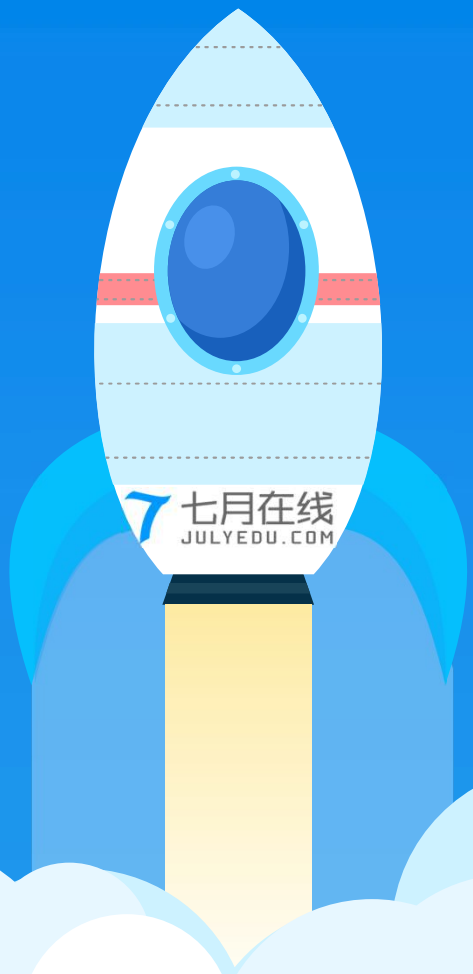
《图论理论基础》

主讲： 彭老师

https://www.julyedu.com/



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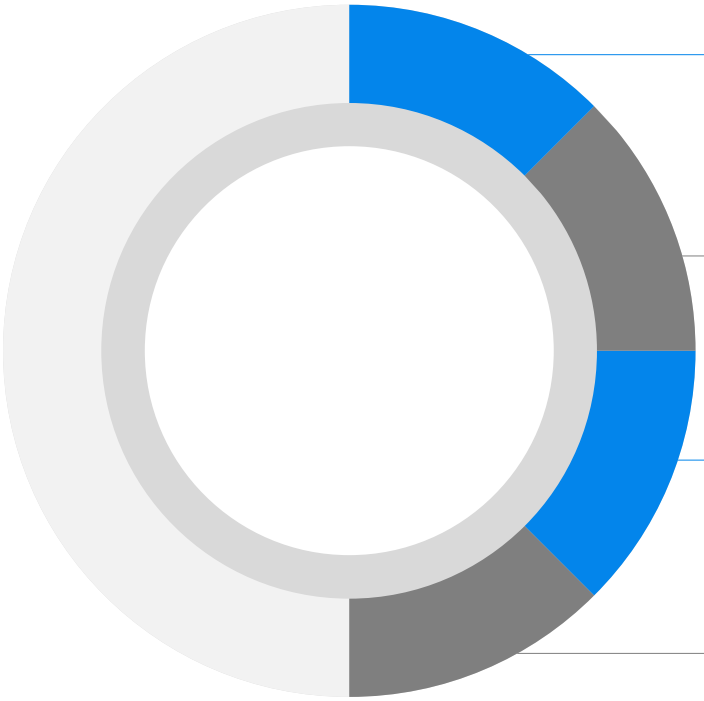


图神经网络简介

Overview of Object GNN

系统与环境配置

Operating System

开源框架速安装

Deep Learning Frame

Project I： NetworkX

项目实战： **NetworkX**

/01 Overview of Object GNN

图神经网络简介

Graph

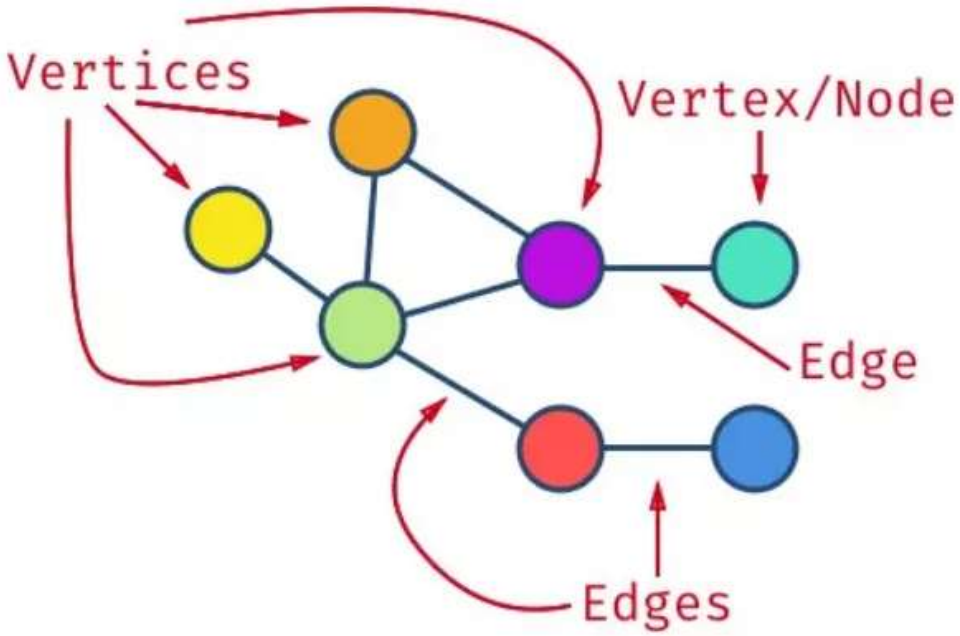
What is Image? What is **Graph**?

Graphs are a kind of data structure which models a set of **objects** (nodes) and their **relationships** (edges).

Graph

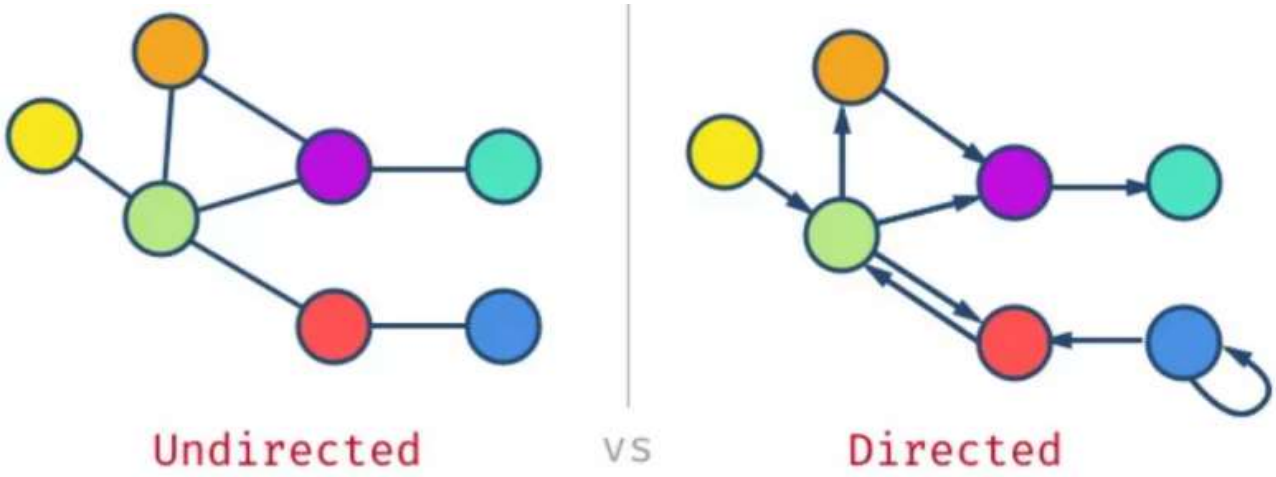
A graph G can be well described by the set of **vertices** (**nodes**) V and **edges** E it contains.

$$G = (V, E)$$



Graph

Edges can be either directed or undirected, depending on whether there exist directional dependencies between vertices.



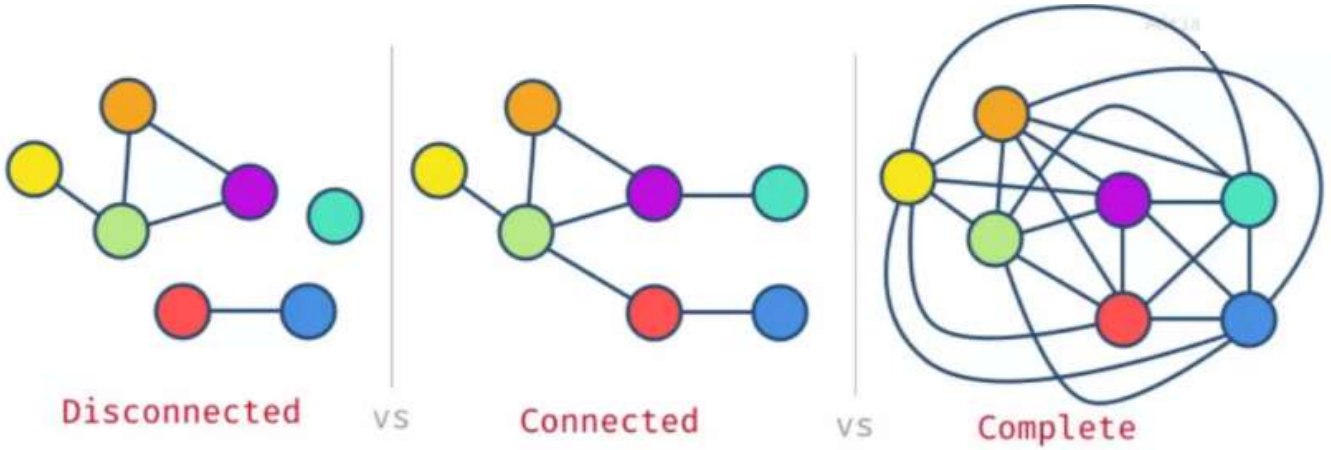
Graph

A graph can have **cycles** which means that if you traverse through the node, you could get to the same node more than once.

The graph without cycles is called **acyclic graph**.

Graph

Not all vertices have to be connected in the graph. You might have isolated nodes or even separated subgraphs.
If all nodes has a least one edge, then we have a **connected graph**. When all nodes are connected to all other nodes, then we have a **complete graph**.

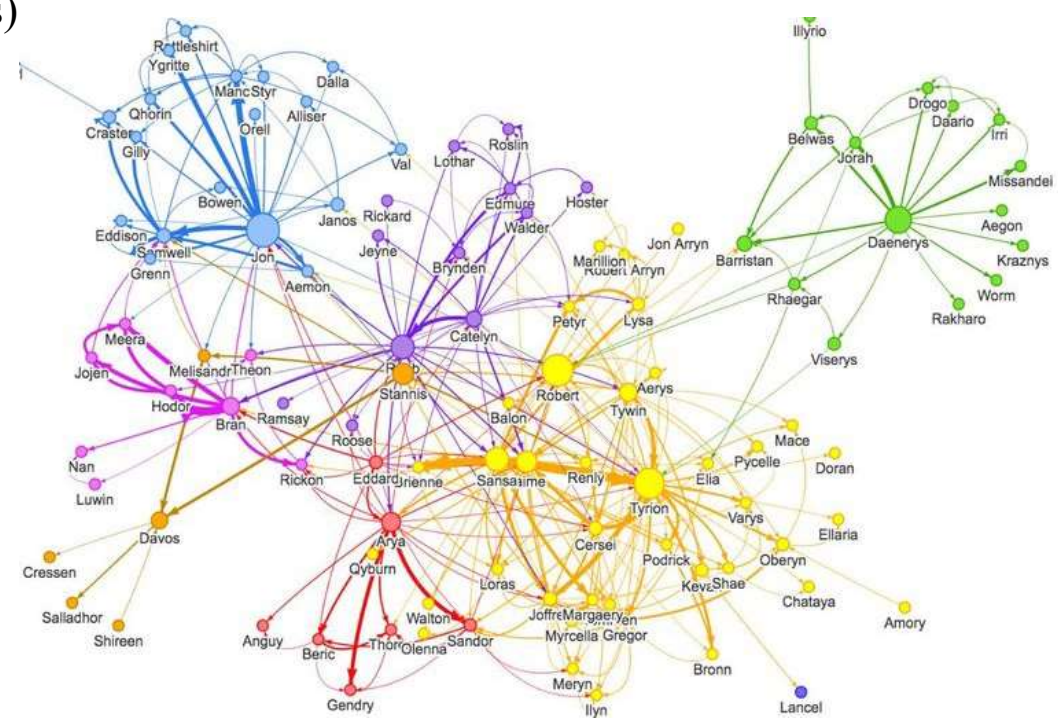


Graph

A graph can represent many things → social media networks, molecules, etc.

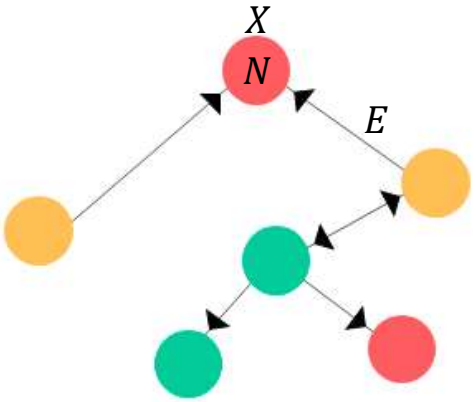
Nodes can be thought of as users/products/atoms while the edges represent connections (following/usually-purchased-with/bonds)

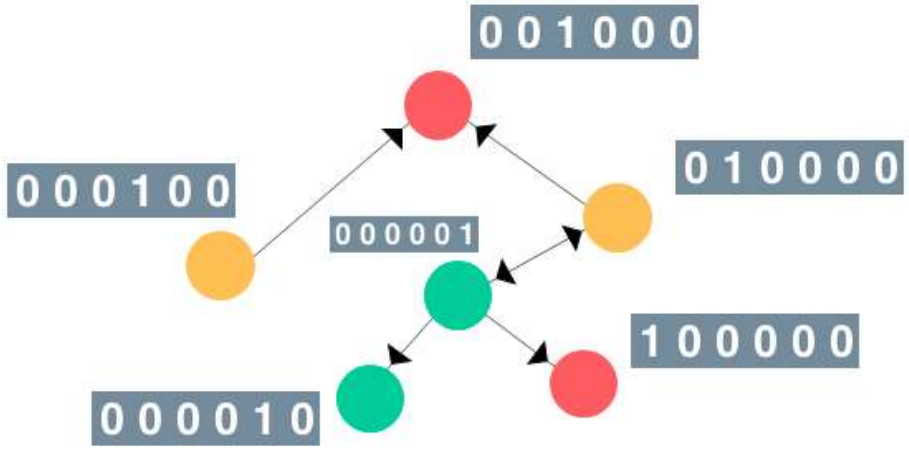
Social media graph:



Graph Neural Network

Graph neural networks (GNNs) are deep learning-based methods that operate on graph domain.

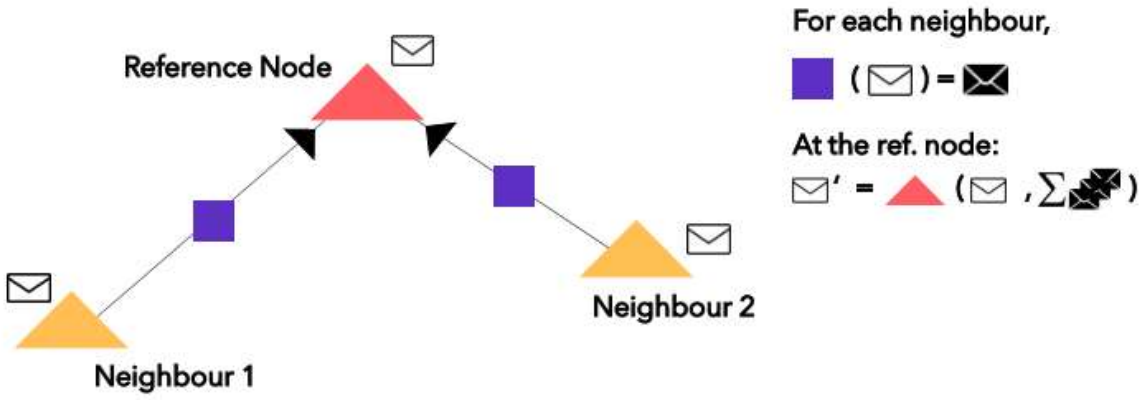




Message Passing

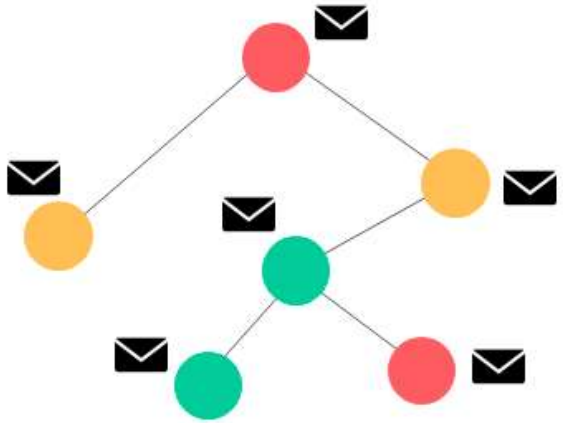
Once the conversion of nodes and edges are completed, the graph performs **Message Passing** between the nodes.

This process is also called **Neighborhood Aggregation** because it involves pushing messages (the embeddings) from surrounding nodes around a given reference node, through the directed edges.



Embedding Aggregation

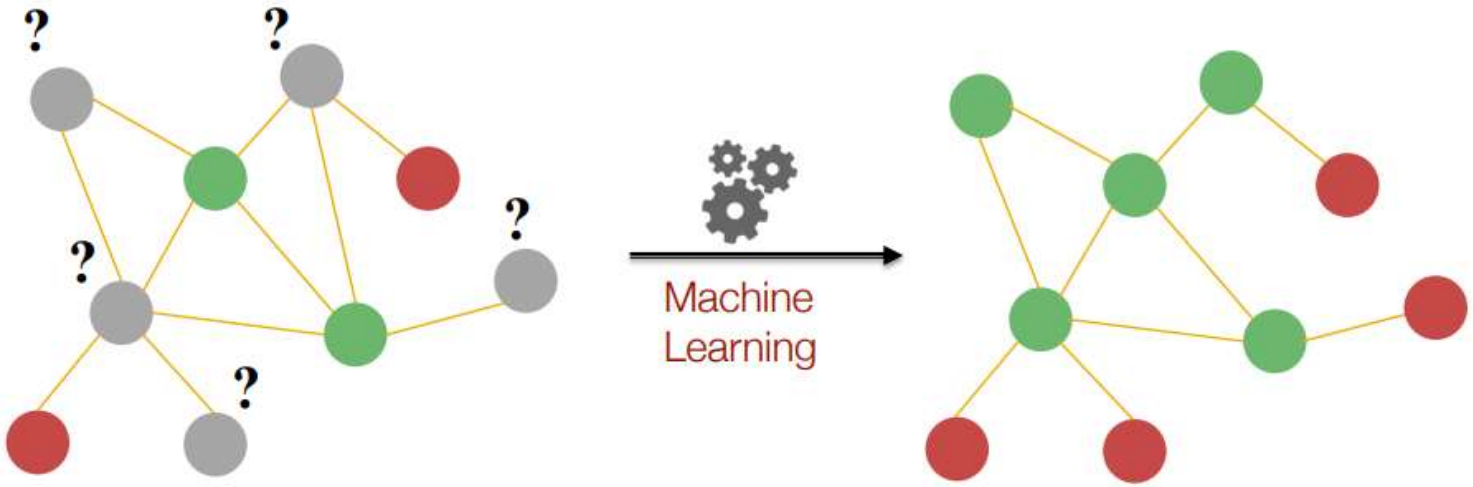
We can take all the embeddings and sum them up together to get vector H that represents the whole graph.



$$H = \sum (\quad)$$

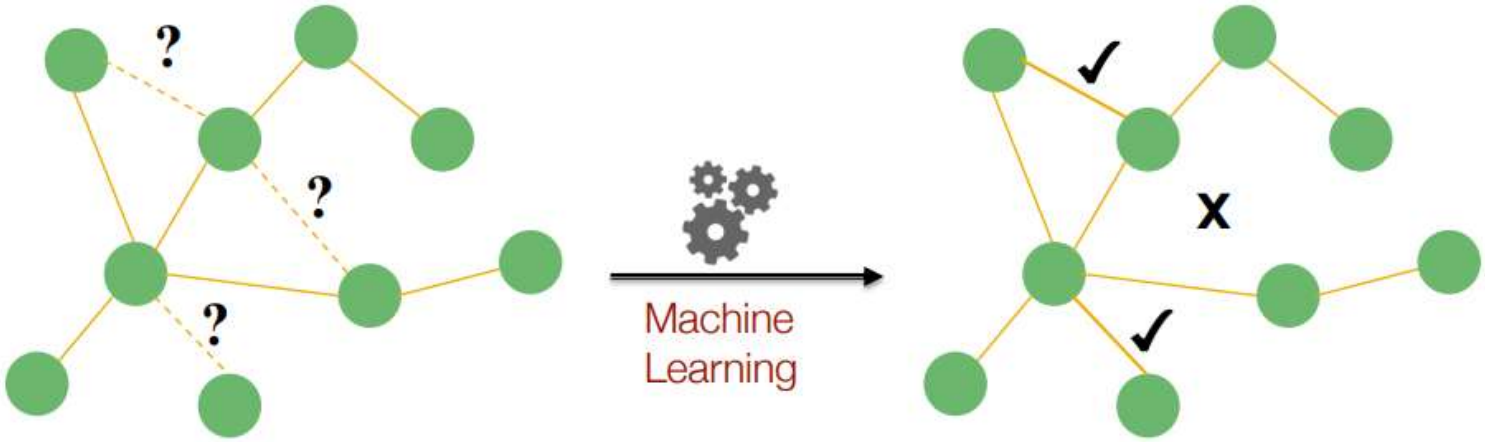
Graph Tasks

Node Classification



Graph Tasks

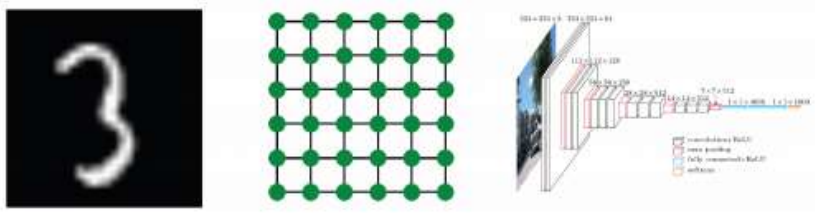
Link Prediction



Why is it hard?

Modern deep learning toolbox is designed for simple sequences or grids.

- ✓ CNNs for fixed-size images/grids….

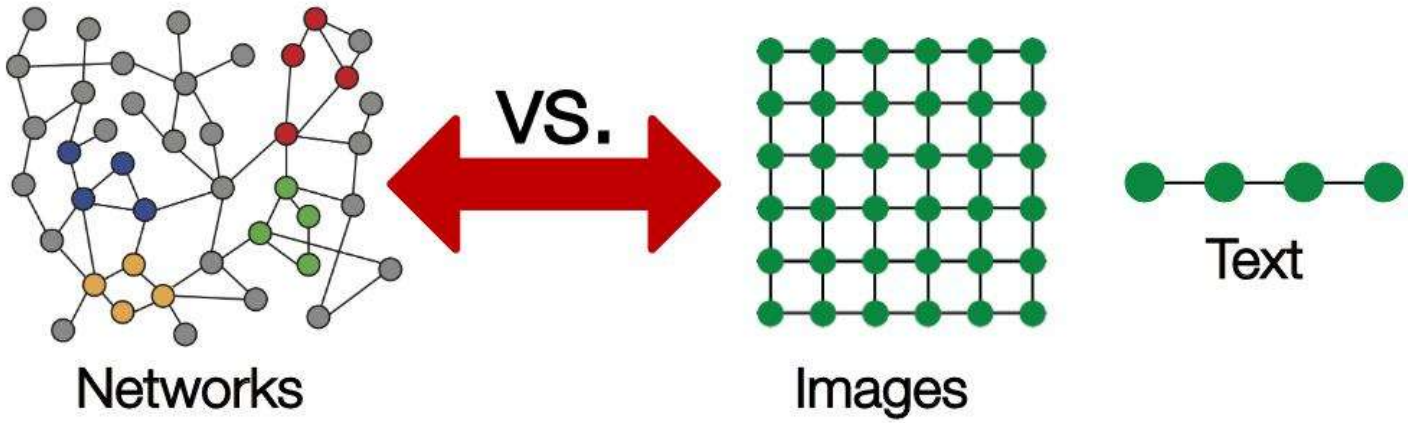


- ✓ RNNs for text/sequences…

Why is it hard?

But networks are far more complex!

- ❖ CNNs/RNNs can only operate on regular Euclidean data like images (2D grid) and text (1D sequence) while these data structures can be regarded as instances of graphs.



Right: image/Text in Euclidean space. Left: graph in non-Euclidean space.

Why is it hard?

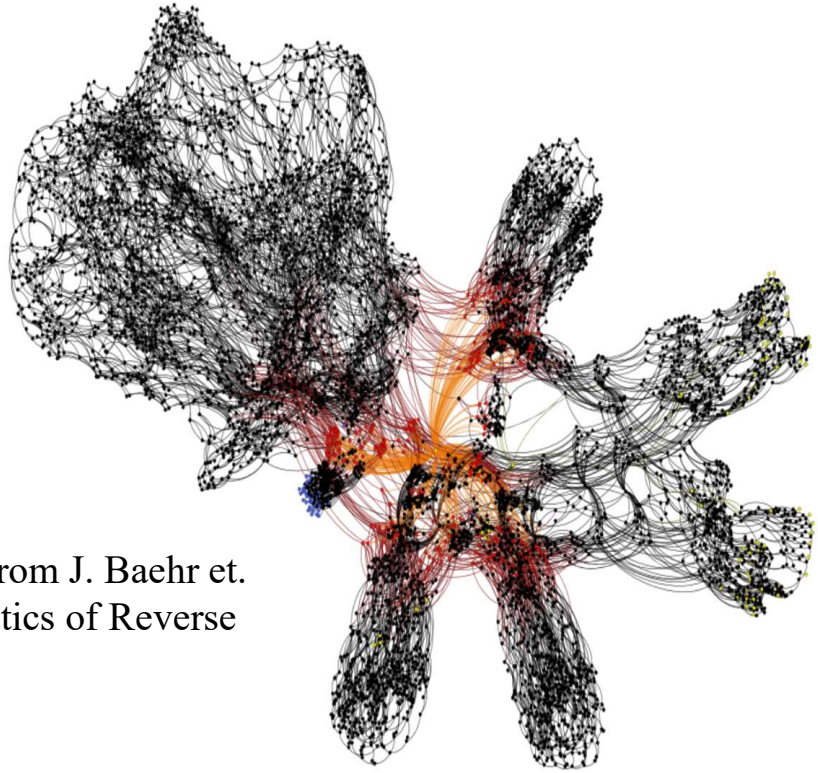
A graph does **not** have a fixed form.

Are these two graphs the same or different?

The above two graphs have a completely different structure and visually different. But when we convert it to adjacency matrix representation, the two graphs have the same adjacency matrix (if we don't consider the weight of edges).

Why is it hard?

A graph is in general **hard to visualize** for human interpretation.



Example of a giant graph: circuit netlist. Figure from J. Baehr et. al. “Machine Learning and Structural Characteristics of Reverse Engineering”

Why Use Graphs?

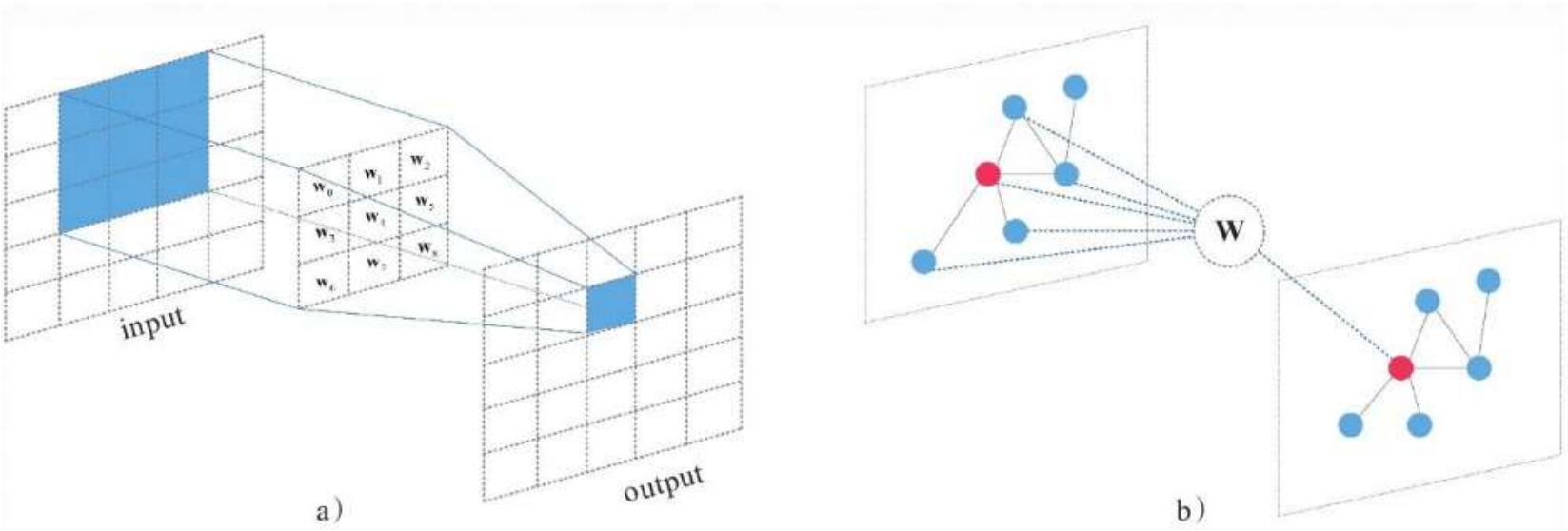
- Graphs provide a better way of dealing with abstract concepts like **relationships** and **interactions**. They also offer an intuitively visual way of thinking about these concepts. Graphs also form a natural basis for analyzing relationships in a social context.

- Graphs can solve more complex problems by **simplifying** the problems into simpler representations or **transforing** the problems into representations from different perspectives.

- ***More applications***. Graph Theories and concepts are used to study and model Social Networks, Fraud patterns, Power consumption patterns, Virality and Influence in Social Media. Social Network Analysis (SNA) is probably the best-known application of Graph Theory for Data Science.

Comparison between CNN and GNN

The layer of a Graph Convolutional Neural Network (GCN) :



Comparison between CNN and GNN

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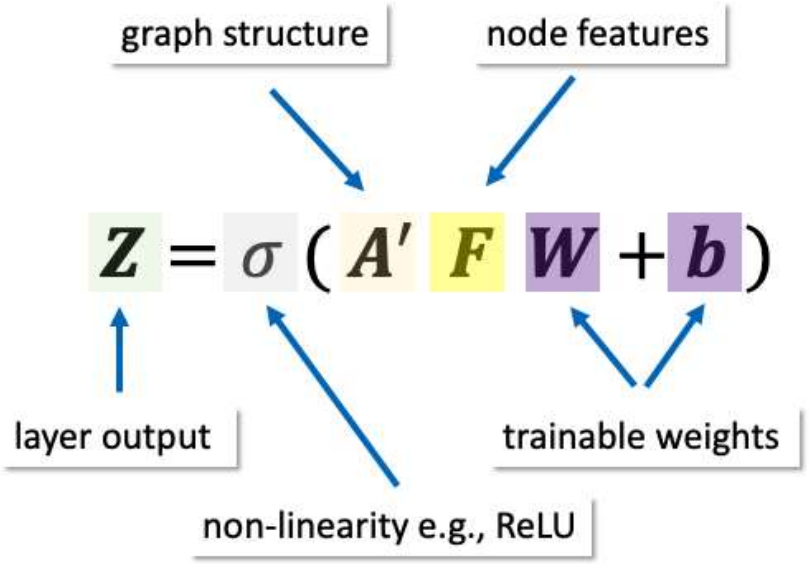
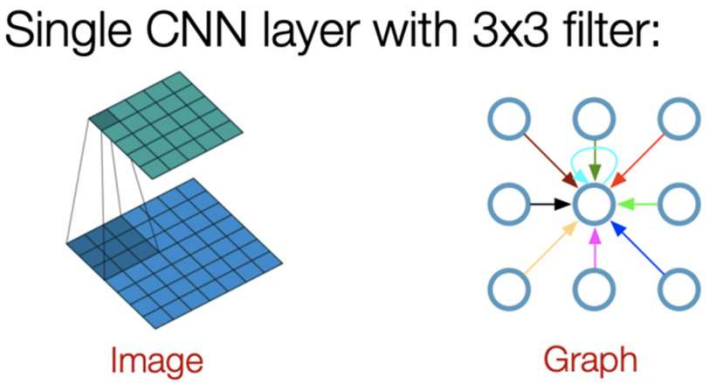


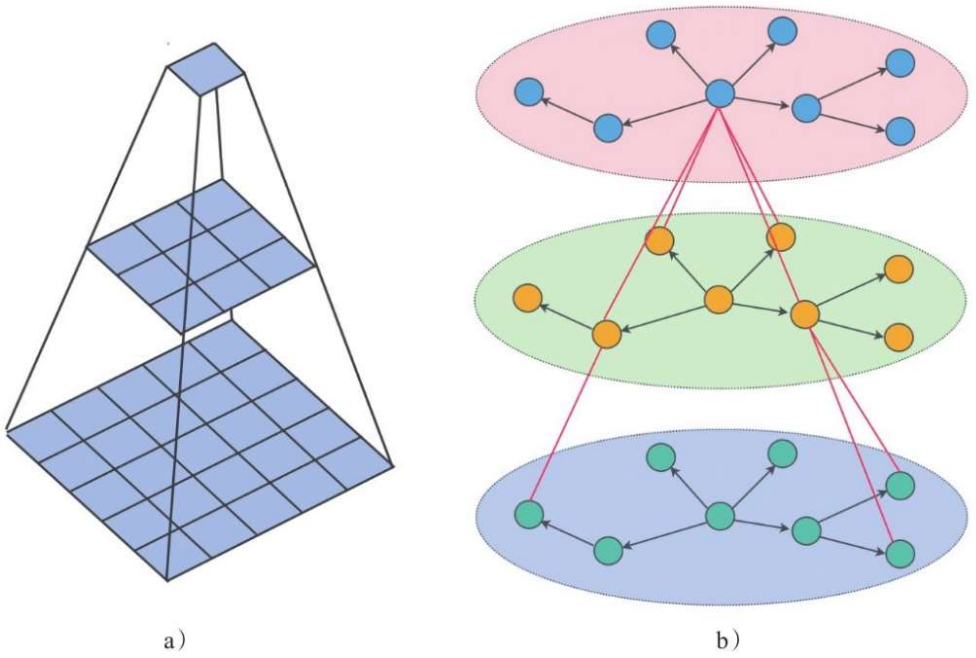


Comparison between CNN and GNN

Receptive Field：

Left: CNN

Right: GNN



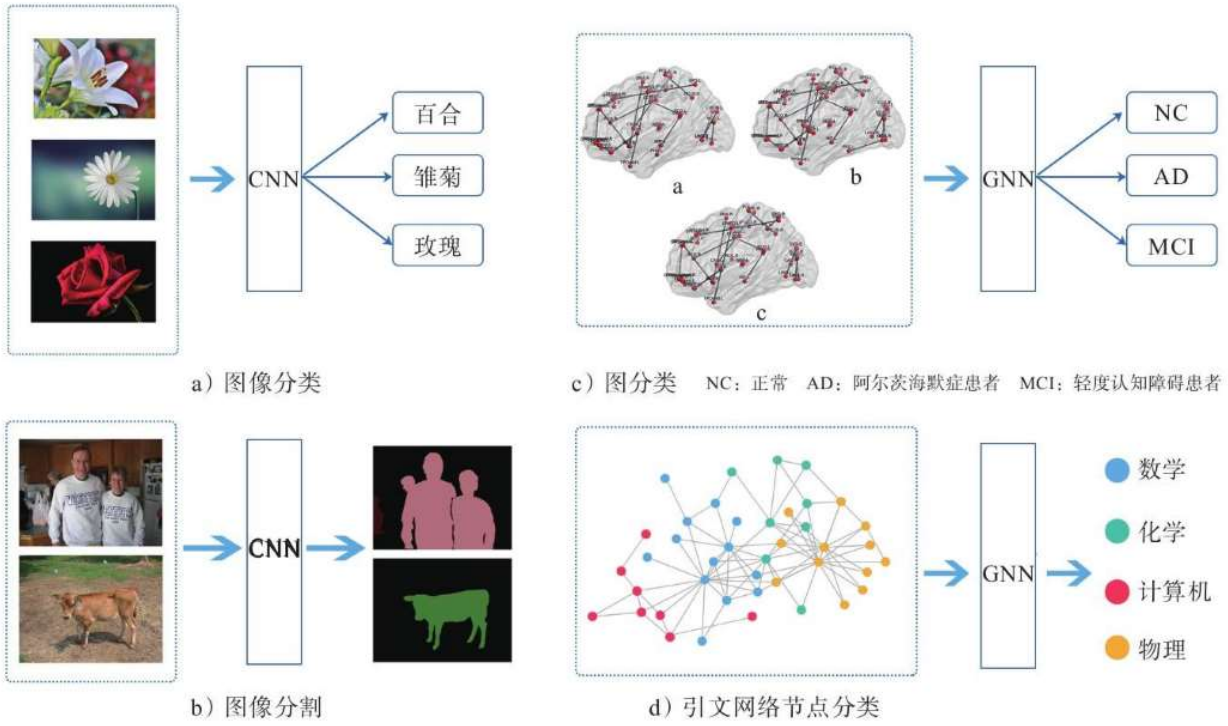
a)　　b)

Comparison between CNN and GNN

Tasks：

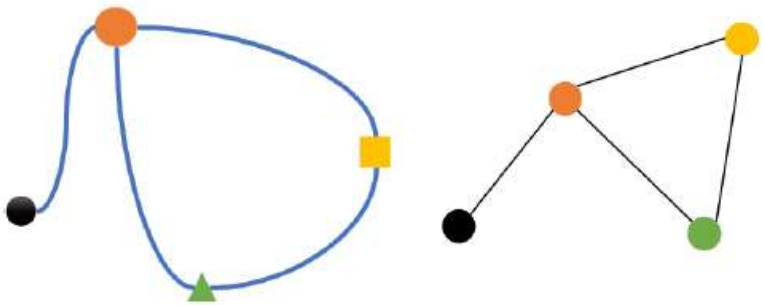
Left: CNN

Right: GNN

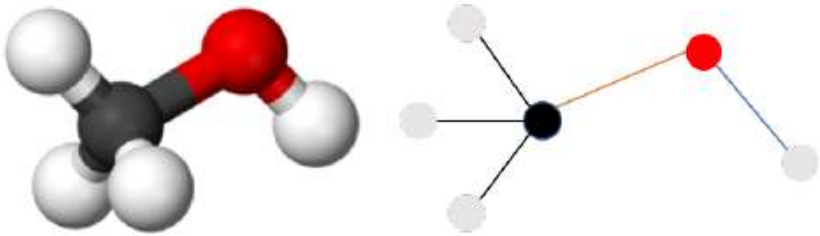


Applications

All is GRAPH !



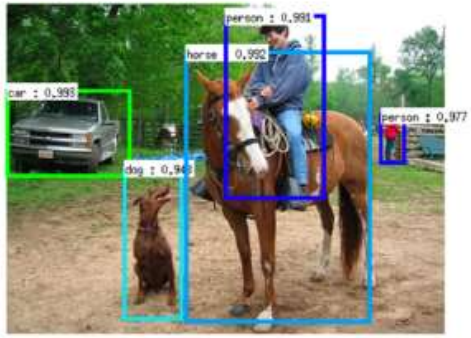
(a) physics

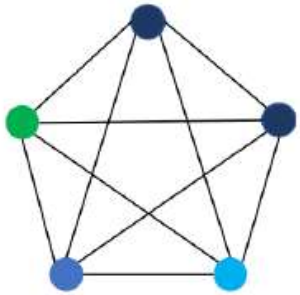


(b) molecule

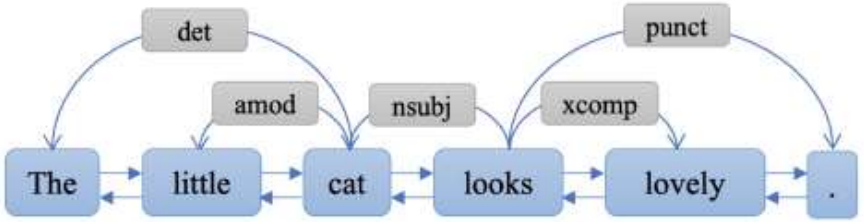
Applications

All is GRAPH !





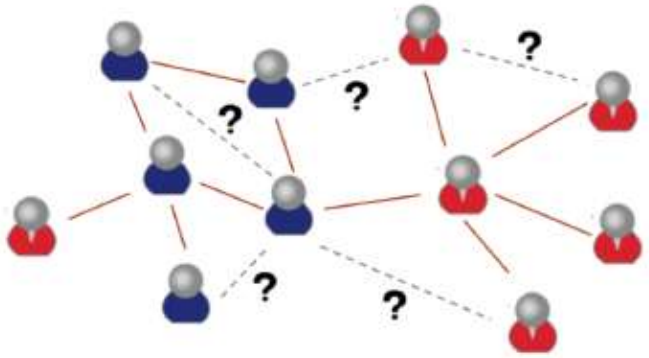
(c) image



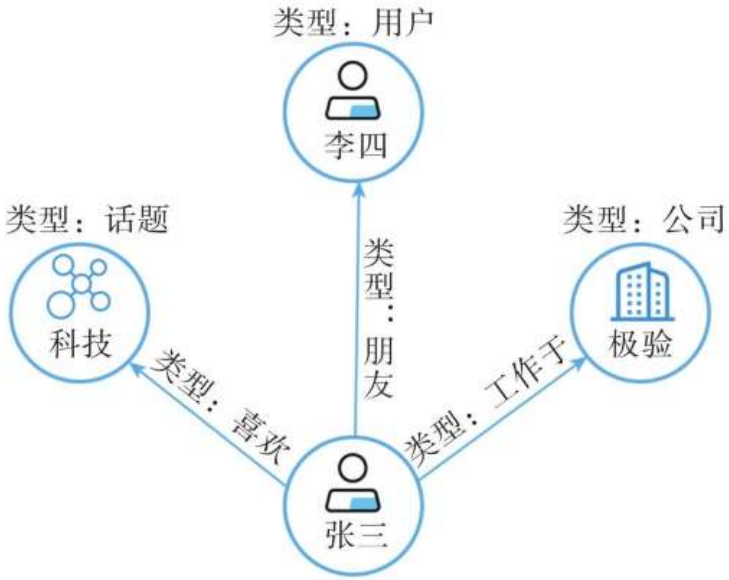
(d) text

Applications

All is GRAPH!



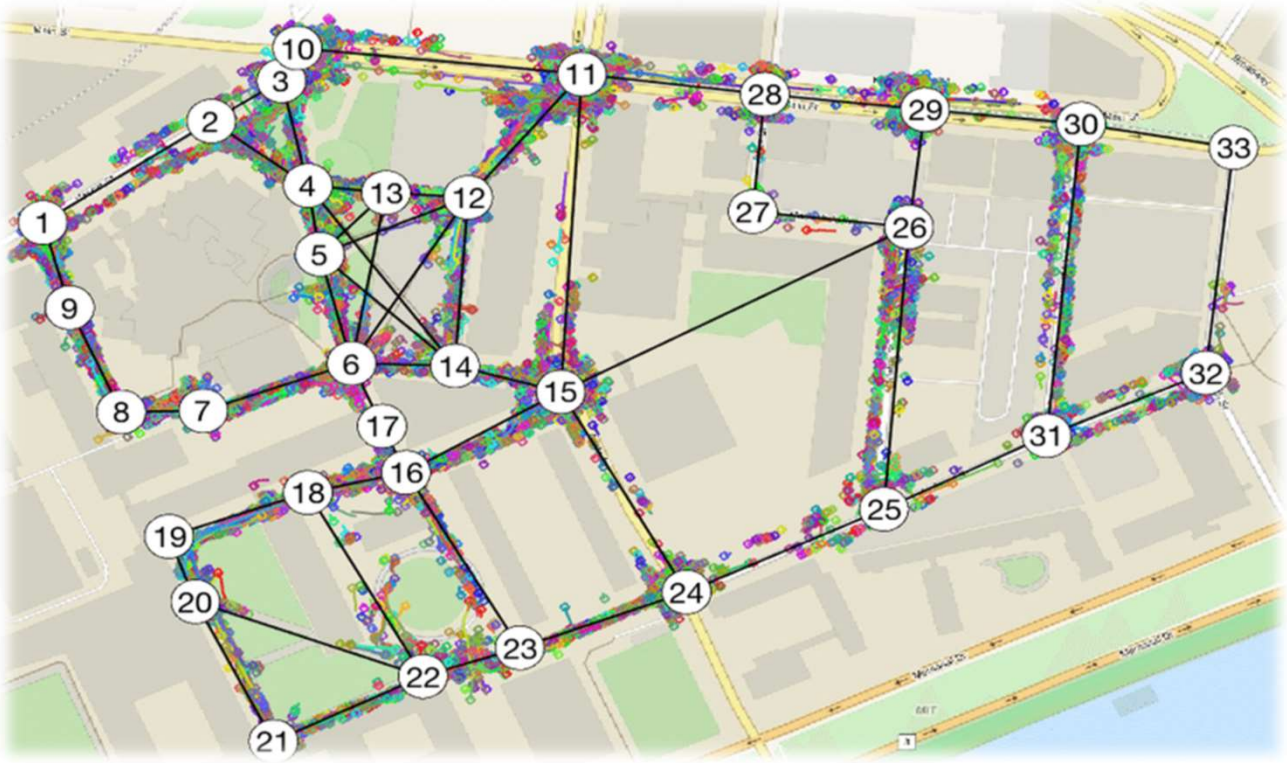
(e) social network



属性图

Applications

All is GRAPH !

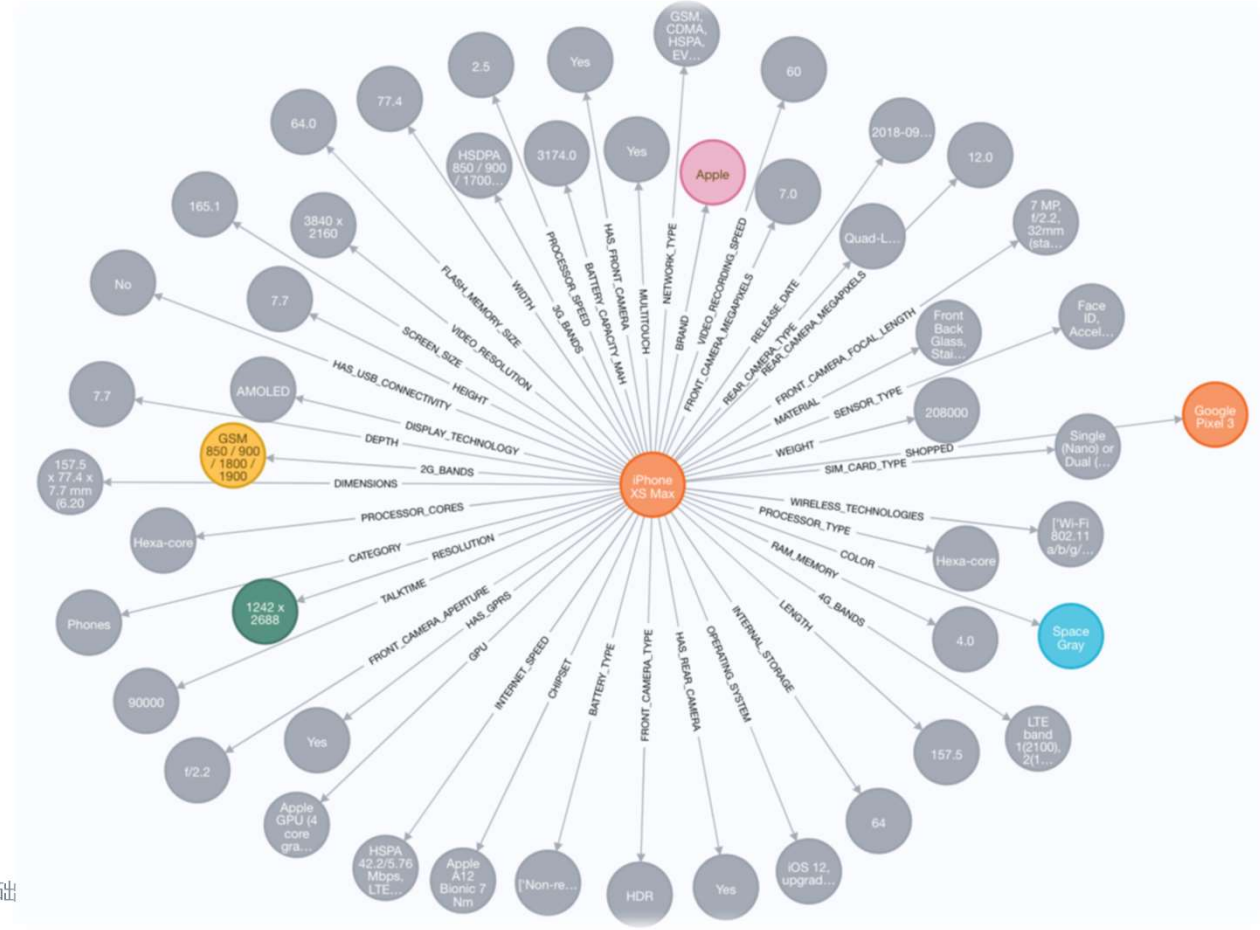


Traffic Network

Applications

All is GRAPH !

Ecommerce Graph



/02 Operating System

系统与环境配置

Operating System

16.04
18.04
20.04

Install Tutorial

Software Installation

Install Packages:

```
$ sudo apt-get install <package_name>
$ sudo apt-get install <package_1> <package_2> <package_3>
$ sudo apt-get install <package_name> --only-upgrade
$ sudo apt-get install <package_name>=<version_number>
```

Remove Packages:

```
$ sudo apt-get remove <package_name>
$ sudo apt-get purge <package_name>

$ sudo apt-get clean
$ sudo apt-get autoclean
$ sudo apt-get autoremove
```

Software Installation

Install Packages:

$ sudo dpkg install *.deb PATH: *.deb

Double Click your mouse to click

Show Packages:

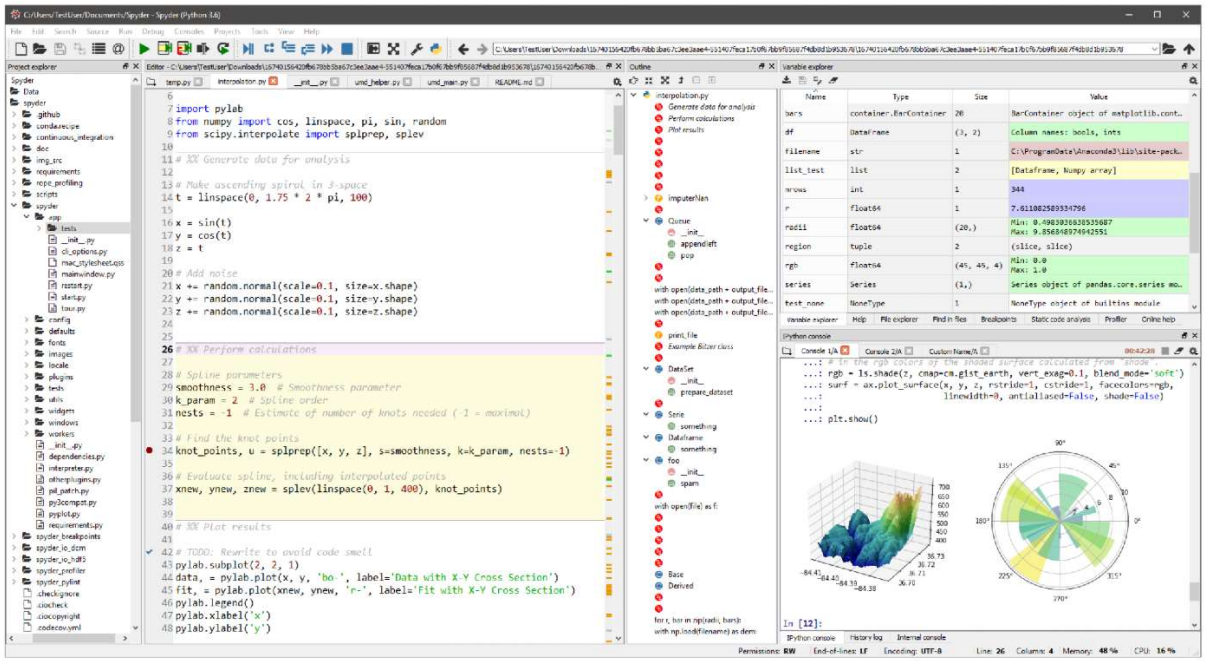
$ sudo dpkg –-list

Remove Packages:

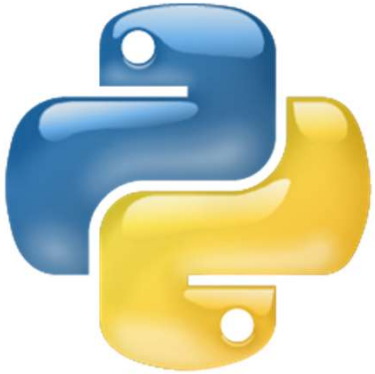
$ sudo dpkg --remove <package_name>
$ sudo dpkg --r<package_name>

Software Installation

sudo apt-get install spyder3



Python Tools




```
sudo apt install python3-pip
```

Python Tools

Installing Packages：

```
$ pip3 install SomePackage            # latest version
$ pip3 install SomePackage==1.0.4     # specific version
$ pip3 install 'SomePackage>=1.0.4'   # minimum version
```

Uninstalling Packages

```
$ pip3 uninstall SomePackage
```

Python Tools

Listing Packages:

```
$ pip3 list
        docutils (0.9.1)
        Jinja2 (2.6)
        Pygments (1.5)
        Sphinx (1.1.2)
```

Show details about an installed package:

```
$ pip3 show sphinx
    ---
    Name: Sphinx
    Version: 1.1.3
    Location: /my/env/lib/pythonx.x/site-packages
    Requires: Pygments, Jinja2, docutils
```

Python Tools

Install some tools:

$ pip3 install opencv-python
$ pip3 install matplotlib
$ pip3 install spyder

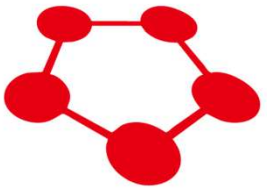
$ pip3 install notebook (请安装，上课演示代码会用)
装好jupyter notebook之后，分别输入下面两条命令
$ pip3 install ipywidgets
$ jupyter nbextension enable --py widgetsnbextension

/03 Deep Learning Frame

开源框架速安装

Frames

Microsoft
CNTK



Chainer

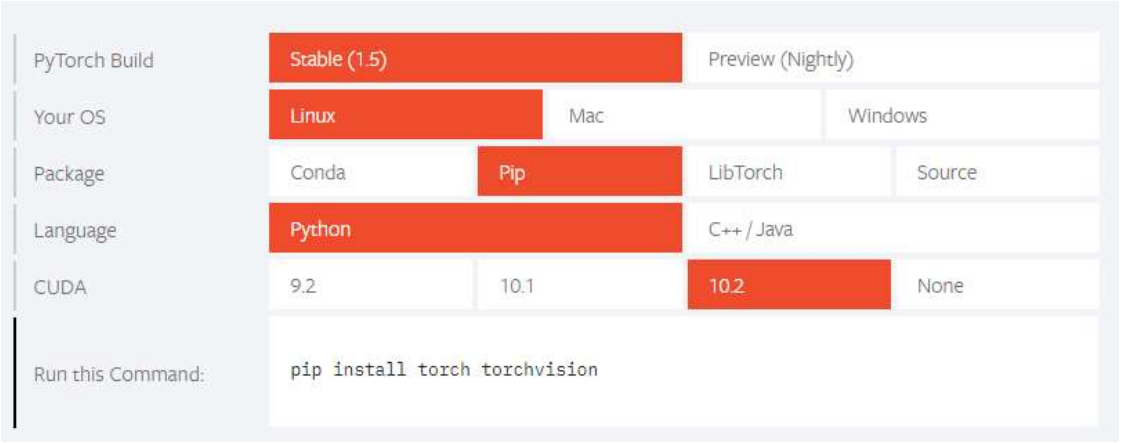
Frames

PyTorch

Tutorials:

https://pytorch.org/tutorials/

Install:



GPU

Installing with Nvidia driver:

```
# Add graphics drivers to your source list:
$ sudo add-apt-repository ppa:graphics-drivers/ppa
$ sudo apt update
$ sudo apt upgrade

# Check what driver will be installed:
$ ubuntu-drivers devices

# Auto install the latest driver:
$ sudo ubuntu-drivers autoinstall

# Then reboot your machine:
$ sudo reboot
```

GPU

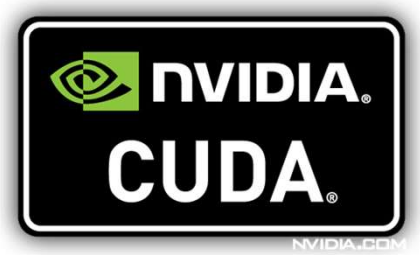
Installing with Nvidia driver:

 # If you boot without any kernel crash,
 # the driver is installed successfully. Y
 # You can check the correct install of the driver:
$ nvidia-smi

```
Tue Oct 16 14:08:49 2018
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 410.57                 Driver Version: 410.57                    |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  TITAN Xp            Off  | 00000000:49:00.0  On |                  N/A |
| 26%   41C    P5    23W / 250W |    426MiB / 12192MiB |      1%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|    0       983      G   /usr/lib/xorg/Xorg                           223MiB |
|    0      1201      G   /usr/bin/gnome-shell                         139MiB |
|    0      1623      G   ...uest-channel-token=16659471694033423175    61MiB |
+-----------------------------------------------------------------------------+
```

GPU



Select Target Platform

Click on the green buttons that describe your target platform. Only supported platforms will be shown.

Operating System	Windows, **Linux**, Mac OSX
Architecture	**x86_64**, ppc64le
Distribution	Fedora, OpenSUSE, RHEL, CentOS, SLES, **Ubuntu**
Version	18.04, **16.04**
Installer Type	runfile (local), **deb (local)**, deb (network), cluster (local)

Download Installer for Linux Ubuntu 16.04 x86_64

The base installer is available for download below.

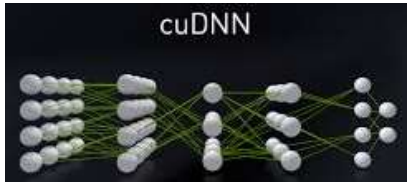
Base Installer

Installation Instructions:

```
$ wget https://developer.download.nvidia.com/compute/cuda/repos/ubuntu1604/x86_64/cuda-ubuntu1604.pin
$ sudo mv cuda-ubuntu1604.pin /etc/apt/preferences.d/cuda-repository-pin-600
$ wget http://developer.download.nvidia.com/compute/cuda/10.2/Prod/local_installers/cuda-repo-ubuntu1604-10-2-local-10.2.89-440.33.01_1.0-1_amd64.deb
$ sudo dpkg -i cuda-repo-ubuntu1604-10-2-local-10.2.89-440.33.01_1.0-1_amd64.deb
$ sudo apt-key add /var/cuda-repo-10-2-local-10.2.89-440.33.01/7fa2af80.pub
$ sudo apt-get update
$ sudo apt-get -y install cuda
```

https://docs.nvidia.com/deeplearning/sdk/cudnn-install/index.html

GPU



https://developer.nvidia.com/cudnn

cuDNN Download

NVIDIA cuDNN is a GPU-accelerated library of primitives for deep neural networks.

☑ **I Agree To the Terms of the cuDNN Software License Agreement**

Note: Please refer to the Installation Guide for release prerequisites, including supported GPU architectures and compute capabilities, before downloading.

For more information, refer to the cuDNN Developer Guide, Installation Guide and Release Notes on the Deep Learning SDK Documentation web page.

- Download cuDNN v7.6.5 (November 18th, 2019), for CUDA 10.2
- Download cuDNN v7.6.5 (November 5th, 2019), for CUDA 10.1
- Download cuDNN v7.6.5 (November 5th, 2019), for CUDA 10.0
- Download cuDNN v7.6.5 (November 5th, 2019), for CUDA 9.2
- Download cuDNN v7.6.5 (November 5th, 2019), for CUDA 9.0

Archived cuDNN Releases

GPU

https://docs.nvidia.com/deeplearning/sdk/cudnn-install/index.html

2.3.2. Installing From A Debian File

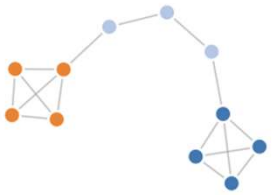
1. Navigate to your `<cudnnpath>` directory containing cuDNN Debian file.
2. Install the runtime library, for example:
   ```
   sudo dpkg -i libcudnn7_7.6.5.32-1+cuda10.2_amd64.deb
   ```
3. Install the developer library, for example:
   ```
   sudo dpkg -i libcudnn7-dev_7.6.5.32-1+cuda10.2_amd64.deb
   ```
4. Install the code samples and the cuDNN Library User Guide, for example:
   ```
   sudo dpkg -i libcudnn7-doc_7.6.5.32-1+cuda10.2_amd64.deb
   ```

/04 Project I： NetworkX

项目实战： NetworkX

Project I： NetworkX

NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.



https://networkx.org/

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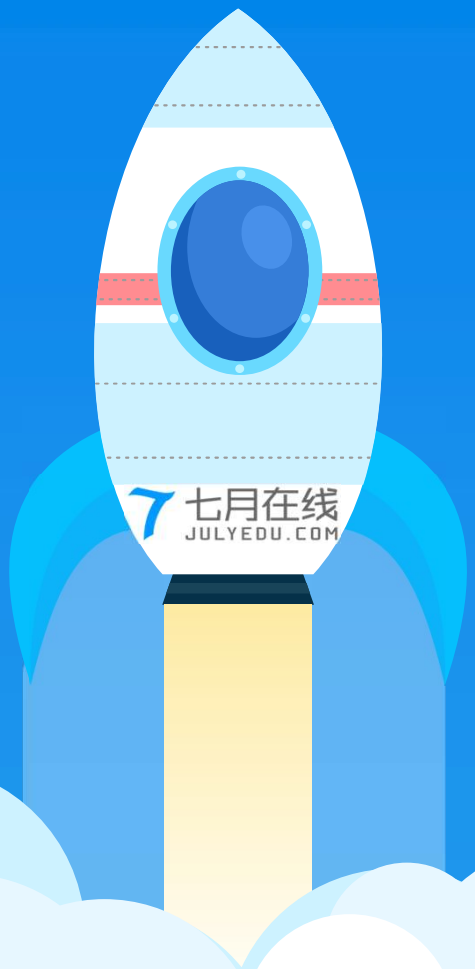

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