WWU MÜNSTER

SPP 2363

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Building Neural Networks with PyTorch

And Graph Neural Networks with PyTorch Geometric

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What is PyTorch?

- Free and open-source machine learning library
- Well documented Python interface (and C++ interface)
- Built-in GPU acceleration
- Originally developed by Meta (Facebook)
- Now governed by the Linux Foundation

```
import torch
```

- Alternatives?

https://pytorch.org/

PyTorch vs Tensorflow

- Free and open-source
- First developed by Meta, now by the Linux foundation

- Used mainly in research/academia but also by Tesla, …

- Strong community movement
- Mobile support is only in beta
- PyTorch code is very “pythonic”
- PyTorch Geometric

- Free and open-source
- Developed by Google

- Used in Googles own apps (Maps, …) and Twitter, …

- Production-ready deployment options
- Advanced mobile support
- Better built-in visualizations
- With Keras: Code looks like PyTorch

➔ By now, both libraries are quite similar and can solve the same problems

https://www.tensorflow.org/
https://developers.google.com/machine-learning/guides/rules-of-ml/
https://github.com/twitter/the-algorithm/

Tensors: Multidimensional Arrays

- Not to be confused with more complicated tensors from physics / differential geometry
- Similar to numpy arrays
- Can be loaded onto the GPU

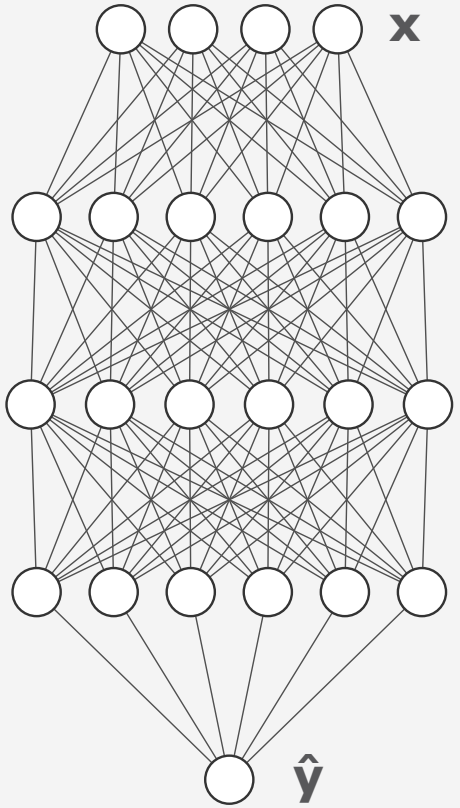
```
torch.tensor(3)
> tensor(3)

torch.tensor([[1, 1], [-1, 0]])
> tensor([[ 1, 1],
          [-1, 0]])

torch.tensor([[1, 1], [-1, 0]]).shape
> torch.Size([2, 2])
```

```
torch.tensor(np.array([[1],[7],[5]]))
> tensor([[1],
          [7],
          [5]])

torch.zeros((2, 3))
> tensor([[0., 0., 0.],
          [0., 0., 0.]])

torch.randn(3,2)
> tensor([[ 1.0128, -0.3360],
          [-0.3667, 1.4099],
          [-2.5155, 0.3394]])

torch.randn(3,2).to('cpu').device # or: 'gpu'
> device(type='cpu')
```

https://pytorch.org/docs/stable/tensors.html

Recap: How do neural networks work?

- What is a NN? → A function that predicts an output $\hat{\mathbf{y}}$ for input $\mathbf{x}$.
- Has different *layers* which perform mathematical operations on $\mathbf{x}$.
- For a linear layer: The parameters of $\mathbf{W}$ (weights) multiplied with $\mathbf{x}$ and other parameters $\mathbf{b}$ (biases) are added. ➔ $\mathbf{x}\mathbf{W}^T+\mathbf{b}$
- Nonlinear activation functions (ReLU, sigmoid, …) transform the input further and allow to predict nonlinear correlations.
- Final operation: linear output (for regression tasks); sigmoid function (for binary classification) or softmax function (for multi-classification)
- Training:
  - The error (loss) between the output $\hat{\mathbf{y}}$ and the true label $\mathbf{y}$ has to be minimized:
  - Derivative of NN with regards to the parameters in $\mathbf{W}$ and $\mathbf{b}$ → gradient
  - $\mathbf{W}$ and $\mathbf{b}$ are changed a little bit depending on the gradient. → backpropagation
  - $\hat{\mathbf{y}}$ is calculated again.

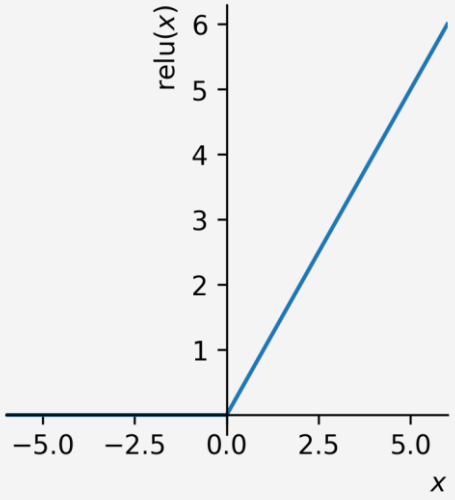


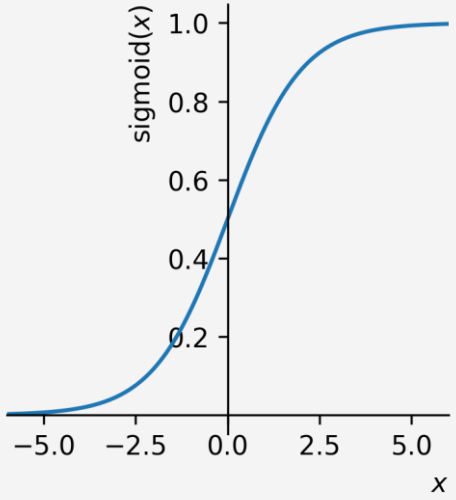
Mathematical Operations with Tensors and Keeping Track

```
t1 = torch.tensor([[ 1.,  2., -1.],
                   [-2., -3.,  0.]])

t2 = torch.tensor([[ 2.,  3.],
                   [-2., -2.],
                   [ 0., -1.]])

torch.matmul(t1, t2)
> tensor([[-2., 0.],
          [ 2., 0.]])
```

```
  1 · 2
+ 2 · (-2)
+ (-1) · 0
= -2
```

```
import torch.nn.functional as F
F.relu(t1)
> tensor([[1., 2., 0.],
          [0., 0., 0.]])
```






```
t1 = torch.tensor([[ 1.,  2., -1.],
                   [-2., -3.,  0.]],
                  requires_grad=True)
torch.matmul(t1, t2)
> tensor([[-2., 0.],
          [ 2., 0.]],
         grad_fn=<MmBackward0>)
```

https://pytorch.org/docs/stable/torch.html

Backpropagation with autograd

Autograd is a “**reverse automatic differentiation system**”

https://pytorch.org/docs/stable/notes/autograd.html
http://blog.ezyang.com/2019/05/pytorch-internals/
https://pytorch.org/blog/overview-of-pytorch-autograd-engine/
https://pytorch.org/blog/computational-graphs-constructed-in-pytorch/

Backpropagation with autograd

- A neural net is just a big function

$$f\big(g(h(\dots(x)))\big) = \hat{y}$$

- Where the nested functions are the different layers and nonlinear activation functions
- Optimizing this function means finding derivative of the error between label y and prediction $\hat{y}$
- The derivative of a nested function can be found with the chain rule

$$\Big(f\big(g(x)\big)\Big)' = f'\big(g(x)\big)\, g'(x)$$

- It's a bit more complicated because we don't want to differentiate for x but for our weights **W** and biases **b**
- Calculate the gradient instead (partial differentiation for all parameters)

$$\frac{\partial f}{\partial w_1}, \frac{\partial f}{\partial w_2}, \dots, \frac{\partial f}{\partial w_n}$$

https://pytorch.org/docs/stable/notes/autograd.html
http://blog.ezyang.com/2019/05/pytorch-internals/
https://pytorch.org/blog/overview-of-pytorch-autograd-engine/
https://pytorch.org/blog/computational-graphs-constructed-in-pytorch/

Backpropagation with autograd

- Possible by hand, but a lot of work.
- What if we want to exchange a function in the middle of the net?

→ We need automatic differentiation.

- Because of the chain rule: relatively easy

https://pytorch.org/docs/stable/notes/autograd.html
http://blog.ezyang.com/2019/05/pytorch-internals/
https://pytorch.org/blog/overview-of-pytorch-autograd-engine/
https://pytorch.org/blog/computational-graphs-constructed-in-pytorch/

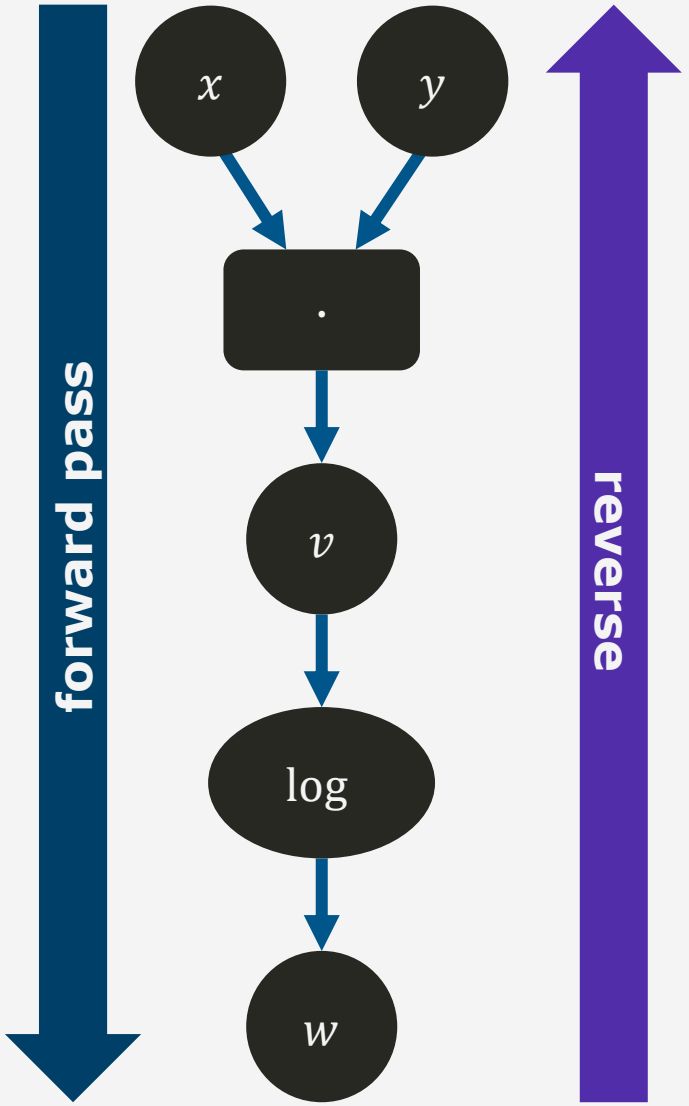
Backpropagation with autograd

- During the forward pass all operations are recorded
- Operations are stored in an acyclic *graph*
- Leaves are the input tensors, the root is the last operation of the neural network

- Example: $f(x, y) = \log(xy)$

- For backpropagation: The graph is traversed in the opposite direction, from root to leaves to calculate the gradient

- Computational graph is created every iteration

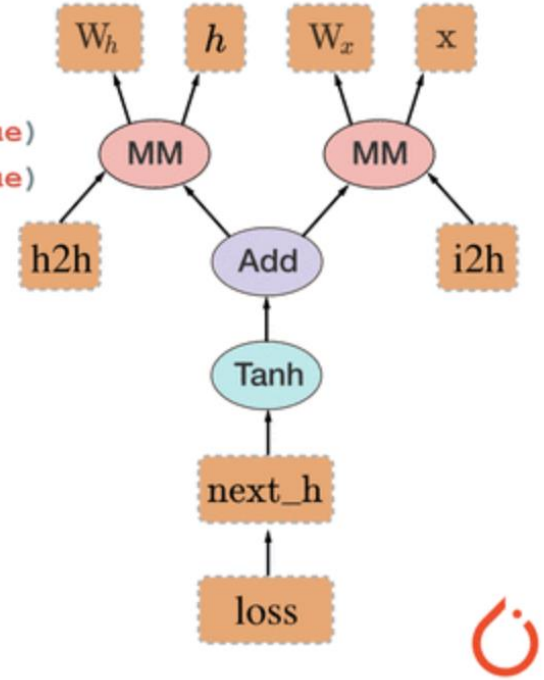


https://pytorch.org/docs/stable/notes/autograd.html
http://blog.ezyang.com/2019/05/pytorch-internals/
https://pytorch.org/blog/overview-of-pytorch-autograd-engine/
https://pytorch.org/blog/computational-graphs-constructed-in-pytorch/

Backpropagation with autograd

Back-propagation
uses the dynamically created graph

```
W_h = torch.randn(20, 20, requires_grad=True)
W_x = torch.randn(20, 10, requires_grad=True)
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)

h2h = torch.mm(W_h, prev_h.t())
i2h = torch.mm(W_x, x.t())
next_h = h2h + i2h
next_h = next_h.tanh()

loss = next_h.sum()
loss.backward()  # compute gradients!
```



Source

Machine Learning Optimization Framework

(Not just for neural networks)

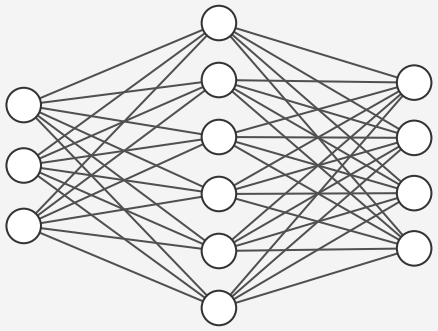
- **Choose a model** describing the relationship between input and output variables
- **Define a loss** (error) function quantifying the fit to the data
  - (optional) chose a regularizer saying how much we prefer different candidates (integration of knowledge)
- **Fit the model** using an **optimization algorithm**

Choose a Model

- Combine basic mathematical operations
- Combine basic layers
  - Using `nn.Sequential`
  - Inheriting from `nn.Module`

```
torch.matmul(x, W.transpose()) + b)

F.linear(x, W, b)

layer1 = nn.Linear(3, 2)
x = torch.tensor([[ 1.,  2., -1.],
                  [-2., -3.,  0.]])
layer1(x)
> tensor([[-1.0423, -1.4743],
          [ 1.3903, -0.0618]],
          grad_fn=<AddmmBackward0>)
```

```
model = nn.Sequential(
          nn.Linear(3,6),
          nn.ReLU(),
          nn.Linear(6,4),
          nn.ReLU()
        )
model(x)
> tensor([[0.0692, 0.4618, 0.4903, 0.0000]
          [1.5100, 0.0000, 0.0000, 0.0000]],
          grad_fn=<ReluBackward0>)
```



https://pytorch.org/docs/stable/nn.html

Choose a Model

```python
class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.lin1 = nn.Linear(3, 6)
        self.lin2 = nn.Linear(6, 4)

    def forward(self, x):
        x = F.relu(self.lin1(x))
        return F.relu(self.lin2(x))

model = Model()
model(x)
> tensor([[0.4112, 0.0000, 0.0000, 0.0000],
          [0.9921, 0.6823, 0.0000, 0.0000]],
          grad_fn=<ReluBackward0>)
```

- Send model to device

```python
model.to('cuda')
```

- Can be nested
- Change training mode:

```python
model.train()
model.eval()
```

  - Important for `nn.Dropout` and `nn.BatchNorm`

- Many more specialized layers (convolutional, recurrent, …)

https://pytorch.org/docs/stable/nn.html

Define a Loss

- Function to calculate error / distance between the prediction **ŷ** and the label **y**

- For regression tasks (predicting a single numerical value)
  - Mean squared error (MSE)

```
loss = nn.MSELoss()
```

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

- For classification tasks
  - Crossentropy loss

```
loss = nn.CrossEntropyLoss()
```

  - For binary classification tasks
    - Binary crossentropy loss

```
loss = nn.BCEWithLogitsLoss()
```

- More functions available

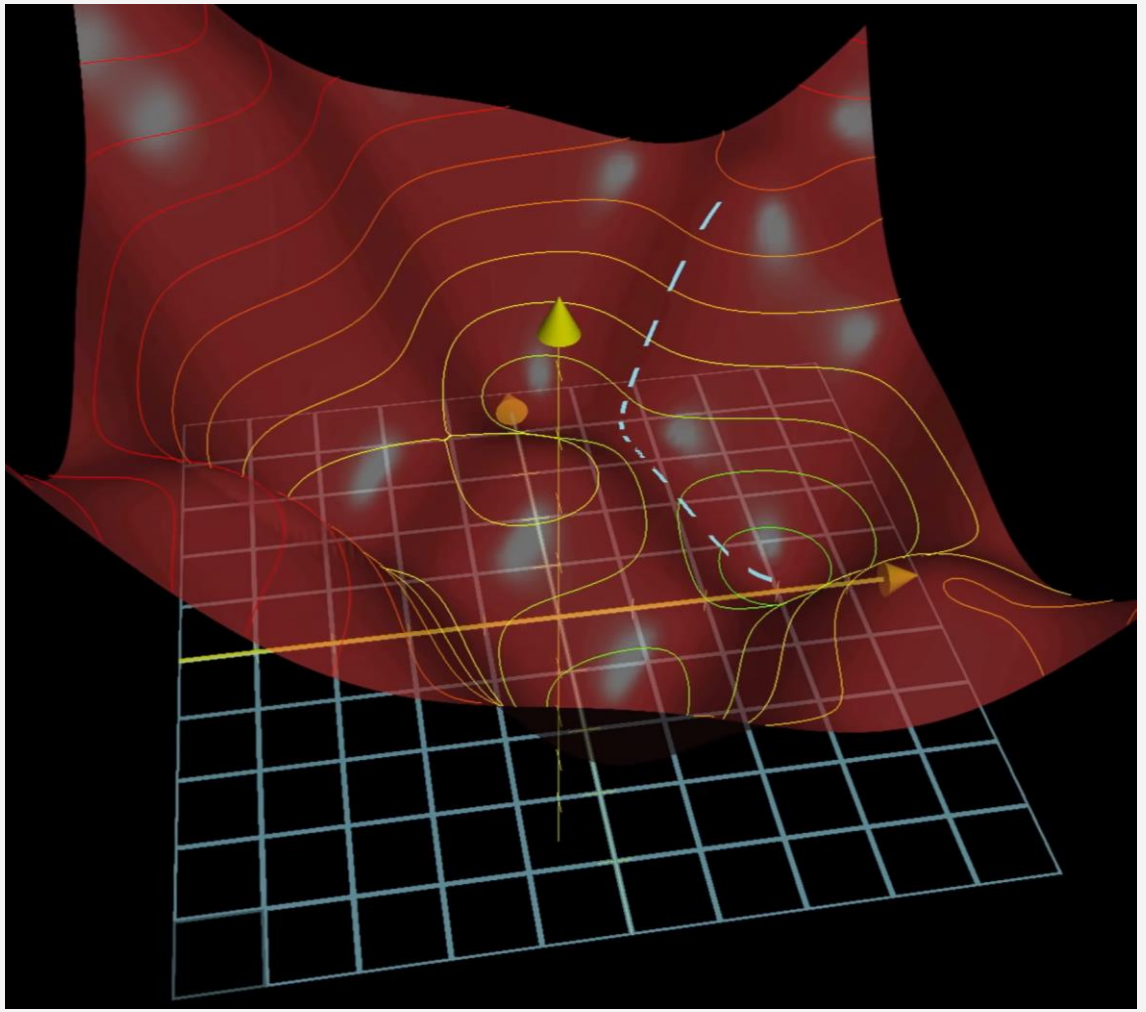
https://pytorch.org/docs/stable/nn.html

Choose an optimizer

- Algorithm to find the minimum of the loss function
  - Gradient points in the direction of the greatest increase
  - Step into the opposite direction
  - “Walking from a mountain into a valley”

- Different algorithms implemented
  - Stochastic gradient descent
  - Adam
  - …

```
from torch import optim
optimizer = optim.Adam(model.parameters(),
                       lr=0.001)
```



https://pytorch.org/docs/stable/optim.html

Gradient descent, how neural networks learn | Chapter 2, Deep learning - YouTube

Train the Model

```
for epoch in range(5):
    model.train()
    for (X, y) in dataloader:

        # Compute prediction error
        pred = model(X)
        loss = loss(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```

- dataloader → see Jupyter Notebook

- After one epoch: the network has seen all training data once
- Between epochs the gradients have to be set back to zero
- Other things to add to the trainings-loop / trainings-function:
  - Sending data to the device the model is on
  - Updating the engineer on the training-process
  - **Evaluate the model**

https://pytorch.org/tutorials/beginner/basics/quickstart_tutorial.html

Evaluate the Model

```
for epoch in range(5):
    model.eval()
    test_loss = 0
    with torch.no_grad():
        for X, y in testdataloader:
            pred = model(X)
            test_loss += loss(pred, y).item()
    print(test_loss)
```

- Evaluate on data different from the training set
- Use different metrics for evaluation

A. Bender, N. Schneider, M. Segler, W. Patrick Walters, O. Engkvist, T. Rodrigues, Evaluation guidelines for machine learning tools in the chemical sciences, *Nat. Rev. Chem.* **2022**, *6*, 428.

Other things to know

- Datasets: torchvision, torchaudio
  - Not relevant for chemistry

- Saving and loading models

```python
# saving
torch.save(model.state_dict(), "model.pt")

# loading
model = Model()
model.load_state_dict(torch.load("model.pt"))
```

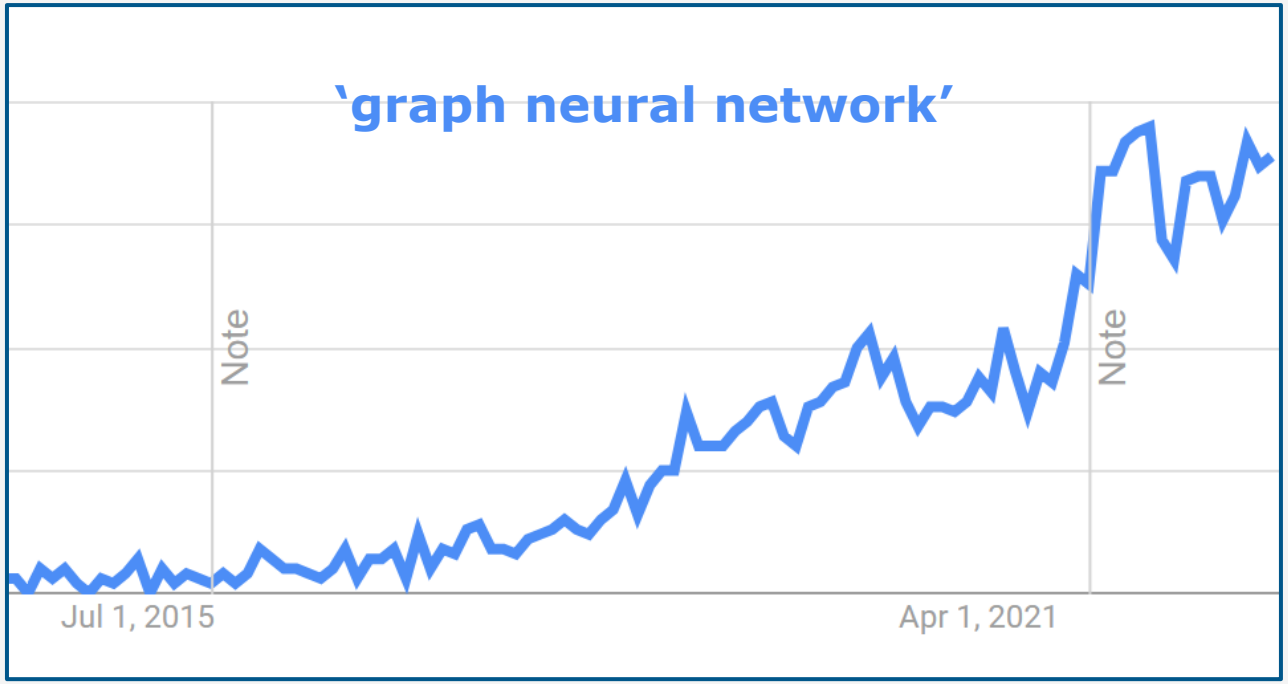
- TorchScript: Build models with Python and run without python dependency
- PyTorch Mobile
- Captum
- Profiler

Questions?

Building Graph Neural Networks with PyTorch Geometric

- What is PyTorch Geometric?

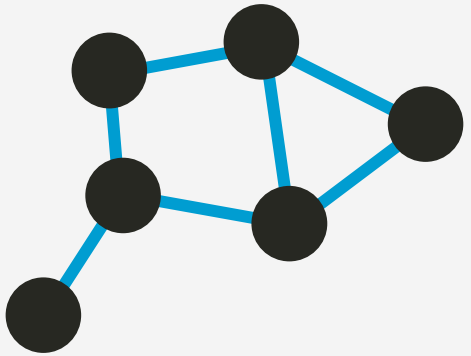
  → Library built upon PyTorch to easily write and train GNNs



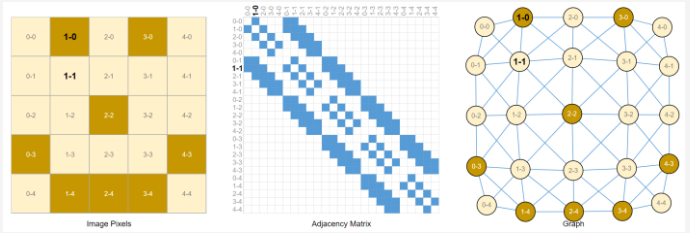
https://trends.google.com/

What is a Graph?

- Mathematical structure used to model pairwise relations between objects (Wikipedia)
- Models for networks in the real world
  - Social networks (in real life and online)
  - Street networks
  - **Molecules**
  - …



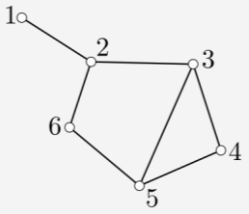
- Made up of nodes (vertices) connected by edges (links)



- Anything can be modeled as a graph

Graphs in PyTorch Geometric

- Adjacency matrix
- Edge index
- Node feature matrix
- (Edge feature matrix)



$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array} \quad \begin{array}{l} \{1,2\} \\ \{2,3\} \\ \{3,4\} \\ \{3,5\} \\ \{4,5\} \\ \{5,6\} \\ \{6,2\} \end{array}$$

```
edge_index = torch.tensor(
    [[0, 1, 1, 2, 2, 3, 2, 4, 3, 4, 4, 5, 5, 1],
     [1, 0, 2, 1, 3, 2, 4, 2, 4, 3, 5, 4, 1, 5]],
     dtype=torch.long)
torch_geometric.utils.to_dense_adj(edge_index)
> tensor([[[0., 1., 0., 0., 0., 0.],
           [1., 0., 1., 0., 0., 1.],
           [0., 1., 0., 1., 1., 0.],
           [0., 0., 1., 0., 1., 0.],
           [0., 0., 1., 1., 0., 1.],
           [0., 1., 0., 0., 1., 0.]]])
```

```
x = torch.tensor([[1], [2],
                  [3], [4],
                  [5], [6]],
                 dtype=torch.float)
data = torch_geometric.data.Data(x=x,
            edge_index=edge_index)
print(data)
> Data(x=[6, 1], edge_index=[2, 14])

# dictionary structure
print(data.x)
> tensor([[1.], [2.], [3.], [4.],
  [5.], [6.]])

print(data.keys)
> ['x', 'edge_index']
```

https://pytorch-geometric.readthedocs.io/en/latest/get_started/introduction.html

What do we learn?

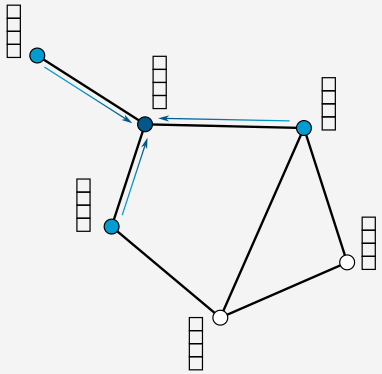
- Node prediction → Does this node belong to class xy?
  - Example citation graph: Is this a neuroscience paper?

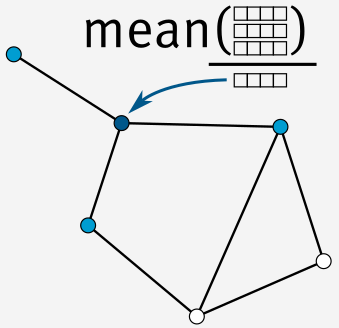
- Edge prediction
  - Edge classification
  - Predicting the existence of an edge between nodes i and j
    - Facebook/Twitter: You might know / like …

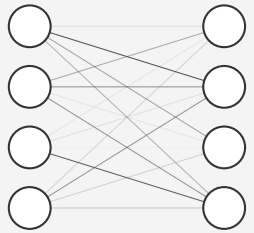
- Graph prediction
  - Molecular properties / activities …

How do we learn?

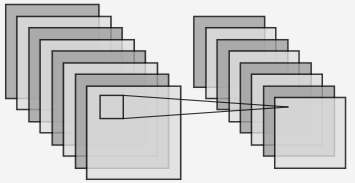
- Message passing:
  - For each node, get all the neighboring nodes/node embeddings
  - Aggregate all messages (sum / mean / max; permutation invariant)
  - Pooled messages are updated by a neural network function (linear layer)







- Similar to pixel-convolutions from image recognition
- In practice: Now many implementations

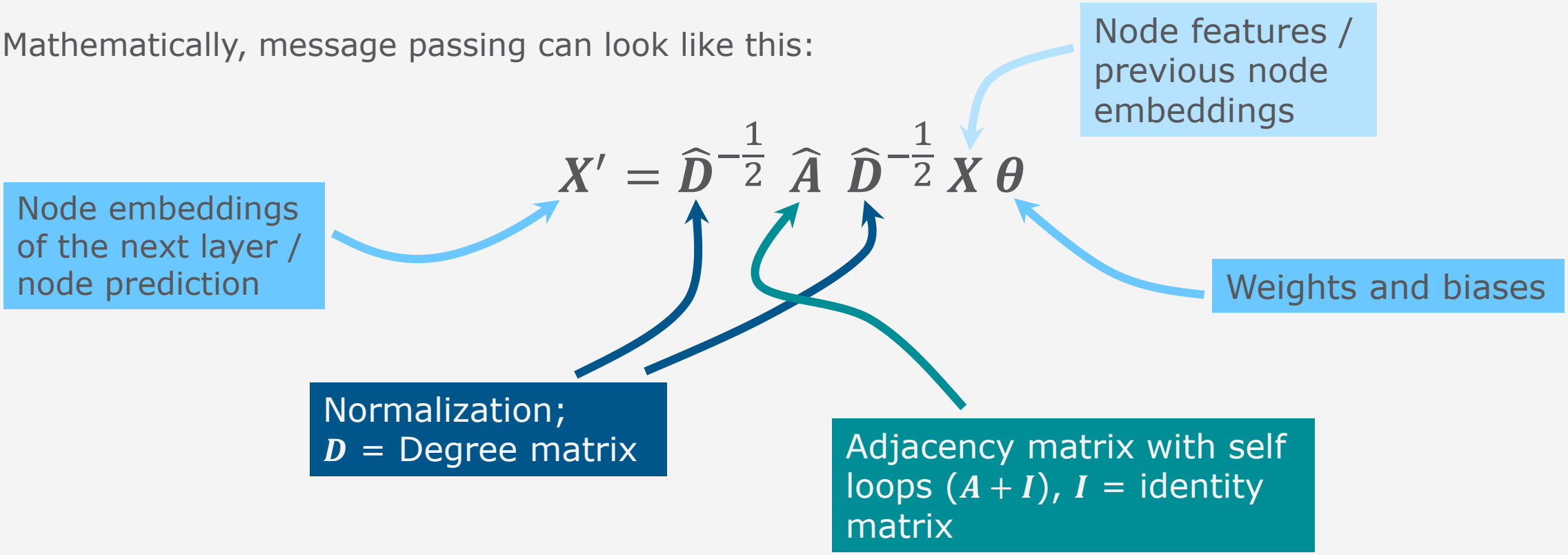


https://distill.pub/2021/gnn-intro/

https://tkipf.github.io/graph-convolutional-networks/

GCNConv – A Simple Graph Convolution

- Mathematically, message passing can look like this:



- Note: For graph-level tasks we need to pool the node embeddings (and add a fully connected layer)

Kipf, T. N.; Welling, M. Semi-Supervised Classification with Graph Convolutional Networks. *ICLR* **2017.**
https://pytorch-geometric.readthedocs.io/en/latest/generated/torch_geometric.nn.conv.GCNConv.html#torch_geometric.nn.conv.GCNConv

Building a GNN

```python
from torch_geometric.nn import GCNConv
from torch_geometric.nn import \
       global_add_pool

class GCN(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = GCNConv(1, 3)
        self.conv2 = GCNConv(3, 1)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = F.relu(x)
        x = self.conv2(x, edge_index)
        # x = global_add_pool(x, batch)
        return F.log_softmax(x, dim=1)
```

```python
model = GCN()
model(data.x, data.edge_index)
> tensor([[0.],
          [0.],
          [0.],
          [0.],
          [0.],
          [0.]],
         grad_fn=<LogSoftmaxBackward0>)
```

More Noteworthy Stuff

- PyTorch Geometric
  - Datasets (KarateClub, **TUDataset**, …, **MoleculeNet**, …, **ZINC**, …)
  - Explain → XAI Algorithms
  - Transforms (ToUndirected, KNNGraph, …)
  - Utils (add_self_loops, to_dense_adj, **from_smiles**, …)
  - GraphGym: Design/evaluate pipeline
  - Profiler

- Other packages:
  - NetworkX → More graph analysis/creation/… tools

- (Graph) Neural Networks are not necessarily the best model for your application! (Also try RF, SVM, …)

Questions?

Exercises / Jupyter Notebooks

https://github.com/SamuelHomberg/SPP2363_Tutorial_PyTorch

- PyTorch:
  - https://github.com/kochgroup/intro_pharma_ai

    → Notebook 8 (GER/EN; Google Colab; with exercises)
  - Other notebooks (Cheminformatics, Datascience, NNs from scratch, GNNs without PyTorch Geometric, …)

- PyTorch Geometric:
  - Jupyter notebook with chapters on
    - Installation of PyG
    - Loading of existing datasets
    - Creating your own dataset
    - Training a simple GNN
  - No exercises; no Google Colab