PyTorch and Graph Neural Networks (GNNs)

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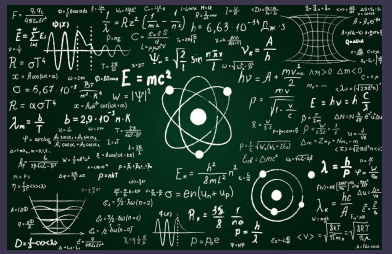
What does it mean to use ML?

Classically



We get answers using rules and data!

Machine Learning

We get the rules given the data and their answers!

What makes PyTorch so advantageous?

What is PyTorch?

- Machine learning framework produced by Facebook in 2016
- Designed to provide good flexibility and high speeds
- Uses dynamic computation graphs

Advantages

- Pythonic Nature
- Easy to Learn
- Strong Community
- Easy Debugging

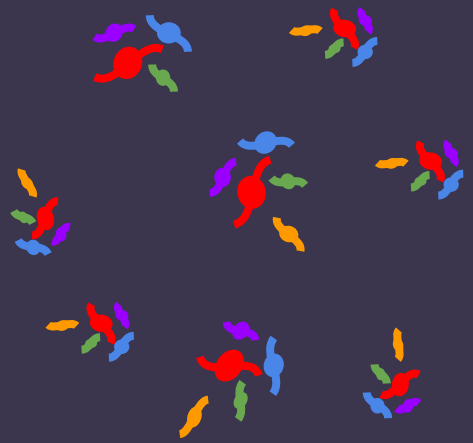
- Dynamic X Static
- **Data parallelism:** asynchronous X manual
- Flexibility, debugging capabilities, and short training duration: >

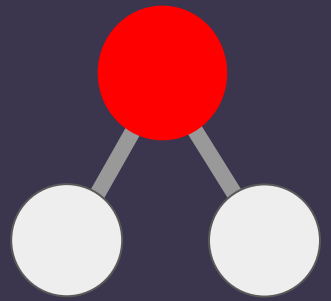
Different datasets

Tabular data

X	...	Y
15.7	...	24.2
12.1	...	14.6
...	...	...
13.0	...	15.9

Structured data





Different datasets

Tabular data

Neural Networks

k Nearest Neighbors

Extremely Randomized Trees

Light Gradient Boosting Machines

Random Forests

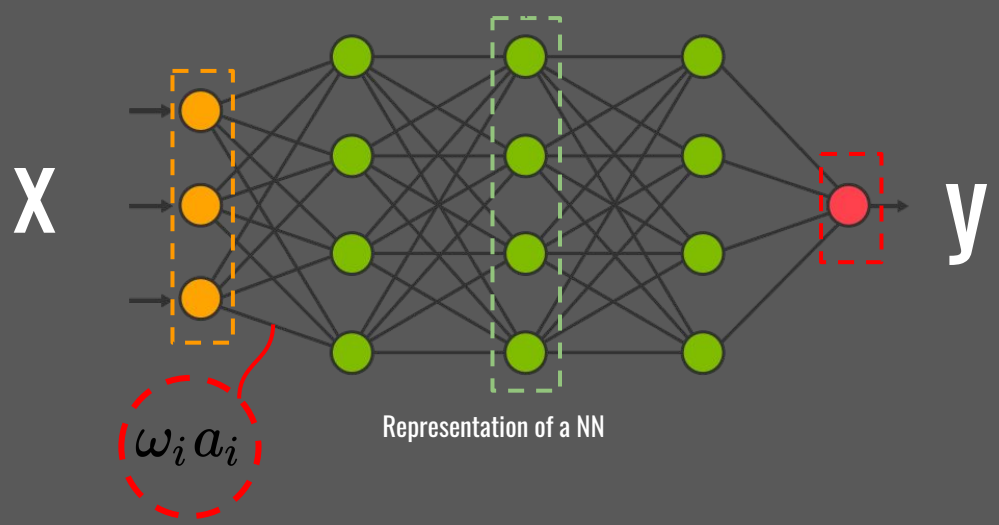
Support Vector Machines

Structured data

Graph Neural Networks

An overview of Neural Networks

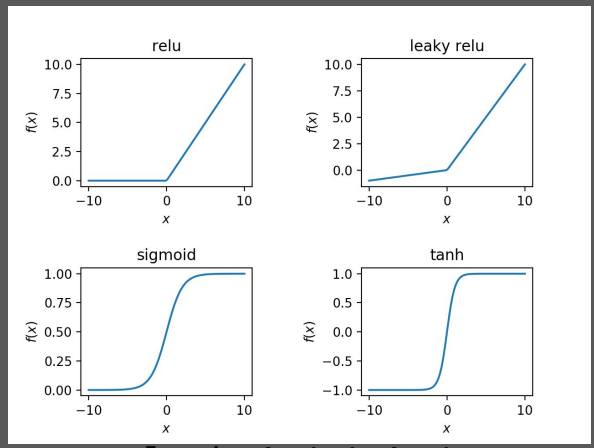
$$b_\mu + \sum_\nu W_{\mu\nu} a_\nu$$



Representation of a NN

Every layer is responsible to employ an **activation function**:

$$y_\mu = f\left(b_\mu + \sum_\nu W_{\mu\nu} a_\nu\right)$$

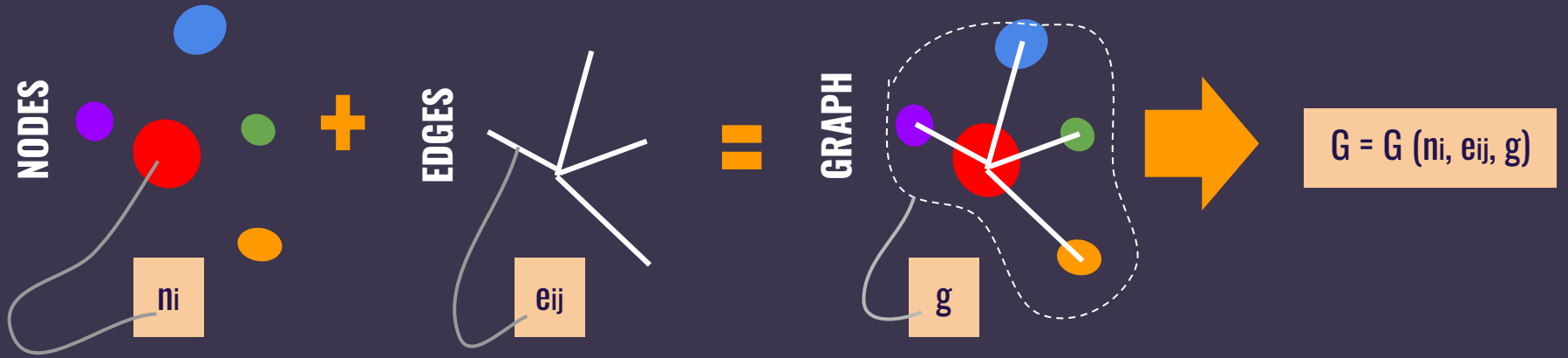


Examples of activation functions

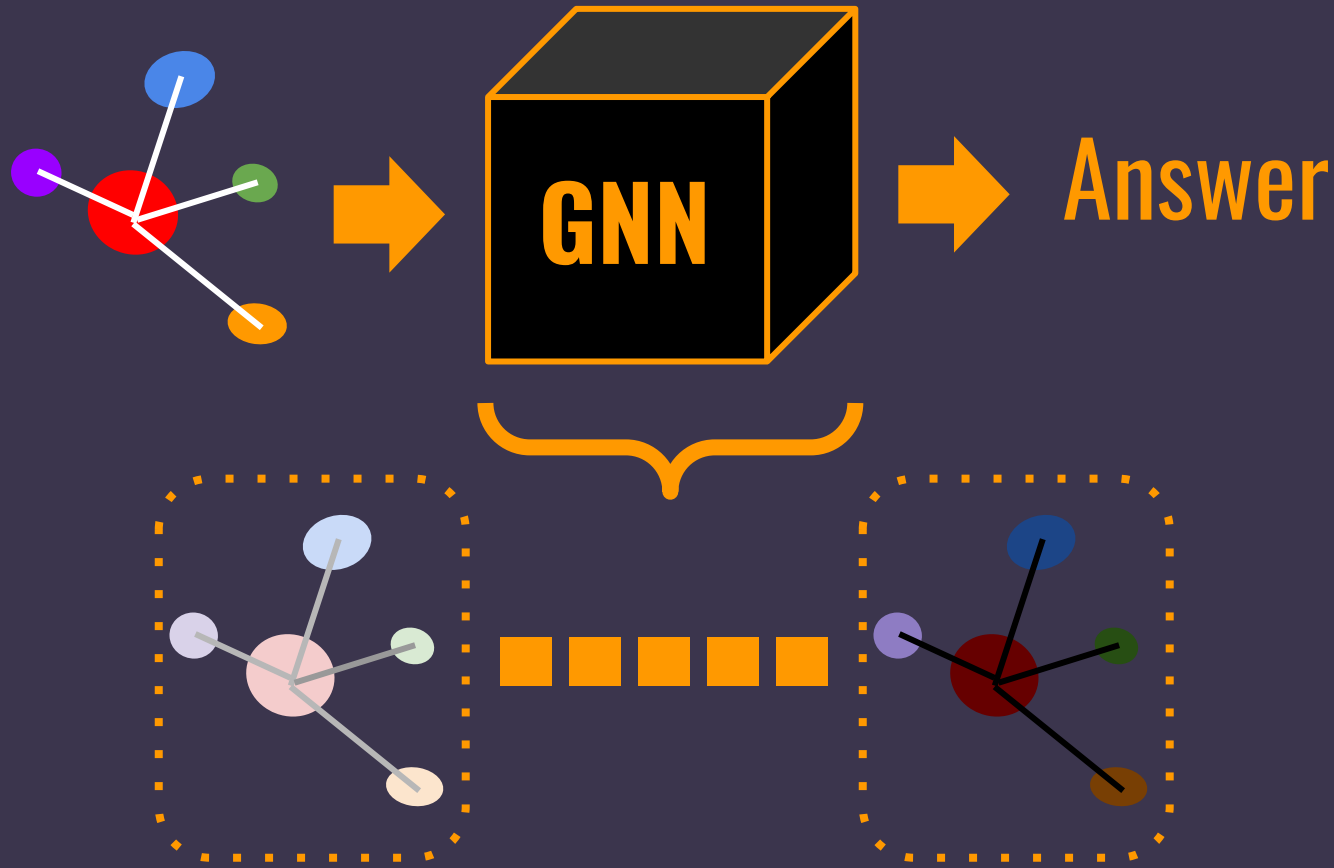
The training process is done is ephocs, minimizing the **loss function**, e.g., ***Mean Square Error*** **(MSE)**:

$$\text{MSE} = \frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$$

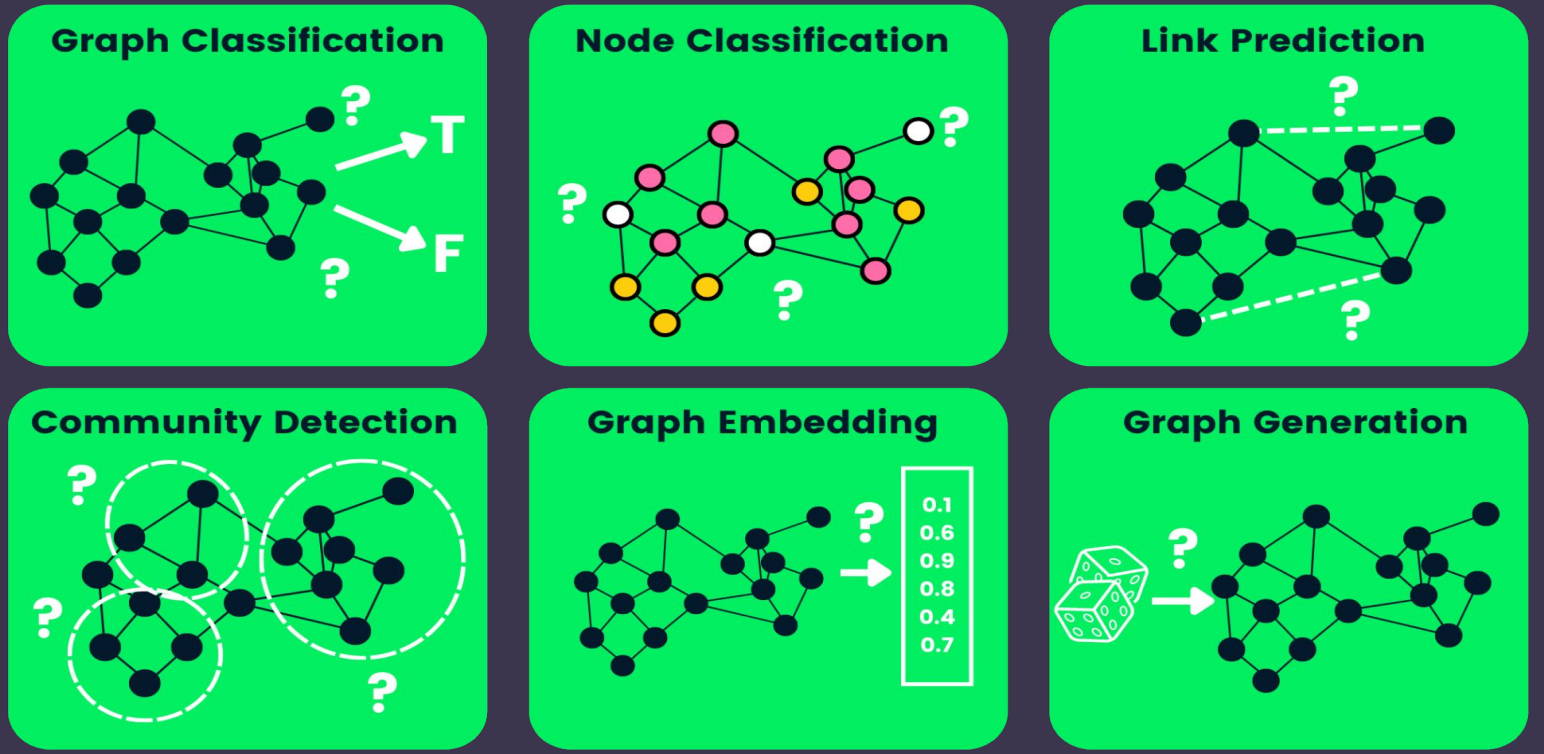
What are graphs?



What are graph neural networks?



How this answer can be?



https://images.datacamp.com/image/upload/v1658404112/Types_of_Graph_Neural_Networks_fd300394e8.png

Hands-on activity

STEP 1: go to github and download the repo using:

$ git clone https://github.com/natalidesanti/pytorch_and_GNNs

STEP 2: open the **pytorch** notebook in your preferred machine (your own or in Google Colab)