\sigma(x) = \frac{1}{1+e^{-x}}$

They introduce nonlinearity and allow the network to model complex functions.

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Output (Readout) Layer

The final layer maps learned representations to the output space:

$$f(x) = g(h_L(x))$$

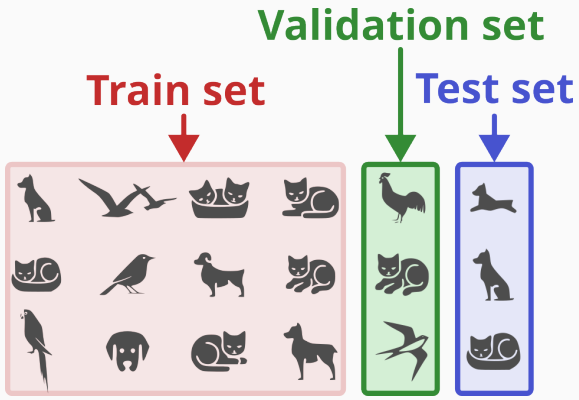
Regression	**Binary clas.**	**Multiclass clas.**
linear output	sigmoid	softmax
Predicting the price of a house.	Fraudulent or legitimate transaction.	Predicting the stage of the tumor.

Training, Generalization and UAT [short]

1. Training (Optimization)

Data is typically split into:

- **Training set**: fit the model
- **Validation set**: model selection/tuning
- **Test set**: final evaluation



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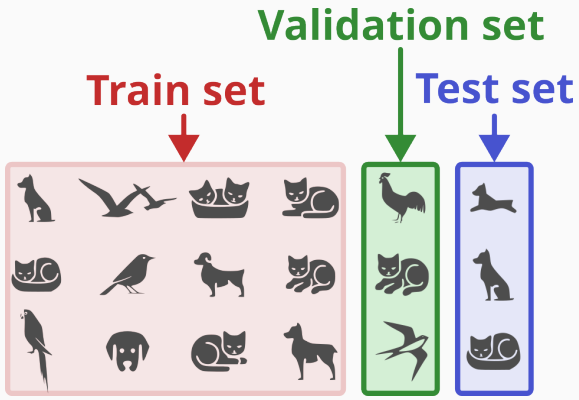

Given training data $\{(x_i, y_i)\}_{i=1}^n$, we define a loss function:

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell\big(f_\theta(x_i), y_i\big)$$

The goal is to find parameters that minimize the loss:

$$\theta^\star = \arg\min_\theta \mathcal{L}(\theta)$$

Training, Generalization and UAT [short]

The loss function measures how well the model fits the data.

Common choices depend on the task:

- **Regression:** Mean Squared Error

$$\ell(y, f_\theta(x_i)) = (y - f_\theta(x_i))^2$$

- **Binary classification:** Binary Cross-Entropy

$$\ell(y, f_\theta(x_i)) = -y \log f_\theta(x_i) - (1 - y) \log(1 - f_\theta(x_i))$$

- **Multiclass classification:** Cross-Entropy

$$\ell(y, f_\theta(x_i)) = -\sum_{c=1}^{C} y_c \log f_\theta(x_i)_c$$

Key idea: learning = minimizing a suitable loss function.

Training, Generalization and UAT [short]

2. Generalization Our goal is not only to fit the training data, but to perform well on unseen (test) data. We distinguish between:

- **Training error:** performance on observed samples
- **Test error:** performance on new data

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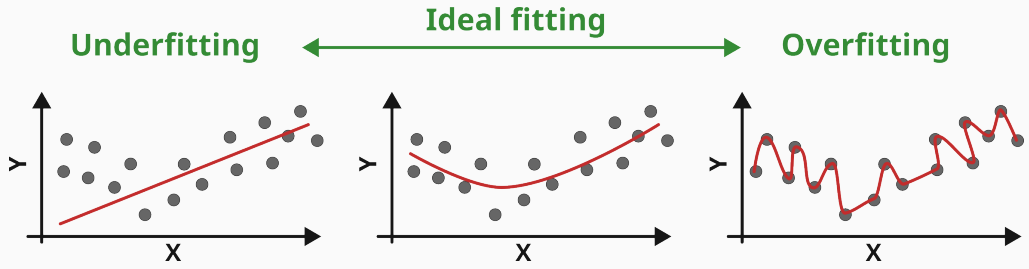
However, minimizing training error alone may lead to:

- **Underfitting:** model is too simple
- **Overfitting:** model memorizes the data



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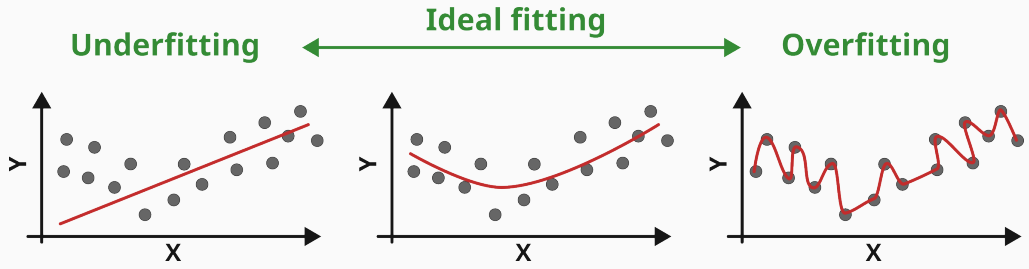


Evaluation metrics To measure performance on unseen data, we use task-dependent metrics:

- **Regression:** i.e. Mean Squared Error
- **Classification:** i.e. Accuracy

Training, Generalization and UAT [short]

3. Expressivity: Universal Approximation Theorem [2]

- A sufficiently wide MLP can approximate any continuous function on a compact domain
- In principle, even a single hidden layer is enough
- However, the theorem is only an **existence result**:
  - it does **not** say how many neurons are needed
  - it does **not** say whether the network can be trained efficiently

Take-home message: MLPs are expressive, but expressivity does not imply practical learnability.

Recap: From Data to Neural Networks

We started from a supervised learning problem:

$$(x, y) \sim \mathcal{D}, \quad f^\star : \mathcal{X} \to \mathcal{Y}$$

Classical approach:

$$f(x) = g(\phi(x)) \quad \text{with handcrafted features}$$

Deep learning:

$$f_\theta(x) = g_{\theta_2}(\phi_{\theta_1}(x)) \quad \text{learned from data}$$

MLPs:

- composition of linear maps + nonlinear activations
- learn representations and predictions jointly

Learning process:

- minimize a loss function
- aim for good generalization on unseen data

Learning on graphs

Limitations of MLPs

So far, we considered inputs as vectors:

$$x \in \mathbb{R}^d$$

MLPs operate on fixed-size, independent inputs.

Limitation:

- They do not model relationships between different data points
- They ignore interactions and dependencies

However, in many real-world problems, data are inherently **relational**.

Relational data can be modeled as a graph.

Graphs

Relational data can be modeled as a graph:

A graph is defined as:

$$G = (V, E, X_V, X_E)$$

where:

- V nodes
- $E \subseteq V \times V$ edges
- $X_V \in \mathbb{R}^{|V| \times d}$ node features
- $X_E \in \mathbb{R}^{|E| \times d'}$ edge features

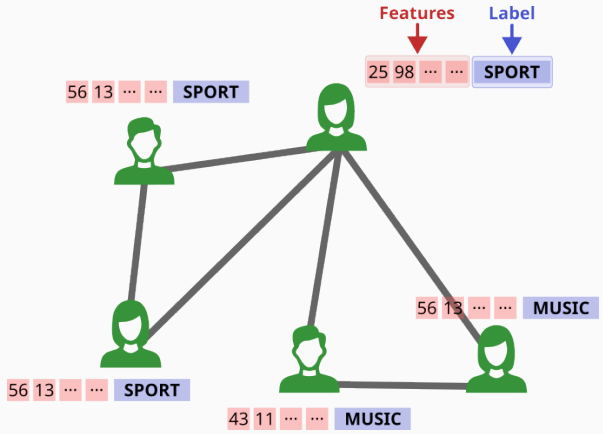
Labels can be associated to different elements:

$$\text{nodes: } y_v, \quad \text{edges: } y_{(u,v)}, \quad \text{graph: } y_G$$

Tasks on Graphs

Node-level tasks. Predict a label for each node:

$$y_v \in \mathcal{Y}, \quad v \in V$$



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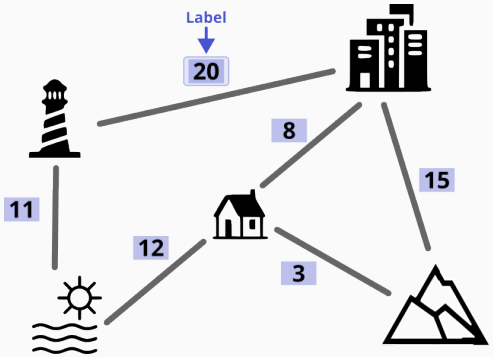

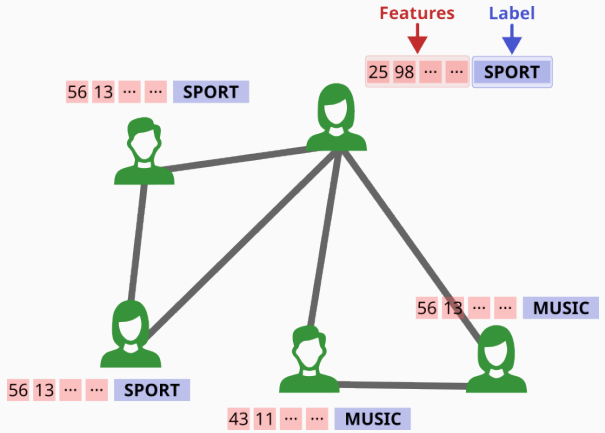

Edge-level tasks. Predict properties of edges or missing links:

$$y_{(u,v)} \in \mathcal{Y}, \quad (u,v) \in E$$

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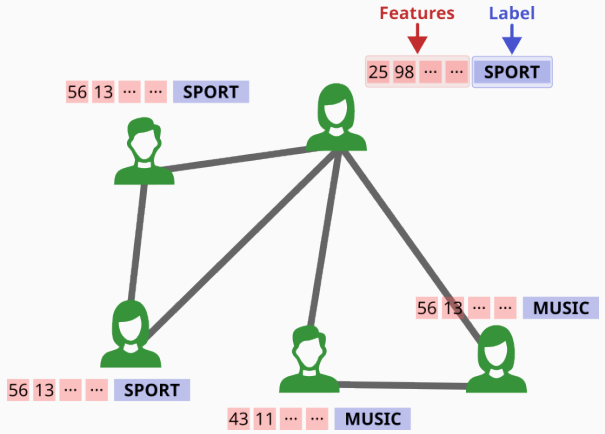
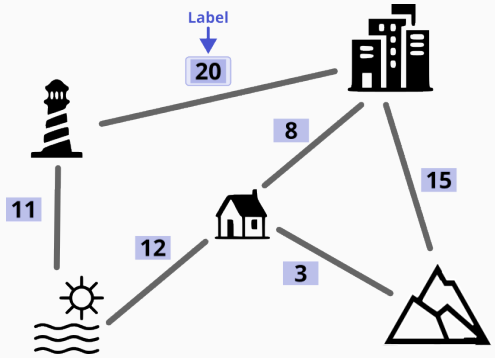


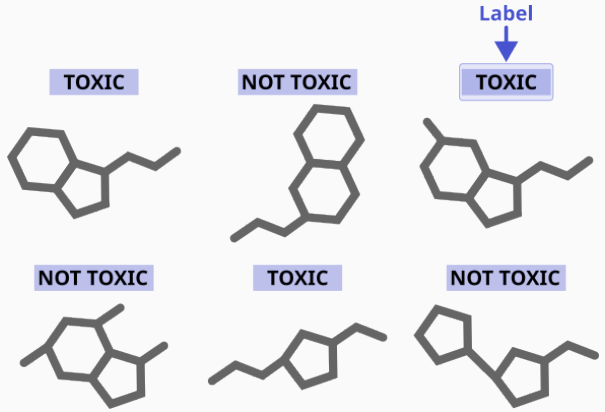


Edge-level tasks. Predict properties of edges or missing links:

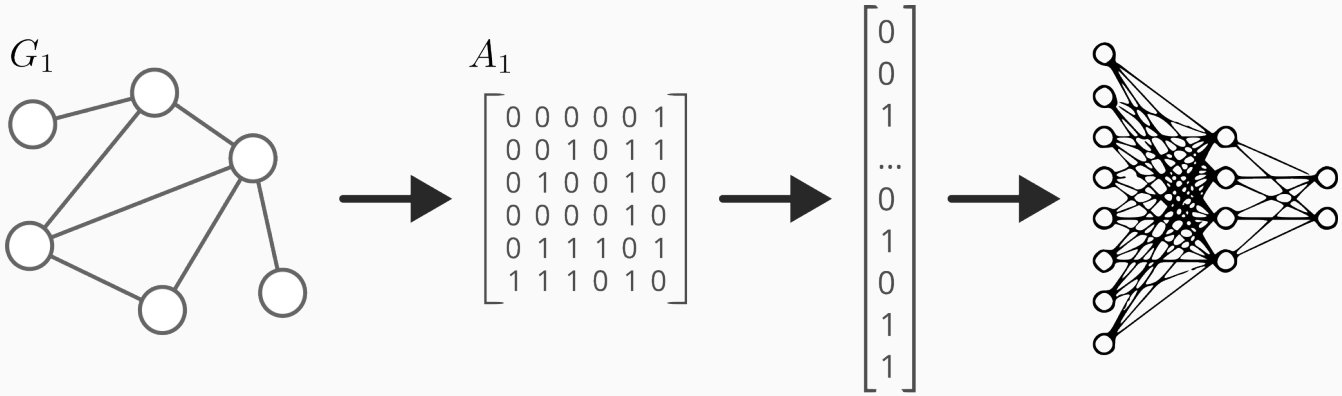
$$y_{(u,v)} \in \mathcal{Y}, \quad (u,v) \in E$$

Graph-level tasks. Predict a label for the entire graph:

$$y_G \in \mathcal{Y}$$



Why not use an MLP on graphs?



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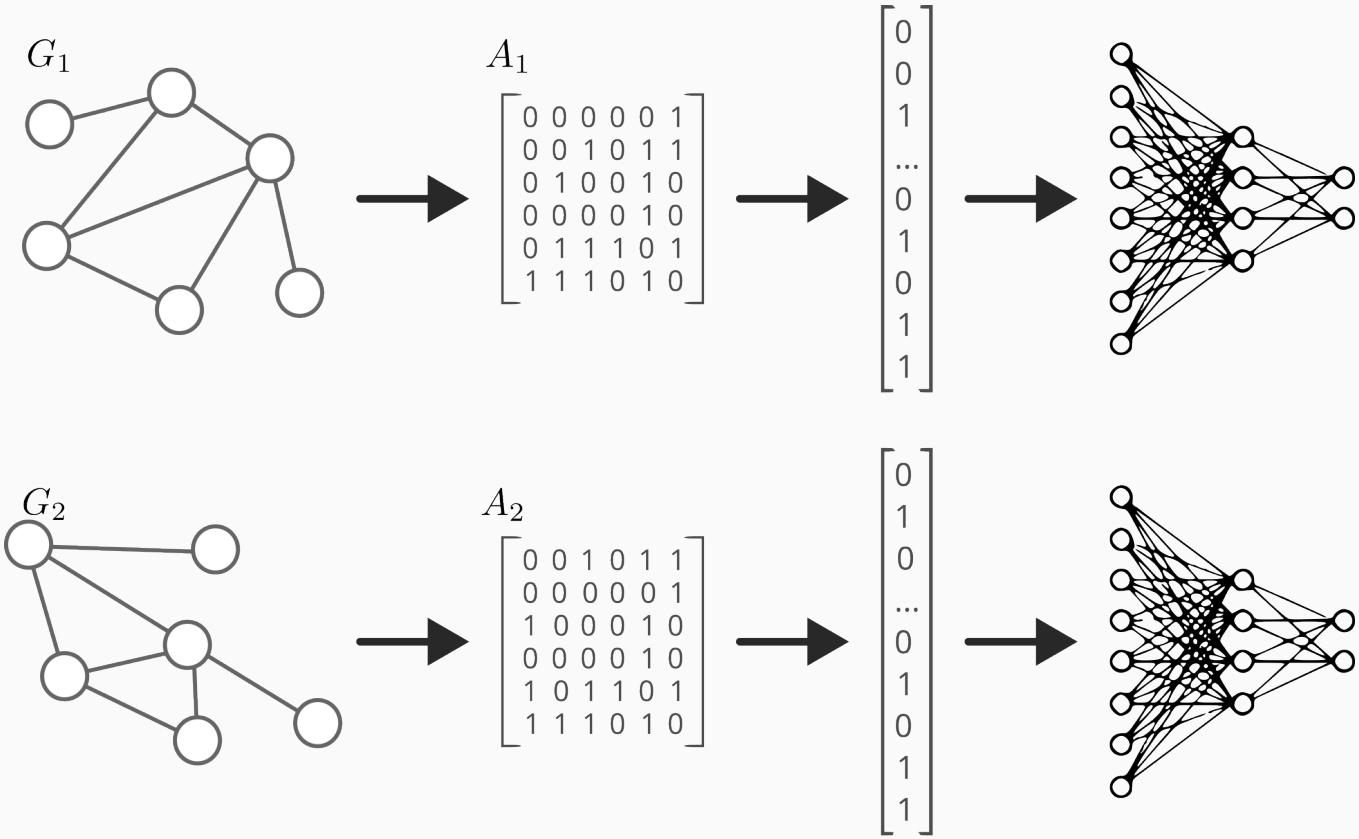


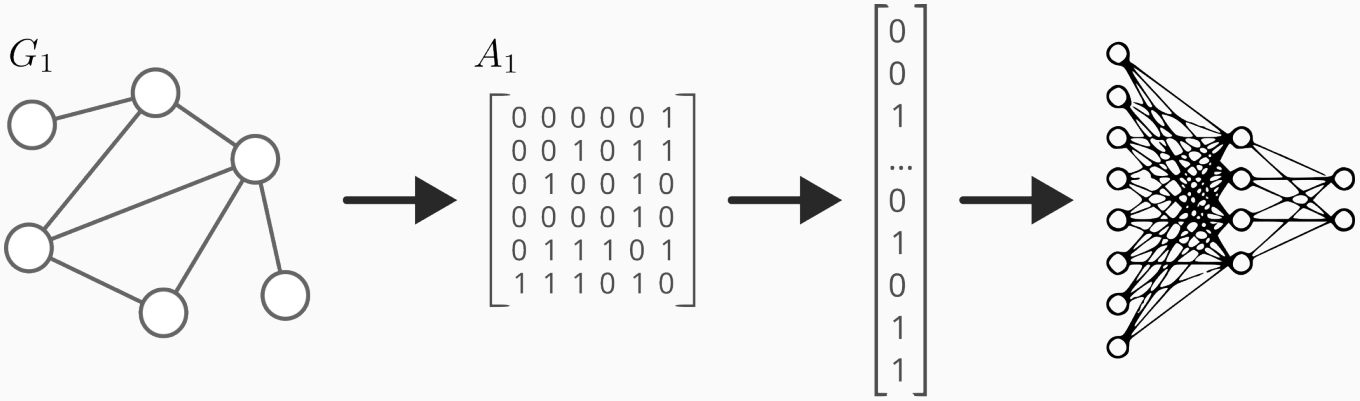
$$G_1 \cong G_2 \quad \text{but} \quad A_1 \neq A_2$$

Two graphs G_1 and G_2 are **isomorphic** ($G_1 \cong G_2$) if there exists a permutation $\pi : V \to V$ such that: $(i, j) \in E_1 \iff (\pi(i), \pi(j)) \in E_2$

Let P be the permutation matrix associated to π. Then: $A_2 = PA_1P^\top$

Why not use an MLP on graphs?

2. Different sizes



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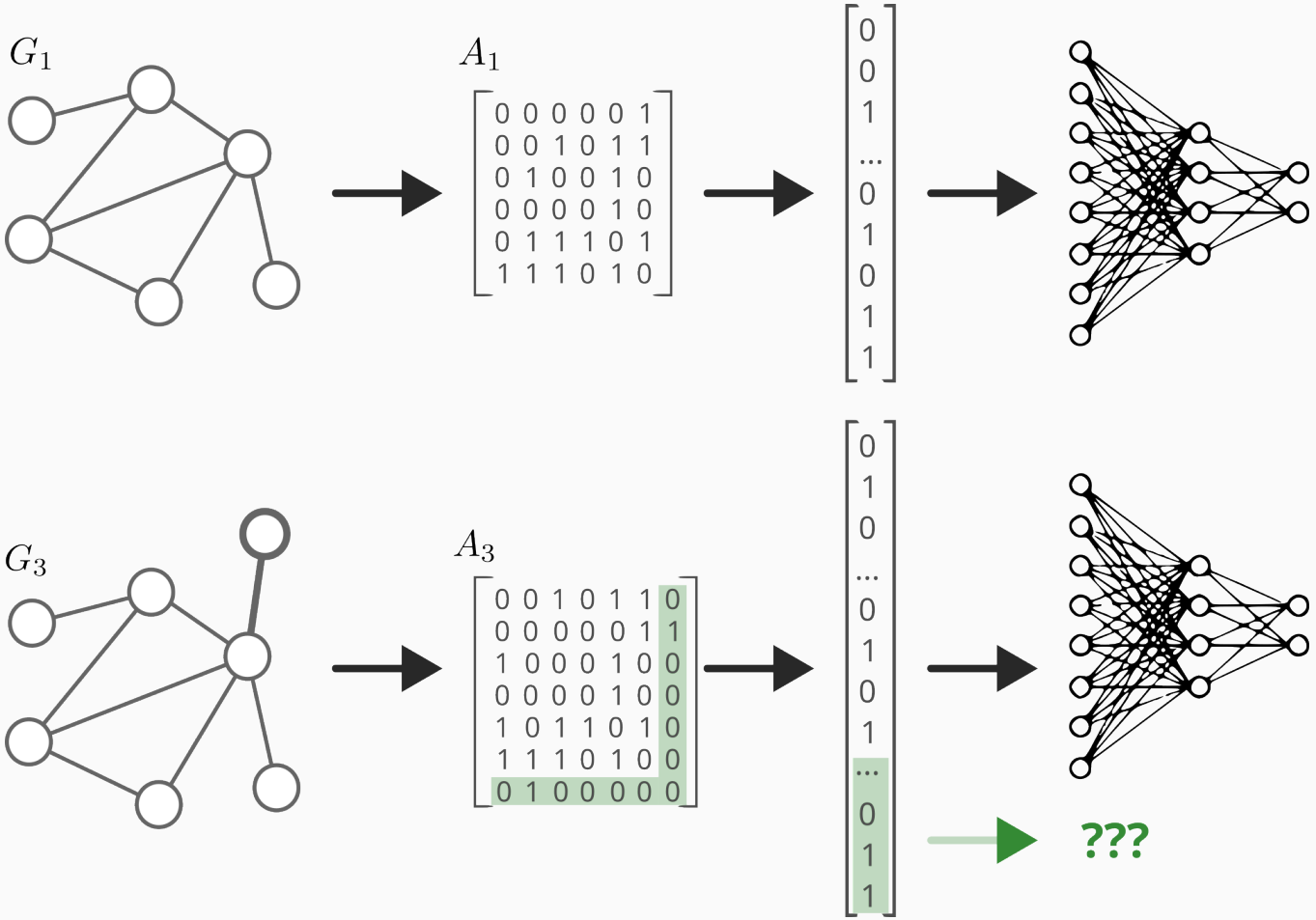


What do we want from a model on graphs?

A good model on graphs should:

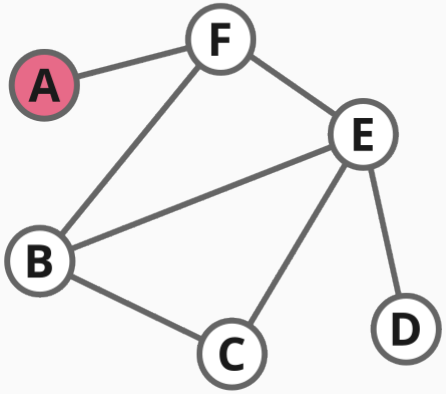
- Be **permutation invariant**
- Handle **variable-size graphs**
- Exploit **local structure** (neighbors matter)
- Share parameters across nodes (scalability)

Key idea: learn representations by aggregating information from neighbors.

Graph Neural Networks

Intuition

Input Graph



Computation Graph

x'_a

Intuition

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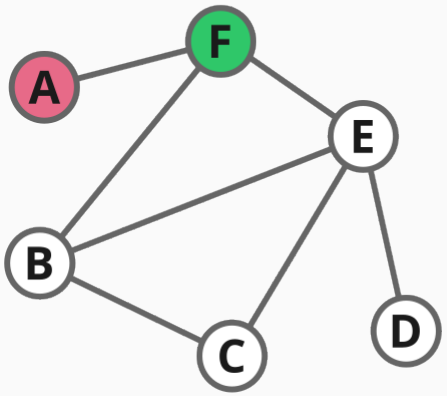
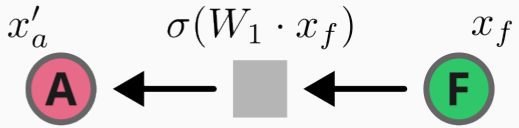


Computation Graph



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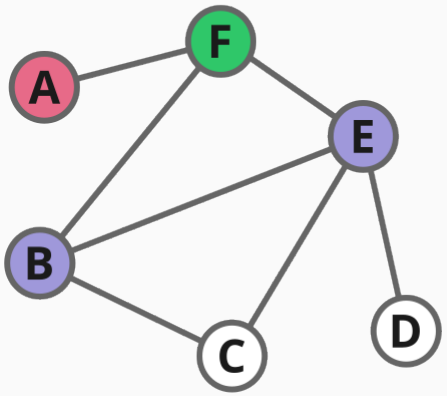

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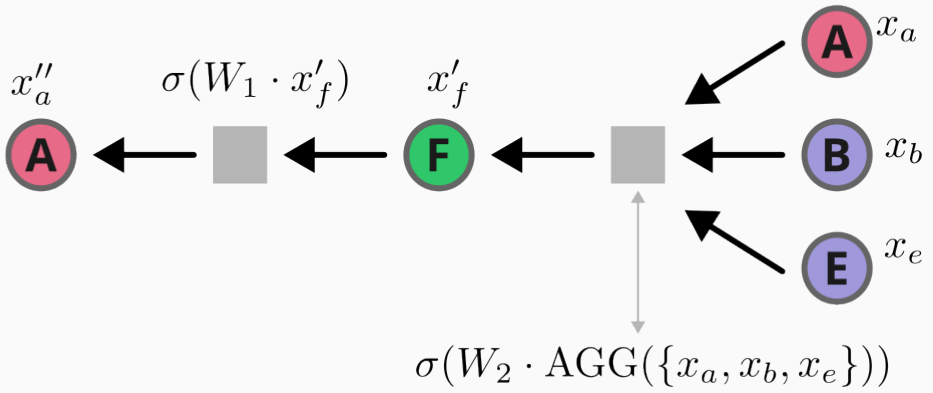

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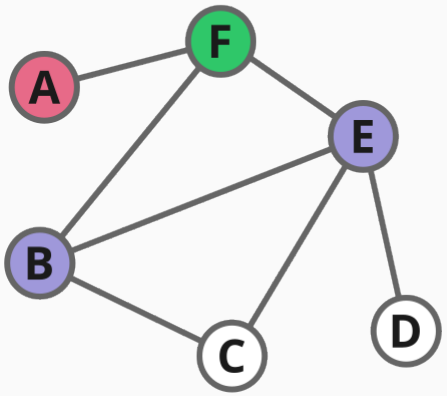

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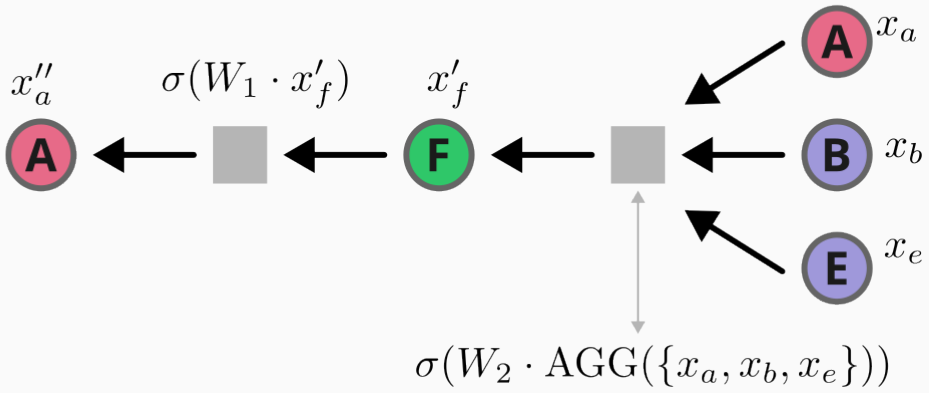

Each node representation is updated by aggregating information from its neighbors.

This process can be decomposed into three steps:

- **Message:** each neighbor sends information
- **Aggregation:** messages are combined
- **Update:** the node updates its feature

Why does message passing work?

Key assumption: local dependency structure

In many real-world graphs, neighboring nodes tend to be **similar** or **correlated**. **Examples:**

- Social networks: connected users share interests
- Citation networks: linked papers discuss related topics
- Molecules: bonded atoms influence each other

Key idea:

- propagate information locally
- progressively enlarge the receptive field

After k layers, each node has access to its k-hop neighborhood.

Message Passing Neural Networks (MPNN)

Let $x_i^{(k)}$ be the feature of node i at layer k.

A general GNN can be written as [3]:

$$m_i^{(k)} = \mathrm{AGG}\Big(\{M(x_i^{(k)}, x_j^{(k)}, e_{ij}) : j \in \mathcal{N}(i)\}\Big)$$

$$x_i^{(k+1)} = U\big(x_i^{(k)}, m_i^{(k)}\big)$$

Components:

- M: message function
- AGG: permutation-invariant aggregation (sum, mean, max)
- U: update function

Key idea: this defines a general class of Graph Neural Networks.

From general to specific models

The MPNN framework defines a large family of models.

Question: how should we choose M and U?

Different choices lead to different GNN architectures.

Example: Graph Convolutional Networks (GCN) [5]

Graph Convolutional Networks (GCN)

A simple and widely used instantiation of message passing is given by [5]:

$$X^{(k+1)} = \sigma\left(\tilde{D}^{-1/2}\tilde{A}\,\tilde{D}^{-1/2}X^{(k)}W^{(k)}\right)$$

where:

- $\tilde{A} = A + I$ is the adjacency matrix with self-loops
- $\tilde{D}$ is the degree matrix of $\tilde{A}$
- $X^{(k)}$ is the node feature matrix at layer k
- $W^{(k)}$ is a learnable weight matrix

GCN corresponds to choosing a very simple message function: a normalized linear aggregation.

A spectral perspective on graphs

So far, we defined GNNs in a **spatial way**, i.e. nodes aggregate information from neighbors.

An alternative viewpoint comes from **spectral graph theory**.

Let G be a graph with normalized Laplacian:

$$L = I - D^{-1/2} A D^{-1/2}$$

Since L is symmetric, it admits an eigendecomposition:

$$L = U \Lambda U^{\top}$$

Interpretation:

- U: graph Fourier basis
- Λ: frequencies

This allows us to define convolution on graphs in the spectral domain.

From spectral convolution to GCN

A spectral graph convolution can be defined as:

$$x \mapsto U\, g(\Lambda)\, U^\top x$$

where $g(\Lambda)$ is a filter in the spectral domain.

However:

- requires eigen-decomposition ($\mathcal{O}(n^3)$)
- not scalable/localized

Key idea: approximate $g(\Lambda)$ with a low-degree polynomial.

This leads to **localized filters** that depend only on neighbors.

From spectral convolution to GCN

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This leads to **localized filters** that depend only on neighbors.

Result (Kipf & Welling)[5]:

$$X^{(k+1)} = \sigma\left(\tilde{D}^{-1/2}\tilde{A}\,\tilde{D}^{-1/2}X^{(k)}W^{(k)}\right)$$

Conclusion: GCNs can be seen as a **first-order approximation** of spectral graph convolutions.

Spatial vs Spectral View

Spectral view:

- convolution = filtering in the graph Fourier domain
- based on the Laplacian spectrum

Spatial view:

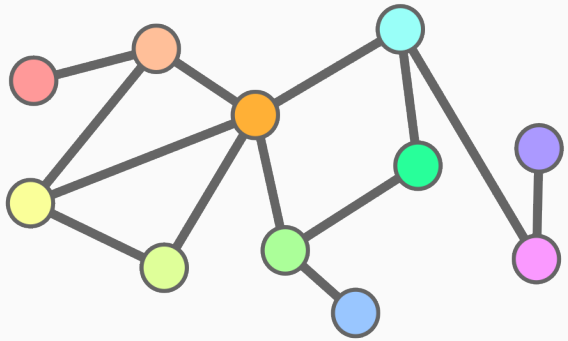
- convolution = aggregation from neighbors
- local, permutation-invariant operations

Key insight: many spatial GNNs can be interpreted as approximations of spectral filters.

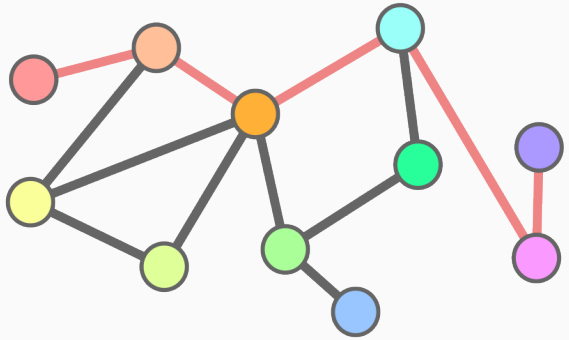
GNN Limitations. Over-smoothing: how many layers do we need?

How many message passing layers should we use

Input graph



Diameter



GNN Limitations. Over-smoothing: how many layers do we need?

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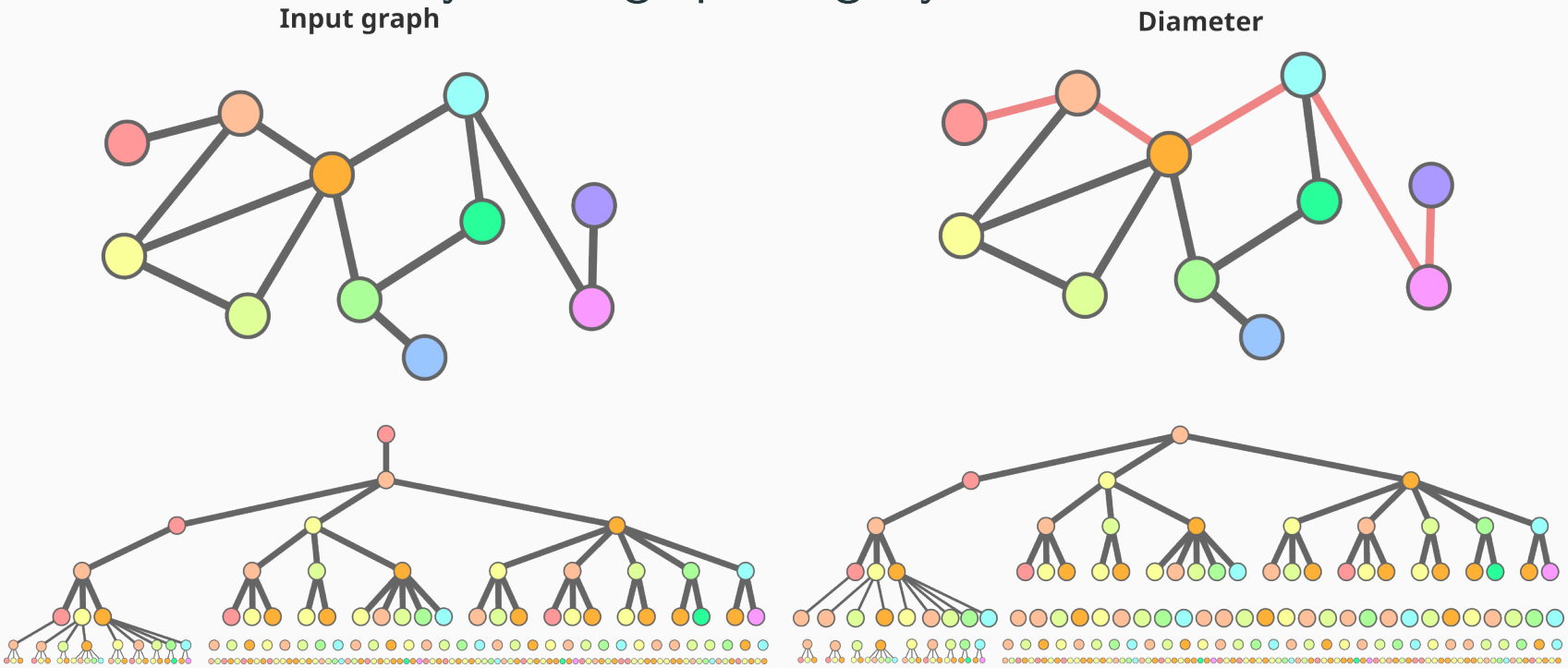


Do we really want to propagate information across the entire graph?

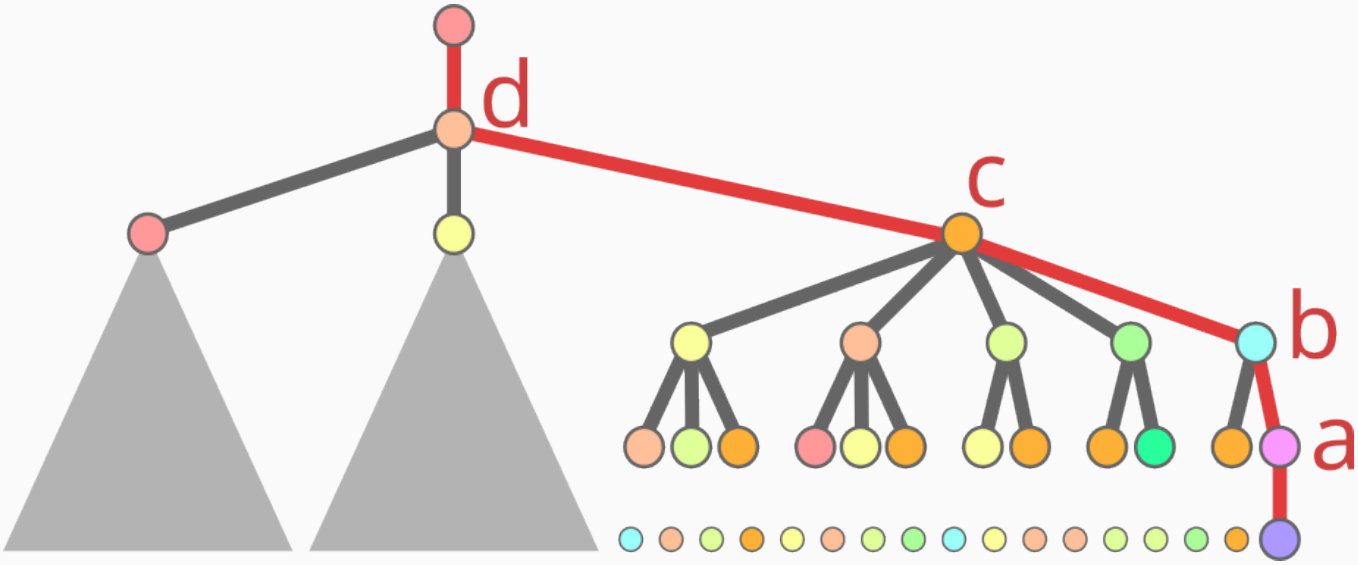
Over-smoothing: node representations become indistinguishable [11]

GNN Limitations. Over-squashing: long-range dependencies

can GNNs capture long-range interactions?

Example: consider a graph where the label of a node depends on a distant node. (information must travel across many intermediate nodes)

Over-squashing: long-range information is **compressed** and becomes hard to recover.[10]



GNN Limitations. Expressivity

Question: how expressive are GNNs?

Weisfeiler–Lehman (WL) test: an iterative procedure that updates node labels by aggregating the labels of neighboring nodes.

At each iteration:

$$\text{label}_i^{(k+1)} = \text{hash}\left(\text{label}_i^{(k)}, \{\text{label}_j^{(k)} : j \in \mathcal{N}(i)\}\right)$$

Key fact: many GNNs are at most as powerful as WL.

Implication: if WL cannot distinguish two graphs, neither can these GNNs.[7]

What the NGML group is doing?

Explainability in GNNs [6]

Problem: a GNN makes a prediction, but *why*?

We want to understand:

- which **nodes / edges** matter
- which **features** matter
- which **subgraph** supports the decision

Why important?

- trust
- debugging
- detecting spurious patterns

Main techniques:

- Subgraph explanations
- Counterfactuals

Uncertainty in NNs [9]

Question: how confident is the prediction?

Why?

- detect unreliable predictions
- decision making under uncertainty
- robustness to distribution shifts

Techniques:

conformal predition ensembles stochastic regularization

Roberto, Andrea, Filippo

Pooling in GNNs [1]

Problem: how do we obtain a **global representation** of a graph?

Goal:

- map variable-size graphs $\rightarrow$ fixed-size representation
- preserve relevant **structure**

Why is it non-trivial?

- must be **permutation invariant**
- must avoid losing important information

Main approaches:

global pooling hierarchical pooling learned clustering

Spatio-temporal Graphs [4]

Problem: data evolve over both **structure** and **time**

Setting:

$$G(t) = (V(t), E(t), X(t))$$

- nodes / edges may change over time
- features evolve dynamically

Goal:

- model **temporal dependencies**
- capture interaction between **space (graph)** and **time**

Main approaches:

temporal message passing recurrent models attention over time

Expressivity: beyond WL [8]

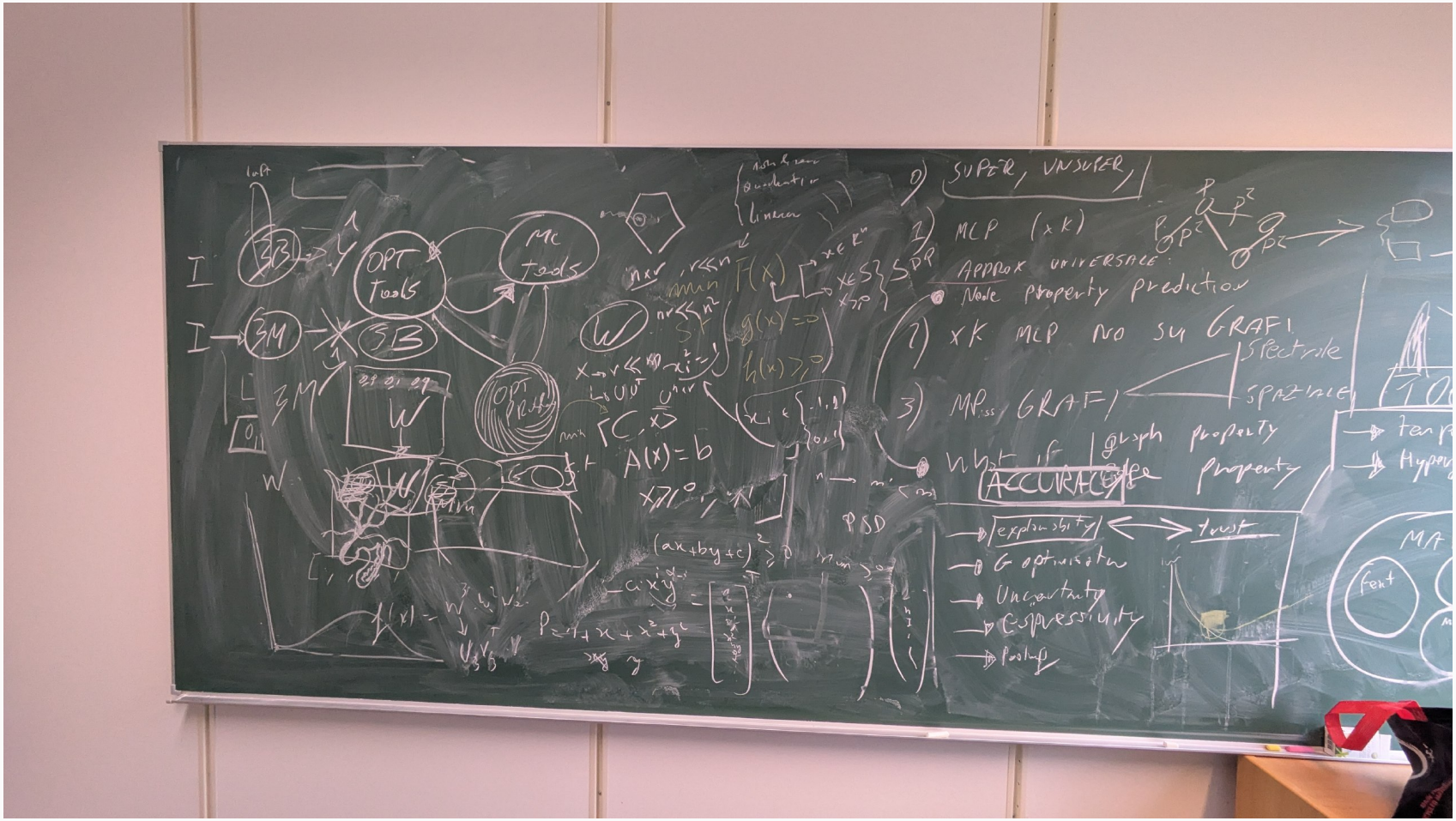
Limitation: standard GNNs $\leq$ Weisfeiler–Lehman (WL)

Research question: how can we go **beyond local aggregation**?

Main directions:

- **Higher-order methods**
  - k-WL, subgraph-based GNNs
- **Richer structures**
  - simplicial complexes, hypergraphs, hyperbolic embeddings
- **Global information**
  - positional encodings, spectral features
- **Breaking symmetry**
  - identifiers, random features

10 Minutes Discussion



Yassine Koubaa

Thank you!

Questions or discussion?

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